The geometry of quantum computation

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Determining the quantum circuit complexity of a unitary operation is closely related to the problem of finding minimal length paths in a particular curved geometry [Nielsen et al. Science 311, 1133-1135 (2006)]. This paper investigates many of the basic geometric objects associated to this space, including the Levi-Civita connection, the geodesic equation, the curvature, and the Jacobi equation. We show that the optimal Hamiltonian evolution for synthesis of a desired unitary necessarily obeys a simple universal geodesic equation. As a consequence, once the initial value of the Hamiltonian is set, subsequent changes to the Hamiltonian are completely determined by the geodesic equation. We develop many analytic solutions to the geodesic equation, and a set of invariants that completely determine the geodesics. We investigate the problem of finding minimal geodesics through a desired unitary, U, and develop a procedure which allows us to deform the (known) geodesics of a simple and well understood metric to the geodesics of the metric of interest in quantum computation. This deformation procedure is illustrated using some three-qubit numerical examples. We study the computational complexity of evaluating distances on Riemmanian manifolds, and show that no efficient classical algorithm for this problem exists, subject to the assumption that good pseudorandom generators exist. Finally, we develop a canonical extension procedure for unitary operations which allows ancilla qubits to be incorporated into the geometric approach to quantum computing.

I. INTRODUCTION

A central problem of quantum computation is to find efficient quantum circuits to synthesize desired unitary operations. These unitary operations are used to solve computational problems such as factoring [1, 2, 3]. Despite intensive effort, few general principles are known either for finding efficient quantum circuits or for proving that a given computational problem has no efficient circuit.

A geometric approach to quantum circuit complexity has recently been developed in [4, 5, 6]. The idea is to introduce a Riemannian metric on the space of n-qubit unitary operations, chosen in such a way that the metric distance d(I, U) between the identity operation and a desired unitary U is equivalent (modulo some technical caveats, discussed below) to the number of quantum gates required to synthesize U. Thus the distance d(I, U) is a good measure of the difficulty of synthesizing U.

This geometric reformulation suggests that the tools of Riemannian geometry may be useful in analyzing quantum circuit complexity. The purpose of this paper is to develop in detail many of the basic geometric notions that can be associated to quantum computation, including the Levi-Civita connection, geodesics, geodesic invariants, curvature, Jacobi fields and conjugate points. We also discuss obstacles to the use of geometric ideas to analyze quantum circuit complexity.

Structure and content of the paper: Section II reviews the relevant background results connecting geometry and quantum circuit complexity, from [4, 5, 6].

Section III derives simple formulae for, and several basic properties of, the Levi-Civita connection on our Riemannian manifold. With these results in hand all other geometric quantities computed later in the paper may be obtained through relatively straightforward computations. In particular, Appendix A computes all the natural curvature quantities for the manifold, including the curvature tensor, the sectional curvature, the Ricci tensor, and the scalar curvature.

Section IV uses the connection to derive the geodesic equation. This is a simple and (we believe) rather elegant equation that determines the locally optimal Hamiltonian evolution for synthesis of any desired unitary. We obtain a complete set of constants of the motion for the geodesic equation, as well as many simple exact solutions, including a completely general exact solution for three qubits.

Section V develops a procedure for numerically finding geodesics passing through a desired endpoint, i.e., a goal unitary. We begin with a review of the theory of Jacobi fields and conjugate points, which make use of the curvature to study the divergence or convergence of geodesics on a manifold. These tools can be used to study when a geodesic is no longer globally minimizing, but is merely a local minimum, and we briefly digress to investigate this phenomenon numerically for a class of unitaries associated with the transverse Ising model. Returning to the main point of the section, finding geodesics to a goal unitary, the basic idea is to smoothly deform the geodesics of a simple and well understood metric to the geodesics of the metric of computational interest. This is done using a notion of a geodesic derivative along a flow through the space of metrics. The idea is to fix the geodesic endpoint, and then the geodesic derivative describes how the initial velocity of the geodesic must change as the metric

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is changed, in order that the deformed geodesic passes through the same endpoint. We develop necessary and sufficient conditions for the geodesic derivative to exist, and a formula for it when it does exist. These necessary and sufficient conditions are naturally expressed in terms of the conjugate points studied earlier in this section. We then use this deformation procedure to numerically find geodesics passing through some unitary operations of interest, including randomly chosen unitaries, and the quantum Fourier transform.

In Section VI we discuss the general prospects for using geometric ideas to analyze quantum circuit complexity. We describe two important obstacles to using geometric ideas to prove nontrivial upper or lower bounds on quantum circuit complexity, and prove two related technical results. The first obstacle is the Razborov-Rudich theorem, a well-known result in classical computational complexity. This is essentially a no-go theorem that, subject to certain assumptions, rules out a wide class of approaches to proving circuit lower bounds. We outline a quantum analogue of the Razborov-Rudich theorem, and use it to argue that the general problem of finding geodesics on a Riemannian manifold is likely to have no efficient (classical) solution. This suggests that proving complexity lower bounds using geometric techniques will require us to use non-generic properties of specific unitaries. The second obstacle discussed in this section is an apparent shortcoming in prior work on the geometric approach to quantum computing, which is that it was developed for the analysis of quantum circuits which do not make use of ancillary working qubits. We show how to avoid this restriction by using a canonical extension procedure for unitary operations which allows ancillas to be incorporated into the geometric point of view. This canonical extension procedure may be of independent interest.

Background: We assume throughout that the reader is familiar with quantum circuits at the level of, e.g., Chapter 4 of [3], and with elementary Riemannian geometry, at the level of, e.g., [7, 8]. In particular, we assume a working knowledge of notions such as tensor fields, the Levi-Civita connection, the geodesic equation, and the curvature tensor. Much of our presentation is concerned with properties of a special type of Riemannian manifold, known as a right-invariant manifold. However, the results we need about right-invariant Riemannian manifolds are not easily accessible in a single (or even a few) publications, so far as we are aware. Therefore, to make the paper accessible, we have developed in a self-contained way the main results about right-invariant manifolds. The reader curious to investigate the literature further should be warned that both left- and rightinvariant manifolds are widely studied, but differ only trivially, and results about one can always be transformed into results about the other, sometimes with changes of sign.

Prior work: Geometric techniques have been used previously in the study of quantum information process-

ing. In particular, Khaneja et al [9, 10, 11] (see also related ideas in [12]) have used powerful techniques from the theory of symmetric spaces to study time-optimal control. This has been extremely successful in the twoqubit case, leading to an essentially complete characterization of two-qubit time optimal control. In the manygubit scenario some successes have been achieved, but the need for the rather specialized symmetric space structure limits the breadth of possible applications. Related ideas have also been investigated by Carlini et al [13, 14], who developed variational principles for time-optimal synthesis of quantum states and of unitary transformations. Time-optimal quantum control of unitary operations has a long history; in addition to the above references, we refer the reader to [15, 16] for recent work, and references to earlier literature.

Perspective: The geometric approach to quantum computation is in its infancy, and its long-term merits remain to be determined. This and earlier papers do not yet offer a killer application of geometric ideas, not available through conventional circuit analysis. However, we believe that there are reasons to hope that the geometric viewpoint will eventually enable insights difficult to obtain in the conventional circuit picture. In particular, by recasting the problem of quantum circuit complexity in terms of smooth mathematical objects, we bring the principles of the calculus of variations into play. This allows us to derive a geodesic equation describing the locally optimal evolutions generating a desired unitary; intuitively, this is to fall freely along a minimal geodesic, with the motion determined entirely by the local geometry of the space, and the initial direction of motion. This is in contrast to the circuit picture, where no such principles are available to derive the locally optimal way to construct a circuit. The present paper develops a fairly complete picture of the basic geometry of quantum computation, and lays the foundation for a more detailed understanding.

II. QUANTUM CIRCUIT COMPLEXITY AND GEOMETRY

In this section we review the connections between Riemannian geometry and quantum circuit complexity, as developed in [4, 5, 6].

We begin by recalling a few basic ideas from Riemannian geometry. We will actually consider Riemannian metrics on two slightly different manifolds, the group $M = U(2^n)$ of n-qubit unitary operations, and the group $M = SU(2^n)$ of n-qubit unitaries with unit determinant. For the most part the development is identical for the two cases, and we will not explicitly delineate them. However, there are a few cases where it is advantageous to use one or the other, and we mention explicitly when this is the case. For definiteness, you may assume that we are working with $SU(2^n)$ unless otherwise specified.

A tangent vector to a point on this manifold (i.e., an n-qubit unitary, U, with unit determinant) can be thought

of as a traceless Hamiltonian, H, i.e., an element of the Lie algebra $su(2^n)$ of traceless $2^n \times 2^n$ Hermitian matrices. More precisely, we can identify a tangent vector at U with the tangent to the curve $e^{-iHt}U$ at t=0. We shall call H the Hamiltonian representation of this tangent vector¹. With these identifications, the Riemannian metric $\langle \cdot, \cdot \rangle_U$ at a point U is a positive-definite bilinear form $\langle H, J \rangle_U$ defined on traceless Hamiltonians H and J. Through most of this paper we assume that this bilinear form is constant as a function of U and so write $\langle \cdot, \cdot \rangle_U = \langle \cdot, \cdot \rangle$. A metric which is constant in this way is known as a right-invariant metric.

Suppose U(t) is a curve in $SU(2^n)$ generated by the Hamiltonian H(t) according to the Schrödinger equation $\dot{U} = -iHU$. Then the length of that curve is given by

$$\int dt \, \langle H(t), H(t) \rangle^{1/2}. \tag{1}$$

The distance d(U, V) between points U and V in $SU(2^n)$ is defined to be the minimal length of any curve joining those two points.

The metric of most interest in this paper is defined as follows. Let \mathcal{P} be the subspace of n-qubit Hamiltonians which contain only 1- and 2-body terms, that is, their Pauli operator expansion contains only terms of weight at most two, e.g., $X \otimes I^{n-1}$, $I \otimes X \otimes Y \otimes I^{n-3}$. Let \mathcal{Q} denote the complementary subspace of n-qubit Hamiltonians containing only 3- and more-body terms. Observe that $su(2^n) = \mathcal{P} + \mathcal{Q}$, i.e., any Hamiltonian can be (uniquely) decomposed as a sum $H = H_P + H_Q$ of one-and two-body terms, H_P , and of three- and more-body terms, H_Q . Overloading notation, we now define maps \mathcal{P} and \mathcal{Q} by $\mathcal{P}(H) \equiv H_P$ and $\mathcal{Q}(H) \equiv H_Q$. We define a right-invariant Riemannian metric which we call the $standard\ metric\ by$:

$$\langle H, J \rangle \equiv \frac{\operatorname{tr}(H\mathcal{P}(J)) + q \operatorname{tr}(H\mathcal{Q}(J))}{2^n}.$$
 (2)

The term q is a penalty parameter², which is chosen to be sufficiently large $(q > 4^n$ can be shown to work). The intuition behind this choice of q can be understood by viewing the length $\sqrt{\langle H(t), H(t) \rangle}$ as a cost for applying the Hamiltonian H(t), and so choosing q exponentially large imposes a very large cost for the direct application of three- and more-qubit gates.

The metric of Equation (2) induces a distance $d(\cdot, \cdot)$ on $SU(2^n)$, as described above. This distance function may be related to quantum gate complexity by the following inequalities, proved in [4, 5]:

$$\frac{b_0 G(U,\epsilon)^{b_1} \epsilon^{b_2}}{n^{b_3}} \le d(I,U) \le G(U). \tag{3}$$

In the first inequality, $G(U,\epsilon)$ is the approximate gate complexity $G(U, \epsilon)$ of U, defined to be the minimal number of one- and two-qubit gates required to synthesize some *n*-qubit unitary operation V such that $||U-V|| \leq \epsilon$, where $\|\cdot\|$ is the usual matrix norm, and no ancilla qubits are used in the computation. The values b_0, b_1, b_2 and b_3 are positive constants. The papers [4, 6] proved this result for $b_1 = 1/3$, $b_2 = 2/3$ and $b_3 = 2$; a value for b_0 was not calculated explicitly, and won't be needed in this paper in any case. Examination of [4, 6] reveals that it is certainly possible to obtain stronger bounds on these constants, but a tight analysis remains to be done. In the second inequality in Equation (3), G(U) is the exact gate complexity of U, i.e., the minimal number of one- and two-qubit gates required to synthesize U exactly, with no ancilla qubits used in the synthesis. Thus, these two inequalities may be summarized by saying that the distance d(I,U) gives us both a lower bound on the exact gate complexity, and an upper bound on the approximate gate complexity of synthesizing U.

Equation (3) can be generalized by using universal families of Hamiltonians other than the one- and two-qubit Hamiltonians. The idea is to choose a subspace \mathcal{P}' of n-qubit Hamiltonians which has only polynomial (in n) dimension, and which is universal for computation. We choose a subspace \mathcal{Q}' such that $su(2^n) = \mathcal{P}' + \mathcal{Q}'$. Overloading notation as before, we define a new metric,

$$\langle H, J \rangle' \equiv \frac{\operatorname{tr}(H\mathcal{P}'(J)) + q \operatorname{tr}(H\mathcal{Q}'(J))}{2^n}.$$
 (4)

It can be shown using the techniques of [4, 6] that provided q is sufficiently large, then

$$poly(G'(U,\epsilon), n, \epsilon) \le d'(I, U) \le G'(U), \tag{5}$$

where poly is some polynomial (with constant but possibly non-integer powers), and the primes indicate the change in choice of universal gates and of metric. More generally, we shall say that any metric related to gate complexity by a relationship of the form of Equation (5) is a *computational metric*.

The metric of most interest to us in the remainder of the paper is the standard metric of Equation (2). However, many of the results we prove will hold in more generality, for *projective metrics*, by which we mean a metric of the form of Equation (4), or even more generally for right-invariant metrics.

III. THE CONNECTION

In this section we derive several explicit formulae for the Levi-Civita connection, which is the basic geometric object on the manifold. These results are standard in the literature on right-invariant Riemannian manifolds (see, e.g., Appendix 2 in [17] for an introduction), although our derivation is from a slightly unusual point of view, being based on the background in differential geometry

¹ In an earlier paper [5] the Pauli expansion coefficients of *H* were referred to as local co-ordinates for the tangent vector. We shall not use this terminology here.

Note that our definition and notation for the penalty parameter has changed slightly from [4, 5, 6].

most common to physicists. Many of the same results can be derived from a more abstract point of view by starting with the general formula for the Levi-Civita connection (e.g., Equation (5.1) on page 69 of [8]). We derive these results here in part for completeness, and also because it provides an opportunity to introduce many items of notation and nomenclature used in subsequent sections. Note that Appendix A uses these results to compute all the natural curvature quantities associated to our metric.

If Y and Z are vector fields on a manifold, then in a fixed co-ordinate system $\{x^k\}$ the connection is given by:

$$(\nabla_Y Z)^j = \frac{\partial z^j}{\partial x^k} y^k + \Gamma^j_{kl} y^k z^l, \tag{6}$$

where y^k, z^k are natural co-ordinate representations for the vector fields Y and Z with respect to the co-ordinate system $\{x^k\}$, summation over repeated indices is implied, and Γ^j_{kl} are the Christoffel coefficients. Expressing the metric tensor g_{jk} with respect to the same system of coordinates we have:

$$\Gamma_{kl}^{j} = g^{jm} \Gamma_{mkl} = \frac{g^{jm}}{2} \left(g_{mk,l} + g_{ml,k} - g_{kl,m} \right),$$
 (7)

where a subscript $_{,l}$ denotes a partial derivative with respect to x_l .

We have defined our metric in Equation (2) using a representation for tangent vectors which identifies a Hamiltonian H with the tangent to $e^{-iHt}U$ at t=0. It is natural to hope that there is a co-ordinate representation for this Hamiltonian (e.g., the Pauli expansion coefficients) which can be identified in a natural way with a set of co-ordinates such as the x_j above. Unfortunately, such a representation does not exist. Instead, to evaluate the Christoffel symbol we must first introduce a fixed system of co-ordinates on the manifold, which we shall call Pauli co-ordinates. We then re-express the metric in terms of these Pauli co-ordinates, and use this re-expression to evaluate the Christoffel coefficients. This can then be used to obtain co-ordinate independent representations for the connection and other geometric objects.

Pauli co-ordinates: To evaluate the connection it is sufficient to introduce co-ordinates defined in a neighbourhood of the origin, $I \in SU(2^n)$. This enables us to evaluate the connection at the origin, and the rightinvariance of the metric then gives a general expression for the connection everywhere on the manifold. We define Pauli co-ordinates by representing U in a neighbourhood of the origin as $U = e^{-iX}$. Such an X can be defined in a unique way using the standard branch of the logarithm. We can associate a co-ordinate vector x to X via $X = x \cdot \sigma$, i.e., the vector x consists of the Pauli expansion coefficients of X. Note that $x^{\sigma} = \operatorname{tr}(X\sigma)/2^n$. We call the matrix X the Pauli representation for U, and the components x^{σ} the Pauli co-ordinates. We shall also use this terminology for the natural corresponding co-ordinates on the tangent spaces, and on the tangent bundle.

We have defined the metric in terms of a Hamiltonian representation for tangent vectors. Our goal now is to reexpress the metric in terms of the Pauli representation. Suppose we are at a point $U = e^{-iX}$ on the manifold, and that a tangent vector is specified there by the Hamiltonian H. What is the corresponding representation of the tangent vector in the Pauli co-ordinate representation for the tangent space $T_U SU(2^n)$?

To answer this question, we rewrite the tangent curve $e^{-iHt}e^{-iX}$ corresponding to H in the form $e^{-iHt}e^{-iX}=e^{-i(X+tJ)}+O(t^2)$. The Baker-Campbell-Hausdorff formula gives us:

$$H = \mathcal{E}_X(J) \equiv i \operatorname{ad}_X^{-1} \left(e^{-i \operatorname{ad}_X} - \mathcal{I} \right) (J), \tag{8}$$

where $\operatorname{ad}_X(Y) \equiv [X,Y], [\cdot,\cdot]$ denotes the matrix commutator, and $\mathcal{I}(Y) \equiv Y$. This formula relates the Hamiltonian representation, H, of the tangent vector, to the Pauli representation, J, of the same tangent vector.

It can be shown that \mathcal{E}_X is invertible near the origin, i.e., for X sufficiently close to 0. We denote the inverse by $\mathcal{D}_X = \mathcal{E}_X^{-1}$, so we have $J = \mathcal{D}_X(H)$. Note that \mathcal{E}_X has the power series expansion

$$\mathcal{E}_X = \sum_{j=0}^{\infty} \frac{(-i\mathrm{ad}_X)^j}{(j+1)!}.$$
 (9)

To compute the connection at the origin it suffices to have expansions of \mathcal{E}_X and \mathcal{D}_X to first order in X:

$$\mathcal{E}_X = \mathcal{I} - \frac{i \operatorname{ad}_X}{2} + O(X^2); \quad \mathcal{D}_X = \mathcal{I} + \frac{i \operatorname{ad}_X}{2} + O(X^2). \tag{10}$$

Finally, it is helpful to note that the adjoint of these superoperators with respect to the trace inner product $(X,Y) \equiv \operatorname{tr}(X^{\dagger}Y)$ satisfies $\mathcal{E}_{X}^{\dagger} = \mathcal{E}_{-X}$ and $\mathcal{D}_{X}^{\dagger} = \mathcal{D}_{-X}$.

The metric in Pauli co-ordinates: In Section II we defined the metric with respect to the Hamiltonian representation. We now rewrite the metric in a neighbourhood of the origin with respect to the Pauli co-ordinates. This procedure can be carried out for a general right-invariant metric with essentially no extra effort beyond what is required for the standard metric. The most general form for a right-invariant metric in the Hamiltonian representation is:

$$\langle H, J \rangle = \frac{\operatorname{tr}(H\mathcal{G}(J))}{2^n},$$
 (11)

where \mathcal{G} is a strictly positive (and thus self-adjoint) superoperator, i.e., a linear operator on matrices such that $\operatorname{tr}(H\mathcal{G}(H)) > 0$ whenever $H \neq 0$. For the standard metric, the explicit form of \mathcal{G} is $\mathcal{G} = \mathcal{P} + q\mathcal{Q}$. It will be convenient for later use to define a Hermitian matrix $L \equiv \mathcal{G}(H)$ dual to the Hamiltonian, H. Note that the dual satisfies $\langle H, J \rangle = \operatorname{tr}(LJ)/2^n$ for all J.

Suppose Y and Z are tangent vector fields defined in a neighbourhood of the origin. We will also use Y and Z to denote the specific values these vector fields take at a point $U = e^{-iX}$ in that neighbourhood. Let Y^P, Z^P

denote the Pauli representation for these vectors, and $Y^H = \mathcal{E}_X(Y^P)$ and $Z^H = \mathcal{E}_X(Z^P)$ denote the corresponding Hamiltonian representation. The metric then is given by:

$$\langle Y, Z \rangle = \frac{\operatorname{tr}(Y^H \mathcal{G}(Z^H))}{2^n}$$
 (12)

$$= \frac{\operatorname{tr}(\mathcal{E}_X(Y^P)\mathcal{G} \circ \mathcal{E}_X(Z^P))}{2^n}$$
 (13)

$$= \frac{\operatorname{tr}(Y^{P}\mathcal{E}_{X}^{\dagger} \circ \mathcal{G} \circ \mathcal{E}_{X}(Z^{P}))}{2^{n}}.$$
 (14)

Define $\mathcal{G}_X \equiv \mathcal{E}_X^{\dagger} \circ \mathcal{G} \circ \mathcal{E}_X$, so $\langle Y, Z \rangle = \operatorname{tr}(Y^P \mathcal{G}_X(Z^P))/2^n$. With respect to the Pauli co-ordinates y^{σ} and z^{σ} we have $Y^P = \sum_{\sigma} y^{\sigma} \sigma$ and $Z^P = \sum_{\sigma} z^{\sigma} \sigma$, and thus in this co-ordinate representation the metric tensor has components

$$g_{\sigma\tau} = \frac{\operatorname{tr}(\sigma \mathcal{G}_X(\tau))}{2^n}.$$
 (15)

The inverse $g^{\sigma\tau}$ is given by

$$g^{\sigma\tau} = \frac{\operatorname{tr}(\sigma \mathcal{F}_X(\tau))}{2^n},\tag{16}$$

where $\mathcal{F}_X \equiv \mathcal{G}_X^{-1} = \mathcal{D}_X \circ \mathcal{F} \circ \mathcal{D}_X^{\dagger}$ and $\mathcal{F} \equiv \mathcal{G}^{-1}$. To compute first derivatives, we note that

$$\mathcal{G}_X = \mathcal{G} + \frac{i}{2}[\operatorname{ad}_X, \mathcal{G}] + O(X^2).$$
 (17)

Using the cyclic property of trace, and the fact $\mathcal{G}^{\dagger} = \mathcal{G}$, a computation shows that at the origin

$$g_{\sigma\tau,\mu} = \frac{i \operatorname{tr}(([\mathcal{G}(\sigma), \tau] + [\mathcal{G}(\tau), \sigma])\mu)}{2^{n+1}}.$$
 (18)

Other equivalent forms are possible; this form seems to us to be particularly easy to recall.

The Christoffel symbol: The Christoffel symbol $\Gamma^{\rho}_{\sigma\tau} = g^{\rho\mu}\Gamma_{\mu\sigma\tau}$ may be computed at the origin by observing that

$$\Gamma_{\mu\sigma\tau} = \frac{1}{2} \left(g_{\mu\sigma,\tau} + g_{\mu\tau,\sigma} - g_{\sigma\tau,\mu} \right) \tag{19}$$

$$= \frac{i}{2^{n+1}} \operatorname{tr} \left(\mu([\sigma, \mathcal{G}(\tau)] + [\tau, \mathcal{G}(\sigma)]) \right). \quad (20)$$

Using $g^{\rho\mu} = \operatorname{tr}(\mathcal{F}(\rho)\mu)/2^n$ we obtain

$$\Gamma^{\rho}_{\sigma\tau} = \frac{i}{2^{n+1}} \operatorname{tr} \left(\mathcal{F}(\rho)([\sigma, \mathcal{G}(\tau)] + [\tau, \mathcal{G}(\sigma)]) \right). \tag{21}$$

It is worth noting that this formula holds in considerable generality. The only critical property of the Pauli matrices used in the derivation is that they are orthonormal (up to a constant factor) with respect to the trace inner product.

The connection: Working in the Pauli representation and using Equations (6) and (21), we have at the origin:

$$(\nabla_Y Z)^P = y^{\sigma} Z_{,\sigma}^P + \frac{i}{2} \mathcal{F}\left([Y^P, \mathcal{G}(Z^P)] + [Z^P, \mathcal{G}(Y^P)] \right).$$
(22)

This equation gives a formula for the connection evaluated at the origin, when the vector fields are written in the Pauli representation. This can be re-expressed in the Hamiltonian representation by observing that at the origin $(\nabla_Y Z)^H = (\nabla_Y Z)^P$, $Y^H = Y^P$ (and thus the y^σ components are the same in both representations), and $Z^H = Z^P$. Finally, we have $Z^P = \mathcal{D}_X(Z^H)$ near the origin, and thus using Equation (10) we obtain $Z^P_{,\sigma} = (i/2)[\sigma,Z^H] + Z^H_{,\sigma}$ at the origin. This gives:

$$(\nabla_Y Z)^H = y^{\sigma} Z_{,\sigma}^H + \frac{i}{2} \left([Y^H, Z^H] + \mathcal{F} \left([Y^H, \mathcal{G}(Z^H)] + [Z^H, \mathcal{G}(Y^H)] \right) \right).$$

$$(23)$$

Note that the partial derivative in $Z_{,\sigma}^{H}$ is still with respect to the Pauli co-ordinates x^{σ} on the manifold.

Suppose now that we have a curve that passes through the origin and that has tangent Y at the origin. Using Equation (23) we see that the covariant derivative along the curve $D_t Z \equiv \nabla_Y Z$ is given in the Hamiltonian representation by:

$$(D_t Z)^H = \frac{dZ^H}{dt} + \frac{i}{2} ([Y^H, Z^H] + \mathcal{F} ([Y^H, \mathcal{G}(Z^H)] + [Z^H, \mathcal{G}(Y^H)])).$$
(24)

Note that because of the right-invariance of the metric this equation is true everywhere on the manifold.

The formula for the connection simplifies in the special case when Z is a right-invariant vector field. In this case Z^H does not vary as a function of position, and so Equation (23) gives:

$$(\nabla_Y Z)^H = \frac{i}{2} \left([Y^H, Z^H] + \mathcal{F} \left([Y^H, \mathcal{G}(Z^H)] + [Z^H, \mathcal{G}(Y^H)] \right) \right).$$

$$(25)$$

Once again, because of the right-invariance of the metric this equation is true everywhere on the manifold. A consequence of this equation that will be useful later is that $\langle X, \nabla_Y Z \rangle = -\langle \nabla_Y X, Z \rangle$ for any triple of right-invariant vector fields, X, Y and Z.

Note that in subsequent sections we work almost entirely in the Hamiltonian representation. As a consequence, when applying formulae like Equations (23) and (24) we will drop the superscript H's.

IV. GEODESICS

In this section we present the geodesic equation (Subsection IV A), develop a complete set of constants of the motion for the geodesic equation (Subsection IV B), and describe several classes of analytic solutions to the geodesic equation (Subsection IV C).

A. The geodesic equation

By definition, a geodesic in $SU(2^n)$ is a curve U(t) whose tangent vector H(t) satisfies the condition $D_tH = 0$, i.e., the tangent vector is parallel transported along the curve. Using Equation (24) this becomes

$$0 = \dot{H} + i\mathcal{F}([H, \mathcal{G}(H)]). \tag{26}$$

This equation is more conveniently rewritten in terms of the dual $L \equiv \mathcal{G}(H) = \mathcal{F}^{-1}(H)$. After a little algebra we obtain the geodesic equation in the form we shall most commonly apply it,

$$\dot{L} = i[L, \mathcal{F}(L)]. \tag{27}$$

We shall refer to this equation as the geodesic equation, to distinguish it from other equivalent forms. A third form which is often used in the literature is the form $\langle \dot{H}, J \rangle = i \langle H, [H, J] \rangle$, valid for any $J \in su(2^n)$. Note that the geodesic equation is a well-known result in the literature on right-invariant Riemannian manifolds (see, e.g., Appendix 2 of [17]). Note also that Equation (27) is in the class of Lax equations well known to mathematicians

In the special case of the standard metric the geodesic equation simplifies nicely. Recalling that $\mathcal{G} = \mathcal{P} + q\mathcal{Q}$, and thus $\mathcal{F} = \mathcal{G}^{-1} = \mathcal{P} + q^{-1}\mathcal{Q}$, we obtain

$$\dot{L} = i (1 - q^{-1}) [L, \mathcal{P}(L)].$$
 (28)

Provided $q \neq 1$ we can remove the dependence on q by defining a rescaled version of L, $M \equiv (1 - q^{-1})L$, obtaining a form of the geodesic equation independent of q, except for the requirement $q \neq 1$:

$$\dot{M} = i[M, \mathcal{P}(M)]. \tag{29}$$

This is a remarkable equation. Because the minimal length path between any two points on a Riemannian manifold is a geodesic, we may assume without loss of generality that the optimal Hamiltonian H(t) generating any unitary operation is determined by a solution M(t) to Equation (29) via the rescaling $H = \mathcal{G}(M)/(1-q^{-1})$. Equation (29) is thus a single universal equation whose solutions determine the paths of minimal length on the manifold. This situation is in vivid contrast with how we usually think about the standard circuit model of quantum computing, where H(t) may have arbitrary time dependence³. It is also notable that Equation (28) is (arguably) the simplest and most elegant equation involving both the Lie group structure, expressed through the Lie

bracket, and also the map \mathcal{P} onto the set of Hamiltonians that are regarded as computationally easy to implement.

As a caveat to this optimistic picture, note that being a geodesic is merely a necessary condition, not a sufficient condition, for a path to be minimal. In particular, there may be many geodesics passing from I to a desired unitary, U, and not all those geodesics will be globally minimizing⁴. The situation is analogous to minimizing a function f(x) in conventional calculus: the condition f'(x) = 0 is a constraint that must be satisfied by x minimizing f(x), but further analysis is necessary to determine if f(x) is a global minimum. Thus finding geodesics is only a first step towards the determination of the distance d(I, U).

B. Constants of the motion

The geodesic equation (Equation (27)) on a right-invariant Riemannian manifold has a corresponding set of constants of the motion which completely determine the geodesics [17]. To see this, observe that for any choice of L_0 the function $L(t) = U(t)L_0U(t)^{\dagger}$ satisfies the geodesic equation, Equation (27). It follows that along any geodesic the function $U(t)^{\dagger}L(t)U(t) = L_0$ is a matrix-valued constant of the motion. Furthermore, by differentiating the equation $L(t) = U(t)L_0U(t)^{\dagger}$ we may recover the geodesic equation, and thus this set of constants of the motion completely determines the geodesics of the system.

As an aside, it is possible to *derive* these constants of the motion (and thus the geodesic equation) by observing that the metric is invariant under a continuous symmetry group, namely, arbitrary right translations of $SU(2^n)$. One may then use Noether's theorem to find the associated constants of the motion, which turn out to be precisely the matrix elements of $U(t)^{\dagger}L(t)U(t)$. This is the approach taken to derive the geodesic equation in [17].

One-body terms are constants of the motion: In the special case of the standard metric, it can be shown that the coefficients of the one-body terms in the Pauli expansion of H(t) are also constants of the motion along geodesics. This fact is useful in developing certain analytic solutions to the geodesic equation, to be described later. To prove that the one-body terms are constant, let S(X) map the n-qubit matrix X onto just its one-body terms. We see that:

$$\frac{d\mathcal{S}(L)}{dt} = \mathcal{S}\left(\frac{dL}{dt}\right) \tag{30}$$

$$= i(1 - q^{-1})\mathcal{S}([L, \mathcal{P}(L)])$$
 (31)

$$= i(1 - q^{-1})\mathcal{S}([\mathcal{Q}(L), \mathcal{P}(L)]). \tag{32}$$

³ This appears to be a major advantage of the geometric approach over the circuit approach. It comes, however, at a cost. In the geometric approach H(t) may include (exponentially small) three-and more-body terms, while in the circuit model only one- and two-body terms appear in the Hamiltonian.

⁴ They are, however, locally minimizing in the sense that any sufficiently small arc along any geodesic is always a global minimum of the length functional ([19], pp 222-226).

The Pauli commutation relations imply that: (1) the commutator of $\mathcal{Q}(L)$ with the one-body terms in $\mathcal{P}(L)$ produces only three- and more-body terms, and (2) the commutator of $\mathcal{Q}(L)$ with the two-body terms in $\mathcal{P}(L)$ produces only two- and more-body terms. As a result $\mathcal S$ annihilates $[\mathcal{Q}(L), \mathcal{P}(L)]$, and so $\mathcal{S}(L)$ is a constant of the motion.

An alternative proof that the one-body terms are constants of the motion may be found by applying Noether's theorem to the continuous symmetry $SU(2^n) \to SU(2^n)$ defined by $U \to VUV^{\dagger}$, where V is an arbitrary one-qubit unitary.

Analytic solutions to the geodesic equation

We now develop a range of partial and full solutions to the geodesic equation. Our results are mostly specialized to projective metrics, and some results are further specialized to the standard metric. In IV C1 we develop general necessary and sufficient conditions for geodesics to be of the form e^{-iHt} for a constant Hamiltonian H. In IV C 2 we find an exact form for the geodesics of the standard metric in the three-qubit case, for the $q \to \infty$ limit. This form is based on an algebraic structure that is also useful in other contexts. Finally, in IVC3 we develop a formal power series solution to the geodesic equation.

Geodesics where the Hamiltonian is constant

Along certain geodesics the Hamiltonian is constant, and thus the geodesic has the form e^{-iHt} . To determine when this is the case it suffices to determine when the dual L(t) is constant along a geodesic, since the dual is related to the Hamiltonian by a fixed invertible transformation. From the geodesic equation for projective metrics, $\dot{L} = i(1 - q^{-1})[L, \mathcal{P}(L)]$, we see that in the q = 1case L is always constant along geodesics. However, the case of most interest to us is when q is very large, where we see that a necessary and sufficient condition for L to be constant is that $[\mathcal{Q}(L), \mathcal{P}(L)] = 0$. This is equivalent to the condition that $[\mathcal{Q}(H), \mathcal{P}(H)] = 0$. When this condition is satisfied, and only when it is satisfied, the geodesic is of the form $\exp(-iHt)$.

In the case of the standard metric, we see that this condition is that the one- and two-body terms in a Hamiltonian should commute with the three- and morebody terms. An appealing consequence is that whenever H contains only one- and two-body terms, then $\exp(-iHt)$ is a geodesic. Over sufficiently short time periods geodesics are guaranteed to be minimal length curves (see, e.g., Section 3.3 of [7]), and so this result accords with the intuition that the fastest way to simulate a physical system is with its own evolution.

Geodesics for three qubits

In the case where there are only three gubits we can derive a solution to the geodesic equation for the standard metric that is exact in the large q limit. In fact, it turns out to be possible to analyze a more general class of metrics, defined by the choice

$$\mathcal{G} \equiv s\mathcal{S} + \mathcal{T} + q\mathcal{Q},\tag{33}$$

where S maps onto the subspace of three-qubit Hamiltonians which contain only one-body terms, \mathcal{T} maps onto the subspace containing only two-body terms, and \mathcal{Q} maps onto the subspace containing only three-body terms. In the case s = 1 this reduces to the standard metric. The limit $s \to 0$ corresponds to the case where onebody Hamiltonians may be applied effectively for free.

The key observation needed to obtain the geodesics is the commutation relations between the matrix subspaces \mathcal{S} , \mathcal{T} and \mathcal{Q} ,

$$[\mathcal{S}, \mathcal{T}] \subseteq \mathcal{T} \tag{34}$$

$$[\mathcal{S}, \mathcal{Q}] \subseteq \mathcal{Q} \tag{35}$$

$$[\mathcal{T}, \mathcal{Q}] \subseteq \mathcal{T}. \tag{36}$$

Note that the derivation which follows depends only on these commutation relations, and not on the specific choice of \mathcal{S} as one-body Hamiltonians, etcetera. It would be interesting to obtain other examples, outside the three-qubit context, where this algebraic structure appears naturally. We do not know whether this particular structure is ever of computational interest in the large n limit. We note that this general approach of using algebraic structure to obtain insight into geometry is reminiscent of the work of Khaneja, Glaser and Brockett [11], who make use of symmetric spaces to solve geometric problems involving two qubits.

Defining $S \equiv \mathcal{S}(L)$, $T \equiv \mathcal{T}(L)$, and $Q \equiv \mathcal{Q}(L)$, we see from the commutation relations of Equations (34)-(36) that the geodesic equation $\dot{L} = i[L, \mathcal{F}(L)]$ becomes:

$$S = 0 (37)$$

$$\dot{T} = i \left[(1 - s^{-1})S + (1 - q^{-1})Q, T \right]$$
 (38)

$$\dot{Q} = i(q^{-1} - s^{-1})[S, Q].$$
 (39)

To solve these equations, observe that S is a constant of the motion. This makes the equation for Q a linear equation that is easily solved. The equation for T is then a time-dependent linear equation that can be solved using standard techniques. The resulting solution is

$$S(t) = S_0 \tag{40}$$

$$T(t) = e^{it(q^{-1} - s^{-1})S_0} e^{it(1 - q^{-1})(S_0 + Q_0)} \times$$

$$T_0 e^{-it(1-q^{-1})(S_0+Q_0)} e^{-it(q^{-1}-s^{-1})S_0}$$
 (41)

$$T_{0}e^{-it(1-q^{-1})(S_{0}+Q_{0})}e^{-it(q^{-1}-s^{-1})S_{0}}$$
(41)

$$Q(t) = e^{it(q^{-1}-s^{-1})S_{0}}Q_{0}e^{-it(q^{-1}-s^{-1})S_{0}}.$$
(42)

The corresponding Hamiltonian has the form:

$$H(t) = s^{-1}S(t) + T(t) + q^{-1}Q(t).$$
(43)

This expression for the Hamiltonian holds for all q and s. We now show how to integrate the corresponding Schrödinger equation in the large q limit to obtain the geodesic U(t).

Without loss of generality we can assume that we are working on a geodesic with $\langle H(t), H(t) \rangle = 1$ for all time. As a result we obtain the bounds $\operatorname{tr}(S^2)/2^3 \leq s, \operatorname{tr}(T^2)/2^3 \leq 1$, and $\operatorname{tr}(Q^2)/2^3 \leq q$. The term $q^{-1}Q(t)$ is therefore of order $q^{-1/2}$, and thus may be neglected in the large q limit, with a resulting error in U(t) of order $tq^{-1/2}$. For similar reasons, we can neglect the q^{-1} terms in the exponentials appearing in T(t). The resulting error in T(t) is at most of order $t(s^{1/2}q^{-1}+q^{-1/2})$, and thus the error in U(t) is at most of order $t(s^{1/2}q^{-1}+q^{-1/2})$. This leads us to define an approximate Hamiltonian

$$\tilde{H}(t) = s^{-1}S_0 + e^{-its^{-1}S_0}e^{it(S_0 + Q_0)} \times T_0e^{-it(S_0 + Q_0)}e^{its^{-1}S_0}.$$
(44)

The corresponding solution $\tilde{U}(t)$ to the Schrödinger equation satisfies

$$||U(t) - \tilde{U}(t)|| \le O(tq^{-1/2} + t^2(s^{1/2}q^{-1} + q^{-1/2})).$$
 (45)

Making the change of variables $\tilde{V} = e^{-it(S_0 + Q_0)}e^{its^{-1}S_0}\tilde{U}$ we see that the Schrödinger equation is equivalent to

$$\tilde{\tilde{V}} = -i \left(S_0 + T_0 + Q_0 \right) \tilde{V}. \tag{46}$$

The approximate solution to the geodesic equation is thus

$$\tilde{U}(t) = e^{-its^{-1}S_0}e^{it(S_0 + Q_0)}e^{-it(S_0 + T_0 + Q_0)}.$$
 (47)

Although this form is an exact solution to the geodesic equation in the $q \to \infty$ limit, it is not obvious which is the minimal geodesic passing through a particular desired unitary U. Developing techniques to find minimal geodesics in this case is an interesting problem for further work.

The special case $s \to 0$ is of some interest in our threequbit example, where it corresponds to zero cost for local unitary operations. In this limit the S_0 terms in the second and third exponentials of Equation (47) may be neglected, and we obtain the solution:

$$\tilde{U}(t) = e^{-its^{-1}S_0}e^{itQ_0}e^{-it(T_0 + Q_0)}. (48)$$

Returning to the case of general s, we now attempt to simplify the expression in Equation (47). Generically, we expect that $S_0 + Q_0$ is large compared with T_0 , and $S_0 + Q_0$ is non-degenerate. First-order perturbation theory can be used to simplify the product of the final two terms to obtain

$$\tilde{U}(t) = e^{-its^{-1}S_0} e^{-it\mathcal{R}_{S_0 + Q_0}(T_0)}, \tag{49}$$

where $\mathcal{R}_{S_0+Q_0}(T_0)$ denotes the diagonal matrix which remains when we work in the eigenbasis of $S_0 + Q_0$ and remove all off-diagonal entries from T_0 . Assuming Q_0 is nondegenerate, in the $s \to 0$ limit we obtain

$$\tilde{U}(t) = e^{-its^{-1}S_0} e^{-it\mathcal{R}_{Q_0}(T_0)}. (50)$$

3. Formal solution of the geodesic equation

In this section we develop a formal power series solution to the geodesic equation. The formal solution is most easily developed for the dual L(t) which satisfies the equation $\dot{L}=i[L,\mathcal{F}(L)]$. We expand L(t) in a power series,

$$L(t) = \sum_{j=0}^{\infty} \frac{L^{(j)}(0)t^{j}}{j!},$$
(51)

where $L^{(j)}(0)$ is the j'th derivative of L(t) at t=0. This derivative can, in principle, be evaluated using the geodesic equation. It is rather inconvenient to do this directly. However, it can be done easily using the vectorization technique, whereby matrices are converted into vectors, and linear operations taking matrices to matrices become matrix operations taking vectors to vectors. We assume readers are familiar with vectorization (see, e.g., Chapter 4 of [18]).

We will write the formal solution for any equation of the form $\dot{L} = \mathcal{E}(L,L)$, where $\mathcal{E}(\cdot,\cdot)$ is a bilinear operation. This class of equations includes the geodesic equation for any right-invariant metric. Vectorization of this equation yields

$$\frac{d|L)}{dt} = E(|L) \otimes |L), \tag{52}$$

where |L) is the vectorized form of the matrix L, and E is the vectorized form of the bilinear operation \mathcal{E} . Note that E is a linear operation mapping from the tensor product of two copies of the space on which |L) lives into a single copy of that space. For the class of operations \mathcal{E} arising from the geodesic equation, standard vectorization techniques show that E has the explicit form $E = iR(I - S)(I \otimes F)$, where F is the vectorized form of \mathcal{F} , S swaps the factors in the tensor product, and R is defined by $R(|X) \otimes |Y) \equiv |XY|$, where XY is the usual matrix product of X and Y.

Taking repeated derivatives, it follows that the j'th derivative may be written

$$|L^{(j)}\rangle = E(E \otimes I + I \otimes E) \dots (E \otimes I^{\otimes (j-1)} + I \otimes E \otimes I^{\otimes (j-2)} + \dots) |L\rangle^{\otimes (j+1)},$$
 (53)

where it is understood that $|L^{(j)}|$ and |L| are evaluated at time t = 0. To simplify this expression, observe that:

$$I^{\otimes k} \otimes E \otimes I^{\otimes l} = S_{1,k+1}(E \otimes I^{\otimes (k+l)})\pi, \tag{54}$$

where $S_{1,k}$ swaps systems 1 and k, and acts trivially on all other systems, and π is some permutation of the systems. It follows that if $|X\rangle$ is a vector in the entire tensor product space such that $|X\rangle$ is symmetric under interchange of any of the systems, then we have

$$(I^{\otimes k} \otimes E \otimes I^{\otimes l})|X) = S_{1,k+1}(E \otimes I^{\otimes (k+l)})|X), \quad (55)$$

where we used the fact that $\pi|X\rangle = |X\rangle$ for all permutations π . Define an operator T_m acting on m systems by

$$T_m \equiv I + S_{1,2} + \ldots + S_{1,m},$$
 (56)

where it is understood that each swap $S_{1,j}$ acts on m systems. Our earlier expression for $|L^{(j)}\rangle$, Equation (53), may now be rewritten as

$$|L^{(j)}\rangle = ET_2(E \otimes I)T_3(E \otimes I^{\otimes 2})$$
$$\dots T_j(E \otimes I^{\otimes (j-1)})|L\rangle^{\otimes (j+1)}.$$
(57)

Thus we have the desired formal expression for the vectorized solution |L(t)| to the equation $\dot{L} = \mathcal{E}(L, L)$,

$$|L(t)| = \sum_{j=0}^{\infty} \frac{\prod_{k=1}^{j} T_k(E \otimes I^{k-1}) |L(0)|^{\otimes (j+1)} t^j}{j!}.$$
 (58)

V. GEODESIC DEFORMATION AND CONJUGATE POINTS

A central problem in developing our geometric approach to quantum computation is to find a minimal geodesic from the identity I to a specified unitary U. In this section we develop two sets of tools that can be used to make progress towards the solution of this problem, and illustrate these tools through numerical examples.

The first set of tools are known as Jacobi fields and conjugate points. They are standard tools in Riemannian geometry, and relate the global problem of determining when a geodesic is minimizing to local curvature properties of the manifold. We will use these tools to give explicit examples of geodesics which are provably not minimizing, i.e., they can be used to find examples of curves which are local length minima, but which are not global length minima. For example, for geodesics of the form $\exp(-iHt)$, with H containing only one- and two-body terms, we use conjugate points to find values of t beyond which these geodesics are not minimal.

The second set of tools is aimed at solving the geodesic equation with fixed endpoints I and U. Traditional methods for solving this two-point boundary value problem (e.g., shooting methods) do not work so well, since the space we are working in has extremely high dimensionality. The idea we use is to deform the geodesics from the q=1 case, where the form of the geodesics is well understood, to much larger values of the penalty, e.g. $q=4^n$. We will show that this deformation can be achieved using a generalization of the Jacobi equation, which we call the lifted Jacobi equation. The lifted Jacobi equation enables us to define a notion of geodesic derivative, which is a way of deforming the geodesic as the penalty q is varied, without changing the endpoints. The lifted Jacobi equation, the geodesic derivative, and the deformation algorithm are all original, so far as we are aware.

The detailed structure of the section is as follows. We begin in Subsection VA by deriving the lifted Jacobi

equation, and obtain as a special case the standard Jacobi equation. This is done on a general Riemannian manifold. In Subsection VB we give explicit forms of these equations which are applicable to the standard metric. In particular, the lifted Jacobi equation describes how geodesics deform as the parameter q is varied in the standard metric. Subsection V C uses the conventional Jacobi equation to numerically investigate conjugate points, and to find examples of geodesics which are provably not minimizing. Subsection VD defines the geodesic derivative, and studies its basic properties, including obtaining necessary and sufficient conditions for the geodesic derivative to exist. The geodesic derivative is then applied in Subsection VE to obtain a numerical procedure for finding geodesics between I and a specified goal unitary, U. We illustrate this procedure with some numerical examples.

A. Lifted Jacobi equation

Suppose $\gamma(t)$ is a geodesic on a smooth manifold, M, with respect to some metric, g, and we smoothly change that metric. Intuitively, it seems it should be possible to smoothly deform the geodesic curve so that it remains a geodesic with respect to the new metric. The lifted Jacobi equation provides a way of making this intuition rigorous. It generalizes a well-known tool of Riemannian geometry known as the Jacobi equation, which describes the behaviour of nearby geodesics of a fixed metric.

We develop the lifted Jacobi equation on a general Riemannian manifold, M, and specialize later to cases of interest in the context of quantum computing. We suppose g_s is a family of metric tensor fields for M parameterized by a single real parameter, s, and smooth with respect to any fixed co-ordinate system. Define a $\binom{0}{2}$ symmetric tensor field g' to be the pointwise derivative of g with respect to s at some fixed value of s, say s=0.

Our strategy is as follows. Imagine $\gamma(s,t)$ is a smooth family of curves on M such that $\gamma(s,\cdot)$ is a geodesic with respect to the metric g_s . We call $\gamma(0,\cdot)$ the base geodesic, and define the lifted Jacobi field $J(t) \in T_{\gamma(0,t)}M$ along the base geodesic by

$$J(t) \equiv \partial_s \gamma(0, t). \tag{59}$$

The lifted Jacobi field is the vector field telling us how the base geodesic is locally deformed as s is varied. We will show as a consequence of the geodesic property that J(t) satisfies the lifted Jacobi equation, which is a second order differential equation. Conversely, given a solution to the lifted Jacobi equation, it is possible to define a corresponding family of deformed geodesics.

To derive the lifted Jacobi equation we expand $\gamma(\Delta, t)$ in a co-ordinate representation as

$$\gamma(\Delta, t) = \gamma(0, t) + \Delta J(t) + O(\Delta^2). \tag{60}$$

By definition $\gamma(\Delta, t)$ satisfies the geodesic equation associated to the metric g_{Δ} . Substituting into the geodesic

equation, expanding in powers of Δ , and considering the term linear in Δ gives

$$0 = \frac{\partial J^{j}}{\partial t^{2}} + \Gamma^{j}_{kl} \frac{\partial J^{k}}{\partial t} \frac{\partial \gamma^{l}}{\partial t} + \Gamma^{j}_{kl} \frac{\partial \gamma^{k}}{\partial t} \frac{\partial J^{l}}{\partial t} + \Gamma^{j}_{kl,m} J^{m} \frac{\partial \gamma^{k}}{\partial t} \frac{\partial \gamma^{l}}{\partial t} + \frac{\partial \Gamma^{j}_{kl}}{\partial s} \frac{\partial \gamma^{k}}{\partial t} \frac{\partial \gamma^{l}}{\partial t}.$$
(61)

The standard Jacobi equation corresponds to the case where g_s is constant, i.e., to the case where the first four terms on the right-hand side of the above equation sum to zero. This allows us to rewrite the above equation in more geometric terms as

$$(D_t^2 J)^j + (R(J, \dot{\gamma})\dot{\gamma})^j + \frac{\partial \Gamma_{kl}^j}{\partial s} \dot{\gamma}^k \dot{\gamma}^l = 0.$$
 (62)

The first two terms here are just the standard terms appearing in the conventional Jacobi equation, with $\dot{\gamma}(t) \equiv \partial \gamma(0,t)/\partial t$ and $J(t) \equiv J(0,t)$. Note that R here is a $\binom{1}{3}$ tensor field formed by raising the last index of the Riemann curvature tensor, and thus has components $R_{jkl}^{\ \ m}$. A lengthy and tedious but essentially straightforward calculation can be used to verify that these first two terms correspond to the first four terms in Equation (61).

Equation (62) can be rewritten in a still more natural geometric form. A calculation shows that

$$\frac{\partial \Gamma_{kl}^{j}}{\partial s} = \frac{g^{jm}}{2} \left(g'_{mk;l} + g'_{ml;k} - g'_{kl;m} \right), \tag{63}$$

where $g'_{mk;l}$ is the standard notation for the covariant derivative of the tensor field g'. We see from this equation that $\partial \Gamma^j_{kl}/\partial s$ is a $\binom{1}{2}$ tensor field. This is a remarkable fact, given that Γ^j_{kl} is not a tensor field. (A simple alternate proof that $\partial \Gamma^j_{kl}/\partial s$ is a tensor field may be obtained by taking the partial derivative with respect to s of the standard (non-tensorial) transformation law for Γ^j_{kl}).

Putting it all together, we obtain the lifted Jacobi equation

$$(D_t^2 J)^j + (R(J, \dot{\gamma})\dot{\gamma})^j + C^j = 0, \tag{64}$$

where

$$C^{j} = \frac{g^{jm}}{2} \left(g'_{mk;l} + g'_{ml;k} - g'_{kl;m} \right) \dot{\gamma}^{k} \dot{\gamma}^{l}$$
 (65)

is a vector field that does not depend on the lifted Jacobi field J^j . Note that the terms $g'_{mk;l}\dot{\gamma}^k\dot{\gamma}^l$ and $g'_{ml;k}\dot{\gamma}^k\dot{\gamma}^l$ appearing in C^j are equal, which may be used to simplify the form of C^j .

We have shown that given a family of curves $\gamma(s,t)$ such that $\gamma(s,\cdot)$ is a geodesic of the metric g_s , the corresponding lifted Jacobi field J(t) must satisfy the lifted Jacobi equation, Equation (64). It is straightforward to turn this reasoning around, and argue that for any solution J(t) to the lifted Jacobi equation there must exist a

family $\gamma(s,t)$ of geodesics for g_s with J(t) as the corresponding lifted Jacobi field.

Solution to the lifted Jacobi equation: The lifted Jacobi equation is a linear, inhomogeneous second order differential equation, and thus it is possible to write a solution to the equation in terms of time-ordered integrals along the geodesic. In co-ordinates the lifted Jacobi equation, Equation (64), may be written as

$$\frac{d^2J}{dt^2} + A\frac{dJ}{dt} + BJ + C = 0, (66)$$

where A and B are time-dependent matrices, and C is a time-dependent vector. This may be rewritten as a first-order system by setting $J_1 = J$, $J_2 = \dot{J}$, and $K = \begin{bmatrix} J_1 \\ J_2 \end{bmatrix}$, so

$$\frac{dK}{dt} = \begin{bmatrix} 0 & I \\ -B & -A \end{bmatrix} K - \begin{bmatrix} 0 \\ C \end{bmatrix}. \tag{67}$$

Let E_t denote the propagator describing the solution to this equation in the homogeneous case, i.e., when C=0 we have $K(t)=E_tK(0)$. This corresponds to the solution of the conventional Jacobi equation. Note that E_t is a time-ordered exponential which may be studied using standard techniques. The solution in the inhomogeneous case is then

$$K(t) = E_t K(0) - E_t \int_0^t dr \, E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix}.$$
 (68)

This expression shows that the solutions to the lifted Jacobi equation may be obtained from the propagator E_t for the conventional Jacobi equation, and an integral involving an expression $C(\cdot)$ determined by g'. An interesting special case of the solution arises when we pick K(0) = 0, which corresponds to keeping the initial position and tangent vector to the geodesic unchanged, and looking to see how the geodesic deforms. We obtain in this case

$$K(t) = -E_t \int_0^t dr \, E_r^{-1} \left[\begin{array}{c} 0 \\ C(r) \end{array} \right]. \tag{69}$$

B. Lifted Jacobi equation for varying penalty

In the last section we derived the lifted Jacobi equation for a general parameterized family of metrics on a Riemannian manifold, M. In this section we derive and present a formal solution to the lifted Jacobi equation for a parameterized family of right-invariant metrics such as arise in the context of quantum computation. Specifically, we choose the parameterized family of metrics $\mathcal{G}_q = \mathcal{P} + q\mathcal{Q}$, so that $\mathcal{G}' = \mathcal{Q}$. We are able to obtain an explicit solution to the corresponding lifted Jacobi equation along geodesics for which the Hamiltonian H is constant

One way of approaching this task is to begin with the lifted Jacobi equation in the form derived in the last section, Equation (64). In fact, for right-invariant metrics

on $SU(2^n)$ there is a simpler alternate approach. We suppose H(t) is a Hamiltonian generating a geodesic U(t) for the metric \mathcal{G}_q , and that there is a nearby $\mathcal{G}_{q+\Delta}$ geodesic of the form

$$\tilde{U}(t) = U(t)e^{-i\Delta J(t)},\tag{70}$$

for some small Δ . We will write the lifted Jacobi equation as a second order differential equation for J(t). To derive this equation, rather than start from Equation (64), which requires converting J(t) into a suitable co-ordinate representation, and then computing all the relevant quantities, it is easiest to rework through the strategy in the last section, but working directly in terms of the quantity J(t) rather than some co-ordinate representation.

To do this, we use Schrödinger's equation to deduce that the Hamiltonian generating $\tilde{U}(t)$ is, to first order in Δ ,

$$\tilde{H}(t) = H(t) + \Delta U(t)\dot{J}(t)U^{\dagger}(t) + O(\Delta^2). \tag{71}$$

We require that $\tilde{H}(t)$ satisfies the geodesic equation for $\mathcal{G}_{q+\Delta}$. To see what this implies we set $\tilde{L} = \tilde{\mathcal{G}}(\tilde{H})$, where $\tilde{\mathcal{G}} = \mathcal{G} + \Delta \mathcal{G}' + O(\Delta^2)$. Substituting into the geodesic equation $\dot{\tilde{L}} = i[\tilde{L}, \tilde{H}]$, and examining the terms linear in Δ , we obtain

$$0 = \dot{K} + \mathcal{F}(i[K, L] + i[H, \mathcal{G}(K)] + (\mathcal{G}' \circ \mathcal{F})(i[L, H]) + i[H, \mathcal{G}'(H)])), \quad (72)$$

where $K = U\dot{J}U^{\dagger}$ is the first-order perturbation to the Hamiltonian. This equation is an inhomogeneous first order differential equation linear in K and thus can be integrated using standard techniques, and then integrated again to obtain J(t). The conventional Jacobi equation corresponds to the case where $\mathcal{G}'=0$, and thus the last two terms vanish. Note that we have used no special features of the standard metric in our derivation, and this form of the lifted Jacobi equation holds for any right-invariant metric.

The case of constant H: Along geodesics where H is constant it is possible to obtain a closed form expression for the solutions to the lifted Jacobi equation corresponding to the standard metric, i.e., with $\mathcal{G}' = \mathcal{Q}$.

To see this, we observe first that the solution to the Jacobi and lifted Jacobi equations coincide when H is a constant. This is because the inhomogeneous contribution $(\mathcal{F} \circ \mathcal{G}' \circ \mathcal{F})(i[L,H]) + \mathcal{F}(i[H,\mathcal{G}'(H)])$ to the lifted Jacobi equation vanishes, since [L,H]=0 and $[H,\mathcal{G}'(H)]=[H,\mathcal{Q}(H)]=0$ along a geodesic with constant H. An interesting consequence is that if we choose J(0)=0 and $\dot{J}(0)=0$, then J(t)=0 for all time, i.e., the geodesic does not deform as the metric is varied. In other words, the geodesics for which H is constant are the same for all q, as can also be seen from the condition derived in Section IV A.

We may thus vectorize the lifted Jacobi equation, obtaining $|\dot{K}\rangle = iA|K\rangle$, with

$$A = F\left[(I \otimes L - L^T \otimes I) + (H^T \otimes I - I \otimes H)G \right],$$
(73)

where G and F are the vectorized forms of \mathcal{G} and \mathcal{F} , respectively. The solution to this equation is $|K(t)| = e^{iAt}|K(0)|$. Vectorizing $\dot{J} = U^{\dagger}KU$ and substituting $U = e^{-iHt}$ gives

$$|\dot{J}(t)\rangle = e^{iBt}e^{iAt}|\dot{J}(0)\rangle.$$
 (74)

where $B = I \otimes H - H^T \otimes I$. Integrating we obtain

$$|J(t)| = |J(0)| + \int_0^t dr \, e^{iBr} e^{iAr} |\dot{J}(0)|. \tag{75}$$

This integral can be performed explicitly by using a second level of vectorization, this time acting on matrices in the space in which A and B live. We denote this vectorization operation using vec, to distinguish it from the map $X \to |X)$, and use unvec to denote the inverse operation. The integral can now be evaluated to yield the explicit solution to the lifted Jacobi equation,

$$|J(t)\rangle = |J(0)\rangle$$

$$+ \operatorname{unvec} \left[\frac{e^{i(A^T \otimes I + I \otimes B)t} - I}{i(A^T \otimes I + I \otimes B)} \operatorname{vec}(I) \right] |\dot{J}(0)\rangle.$$
(76)

This expression looks daunting, due to the multiple layers of vectorization, but is actually quite simple.

C. Conjugate points

In this section we use the theory of conjugate points to derive conditions under which geodesics are no longer minimizing. In particular, we numerically study geodesics of the form e^{-iHt} , where H is a fixed two-body Hamiltonian, and use conjugate points to derive conditions on t such that the geodesic from I to e^{-iHt} is only a local minimum of the length, not a global minimum. This work will also be useful in our later discussion of the geodesic derivative.

Recall the definition of conjugate points from elementary Riemannian geometry [8]. Two points x and y along a geodesic are said to be conjugate if there exists a nonzero Jacobi field defined along the geodesic which vanishes at both x and y. If we write the propagator for the Jacobi equation in block form as

$$E_t = \begin{bmatrix} E_1 & E_2 \\ E_3 & E_4 \end{bmatrix} \tag{77}$$

so that the solution is

then we see that the points at 0 and t are conjugate along the geodesic if and only if E_2 is singular.

Suppose now that we begin at a point x and move along a geodesic. Let $t_c > 0$ be the first time we pass through a point y conjugate to x, assuming such a point

exists. This point is of particular interest, because it can be shown (see [19], pp 268-270) that past the first conjugate point the geodesic is no longer minimizing. Thus, the propagator E_t associated with the Jacobi equation provides a computational machine which lets us determine when geodesics are no longer minimizing⁵.

To illustrate these ideas we analyze geodesics of the form e^{-iHt} , where H is a sum of one- and two-body terms. Intuitively, over short times we expect that the fastest way to simulate a physical system is with its own evolution. This intuition is confirmed by the fact ([19], pp 222-226) that over sufficiently short time periods geodesics are guaranteed to be globally minimal paths.

However, over longer time periods this is no longer the case. A simple illustration is the unitary e^{-iZt} . For $t \leq \pi/2$ this can be implemented by applying the Hamiltonian H=Z for a time t; for $\pi>t>\pi/2$ it is more efficient to apply H=-Z for a time $\pi-t$. More generally, for any Hamiltonian it is true that $e^{-iHt} \approx I$ for sufficiently large t, and so sufficiently long geodesics are never minimizing.

The method of conjugate points offers a powerful general way of studying when geodesics are no longer globally minimal. In particular, by integrating the Jacobi equation it is possible to determine to good accuracy when two points are conjugate using computational resources that scale polynomially with the dimension of the underlying manifold, which is $2^{O(n)}$ in this instance. By contrast, the volume of the space of paths scales as $2^{O(2^n)}$. It is therefore a priori quite remarkable that it is possible to prove a geodesic is not minimizing using $2^{O(n)}$ computational resources.

In general, finding conjugate points seems to require numerical solution of the Jacobi equation, perhaps using an explicit solution such as Equation (76), valid in some special case. In the bi-invariant case, i.e., when q=1, it is possible to write an analytic solution. In particular, Equation (76) simplifies because A=0, and it is easily verified that conjugate points occur at times

$$t_c = \frac{2m\pi}{\lambda_j - \lambda_k},\tag{79}$$

where m is a non-zero integer, and λ_j and λ_k are distinct eigenvalues of H.

Of course, the case of computational interest is when $q \gg 1$. As an example of this case we consider the transverse Ising Hamiltonian in one dimension,

$$H = \sum_{j} Z_{j} Z_{j+1} + h \sum_{j} X_{j}, \tag{80}$$

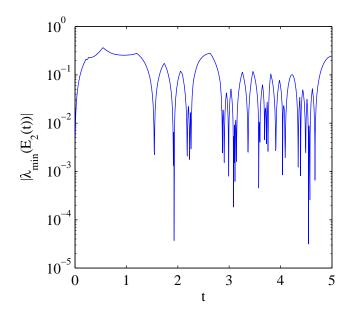


FIG. 1: Log plot of the absolute value of the minimum eigenvalue of E_2 ($\lambda_{\min}(E_2)$) versus time, for the transverse Ising model with external field h=1. The penalty parameter is in the regime of computational interest, $q=4^n=64$. Sharp dips indicate conjugate points.

where h is the strength of the applied field. We numerically investigated conjugate points for the case of n=3 qubits, with external field h=1, and penalty $q=4^n=64$ chosen to be in the regime of computational interest. Figure 1 is a log plot of the minimum eigenvalue of E_2 versus time. The occurrence of sharp dips in this plot strongly suggests the presence of a conjugate point. We see that in this example the first conjugate point occurs at $t_c \approx 1.54$, and thus the geodesic is no longer minimizing past this time. What is remarkable about this observation is that we have deduced the non-minimizing property without explicitly finding a shorter geodesic. We do it instead through the (relatively) computationally easy process of studying the conjugate points. It would be an interesting challenge to generalize this procedure to arbitrary n, perhaps using the known analytic solution to the transverse Ising model.

D. Geodesic derivative

Suppose $\gamma(t)$ is a geodesic passing through the point x at t=0 and y at t=T, and we vary the metric while holding the endpoints fixed. We show in this section that provided x and y aren't conjugate along the geodesic γ , the geodesic deforms in a unique way that can be described by an object we call the *geodesic derivative*.

To define the geodesic derivative, suppose $\gamma(s,t)$ is a family of geodesics, with $\gamma(s,\cdot)$ being a geodesic for the metric g_s , as in Subsection V A. We suppose $\gamma(s,t)$ has the constraints $\gamma(0,t) = \gamma(t)$, and $\gamma(s,0) = x, \gamma(s,T) = x$

Note, however, that while the conjugate point condition is sufficient to say a geodesic is no longer minimizing, it may not be necessary — there could already be a (globally) shorter path before a conjugate point is encountered.

y for all s. We define the geodesic derivative as $D\gamma \equiv \partial_s \partial_t \gamma \in T_x M$ at s=0 and t=0. Note that ∂_s is defined here, since $\partial_t \gamma$ lives in the same vector space, $T_x M$, for all values of s. The geodesic derivative thus represents the way in which the initial tangent $\partial_t \gamma$ is changing as the parameter s is changing near s=0.

Theorem 1 Let $x = \gamma(0)$ and $y = \gamma(T)$ be endpoints on a geodesic $\gamma(t)$. Then a corresponding geodesic derivative $D\gamma$ exists and is uniquely defined if and only if x and y are not conjugate along γ .

Intuitively, at a conjugate point geodesics in a fixed geometry "split" into many nearby geodesics (consider, e.g., antipodal points on a sphere). Thus, in one direction this theorem is not surprising: we expect conjugate points to give rise to many different ways to deform a geodesic as the metric is changed. The converse, however, is rather less obvious.

Proof: The existence and uniqueness of such a $D\gamma$ is equivalent to the existence of a family $\gamma(s,t)$ of geodesics satisfying the appropriate endpoint conditions, and such that the geodesic derivative is the *same* for any such family. Observe that if such a $D\gamma$ exists, then $D\gamma = \dot{J}(0)$, where J(t) is a lifted Jacobi field. Thus $D\gamma$ exists and is unique if and only if the lifted Jacobi equation has a unique solution satisfying J(0) = J(T) = 0. Comparing with the earlier solution to the lifted Jacobi equation, Equation (68), we see that this is equivalent to there existing a unique $D\gamma$ satisfying the constraint:

$$E_2 D\gamma = P E_t \int_0^t dr \, E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix}, \tag{81}$$

where P projects onto the top block in the block representation $K = \begin{bmatrix} J_1 \\ J_2 \end{bmatrix}$ used in the solution of the lifted Jacobi equation, Equation (68). Such a unique solution $D\gamma$ exists if and only if E_2 is invertible. We saw in the last section that this is equivalent to x and y not being conjugate along $\gamma(t)$. **QED**

Note that our proof shows more generally that any $D\gamma$ satisfying Equation (81) is a valid geodesic derivative, even when the geodesic derivative is not uniquely defined. Thus, the analysis of the geodesic derivative is closely tied to understanding the kernel of E_2 .

E. Numerically finding geodesics

In this section we explain how the geodesic derivative may be used to find geodesics reaching a particular desired target unitary, U. The procedure used is to begin by picking a Hamiltonian H(0) which generates U at some fixed time T along the q=1 geodesic. This may be done by picking H(0) so that $U=e^{-iH(0)T}$, i.e., by computing logarithms. We now vary the parameter q in the family of metrics $\mathcal{G}_q=\mathcal{P}+q\mathcal{Q}$, causing a corresponding change $dH_q(0)/dq=D\gamma$ in the initial Hamiltonian. Provided the geodesic derivative $D\gamma$ exists and is unique for

a suitable range of values of q, we can integrate to obtain an initial Hamiltonian $H_q(0)$ generating a geodesic connecting I and U, for any desired value of q.

To implement this procedure we need to develop a method to compute $D\gamma$. We could do this using Equation (81), but in the case of right-invariant metrics on $SU(2^n)$ a more computationally convenient form is possible, which we now derive. Recall that $D\gamma$ is defined to be a value of $\dot{J}(0)$ such that when J(0)=0, the solution to the lifted Jacobi equation satisfies J(T)=0, i.e., no variation occurs at the endpoint as q is varied. To analyze the values of $\dot{J}(0)$ for which this occurs, we examine the solution to the lifted Jacobi equation for right-invariant metrics more explicitly. Observe that since J(0)=0 we have

$$J(T) = \int_0^T dt \, \dot{J}(t) = \int_0^T dt \, U^{\dagger}(t) K(t) U(t), \quad (82)$$

where $K(t) \equiv U(t)\dot{J}(t)U(t)^{\dagger}$, as defined in Subsection VB. The lifted Jacobi equation, Equation (72), has solution

$$K(t) = \mathcal{K}_t(K(0)) - \mathcal{K}_t\left(\int_0^t dr \, \mathcal{K}_r^{-1}(C(r))\right) , \qquad (83)$$

where C is the inhomogeneous part of Equation (72), and \mathcal{K}_t is the propagator for the homogeneous form of Equation (72), i.e., for the standard (not lifted) Jacobi equation. The metric derivative along our family is $\mathcal{G}' = \mathcal{Q}$, and a calculation shows that

$$C = \mathcal{F}^2(i[\mathcal{P}(H), \mathcal{Q}(H)]). \tag{84}$$

Substituting Equation (83) into Equation (82), we obtain

$$J(T) = \mathcal{J}_T(\dot{J}(0))$$
$$-\int_0^T dt \, U(t)^{\dagger} \mathcal{K}_t \left(\int_0^t dr \, \mathcal{K}_r^{-1}(C(r)) \right) U(t), \tag{85}$$

where \mathcal{J}_T is the propagator that generates the standard (not lifted) Jacobi field $J_{\text{stand}}(T) = \mathcal{J}_T(\dot{J}_{\text{stand}}(0))$, assuming that $J_{\text{stand}}(0) = 0$. Requiring that J(T) = 0 and identifying $dH_q(0)/dq = D\gamma = \dot{J}(0)$, we obtain

$$\frac{dH_q(0)}{dq} = \mathcal{J}_T^{-1} \left[\int_0^T dt \, U(t)^{\dagger} \mathcal{K}_t \left(\int_0^t dr \, \mathcal{K}_r^{-1}(C(r)) \right) U(t) \right].$$
(86)

This equation can be simplified by observing that

$$-\mathcal{K}_t \left(\int_0^t dr \, \mathcal{K}_r^{-1}(C(r)) \right)$$

$$= \begin{cases} it[\mathcal{Q}(H), \mathcal{P}(H)], & q = 1, \\ (\mathcal{K}_t(L(0)) - L(t))/q(q - 1), & q > 1, \end{cases}$$
(87)

The top equation can be verified by noting that for q = 1 \mathcal{K}_t is the identity operation for all time and C is constant. For the bottom equation it is sufficient to check that both sides solve Equation (72) with q > 1 and initial condition K(0) = 0. Substituting into Equation (86) and using $U^{\dagger}(t)L(t)U(t) = L(0)$, we obtain

$$\frac{dH_q(0)}{dq} = \begin{cases}
\mathcal{J}_T^{-1}\left(\int_0^T dt \, U^{\dagger}(t) it[\mathcal{P}(H), \mathcal{Q}(H)]U(t)\right), & q = 1, \\
(\mathcal{J}_T^{-1}(L(0))T - L(0))/q(q - 1), & q > 1,
\end{cases}$$

This is our desired expression for the geodesic derivative. In practice, we find it more convenient numerically to work with the corresponding expression for $dL_q(0)/dq$, which is easily obtained from this expression using the chain rule.

Numerical examples: We now illustrate the geodesic deformation procedure for two examples. The first example is unitary operations chosen at random, and the second example is the quantum Fourier transform.

For the first example, we choose a three-qubit unitary operation, U, according to the Haar measure. Then we define a unique corresponding canonical Hamiltonian, H_{canon} , which satisfies $U = \exp(-iH_{\text{canon}}T)$ and has all eigenvalues in the range $(-\pi/T, \pi/T]$. We use this canonical Hamiltonian as our initial condition, since it has the desirable property that the geodesic U(t) = $\exp(-iH_{\rm canon}t)$ has no conjugate points before t=T, and thus is a likely candidate for the shortest geodesic through U = U(T) when q = 1. The results obtained when we apply the deformation procedure are illustrated in Figure 2. Empirically we find that for typical U, if we start with the canonical Hamiltonian and deform to large values of q we never encounter conjugate points, and so the deformation is uniquely defined. This agrees with the general intuition that conjugate points are rare. We also empirically observe (but have not proved) that the value of the dual Hamiltonian $L_q(0)$ converges for large q.

Other choices for the starting Hamiltonian are possible by adding multiples of $2\pi/T$ to the eigenvalues of the canonical Hamiltonian. Thus the set of possible starting Hamiltonians that reach a desired unitary for q=1 at time t=T has the structure of a (displaced) lattice. In contrast to the canonical Hamiltonian, however, our numerical results indicate that conjugate points at t=T do sometimes occur for some of these other starting Hamiltonians, and so the deformation procedure is not always well defined.

Somewhat remarkably, in view of this fact, is that our procedure still works numerically, even when conjugate points appear at t=T. In particular, if we take advantage of the fact that numerically the propagator \mathcal{J}_T is never exactly singular, then it is still possible to invert, and we can numerically integrate straight through the range of values of q where (presumably) a conjugate point occurs. Although we do not know how to justify this mathematically, we find empirically that our algo-

rithm still reaches the desired target unitary. It seems likely that what is going on is that our numerical procedure is picking out one possible way of doing the deformation. In principle, of course, it may be that no such deformation exists, but we have not encountered any circumstance where this appears to be the case. An interesting observation is that in contrast to the canonical case, we find that the initial dual Hamiltonian, $L_q(0)$, tends not to converge for large q, but continues to grow in norm.

In our second example, we generate a geodesic reaching the unitary that implements the quantum Fourier transform on three qubits. Again we start with the canonical Hamiltonian for this unitary. The deformation is illustrated in Figure 3, and only shows the deformation up to q = 16 in order to highlight the interesting behavior around q=6. For values of q in the range 1 through ≈ 6 there is a set of Pauli components of $L_q(0)$ that remain zero. At $q \approx 6$ all of these Pauli components suddenly become non-zero. This phenomena coincides with the propagator \mathcal{J}_T becoming very nearly singular (the magnitude of its smallest eigenvalue is approximately 10^{-6}), and it remains nearly singular up to the final value of q=16as illustrated in panel (b). As in the earlier discussion, however, we find empirically that applying our deformation procedure still appears to generate a valid (though non-unique) geodesic derivative, and this is supported by the fact that we do indeed obtain valid geodesics to the final target unitary, the quantum Fourier transform (see inset of panel (b).

Finding the minimal geodesic: We have used the geodesic deformation procedure to obtain upper bounds on the distance d(I,U) for values of q of computational interest. Of course, there are many geodesics for any given U, not just the geodesics beginning with the canonical Hamiltonian H_{canon} , which is the case we have focused on. Can the geodesic deformation procedure be used to obtain values for the distance d(I,U)?

An idea for how to do this is as follows. Imagine we are trying to determine whether a geodesic of length $< n^k$ (say) exists for U. It is clear that the length of geodesics monotonically increases with q under deformation. At q=1 this allows us to restrict our attention to a finite $(2^{O(n^{k+1})})$ set of possible initial values for the Hamiltonian, and study how the corresponding geodesics deform. A better understanding of the way conjugate points behave under deformation may enable us to substantially narrow this range of choices.

A number of caveats to this approach need to be noted. The first is that for particular choices of unitary, for example the quantum Fourier transform above, the deformation procedure produces conjugate points at the endpoints, and so the deformation procedure is not well defined. A possible way around this difficulty is to consider deforming the metric with two or more parameters, instead of just one. It seems plausible that it may always be possible to deform the metric in such a way that new conjugate points never appear along the geodesics, the

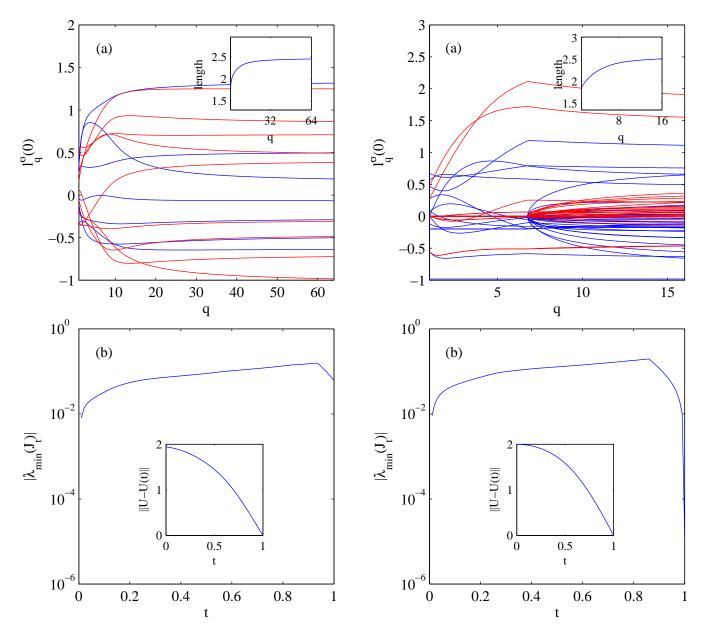


FIG. 2: Geodesic deformation to a randomly-chosen unitary on n=3 qubits. Panel (a) shows how the Pauli components of the initial dual Hamiltonian, $l_q^{\sigma}(0) = \operatorname{tr}(\sigma L_q^{\sigma}(0))/2^n$, vary with the penalty parameter up to $q=4^n=64$. Of the $4^n=64$ Pauli components, only 16 representatives are shown, for clarity, but all converge in the large q limit. Blue lines are components where $\sigma \in \mathcal{P}$, red lines are where $\sigma \in \mathcal{Q}$. The inset shows how the length of the geodesic segment from I to U varies with q. Panel (b) shows the minimum eigenvalue of the vectorized form of the propagator \mathcal{J}_t as a function of time along the geodesic found for q=64. No conjugate points are evident. The inset shows the operator norm of the difference between the target unitary U, and U(t) along the q=64 geodesic, showing that the target is indeed reached at the final time T=1

FIG. 3: Geodesic deformation to the quantum Fourier transform on n=3 qubits. Panel (a) shows how the Pauli components of the initial dual Hamiltonian, $l_q^{\sigma}(0) = \operatorname{tr}(\sigma L_q^{\sigma}(0))/2^n$, vary with the penalty parameter up to q=16. The inset shows how the length of the geodesic segment from I to U varies with q. Blue lines are components where $\sigma \in \mathcal{P}$, red lines are where $\sigma \in \mathcal{Q}$. Panel (b) shows the minimum eigenvalue of the propagator \mathcal{J}_t as a function of time along the final geodesic found for q=16. The sharp dip at the final time T=1 indicates a conjugate point. The inset shows the operator norm of the difference between the target unitary U, and U(t) along the q=16 geodesic, showing that the target is indeed reached at the final time T=1

intuition being that conjugate points are rather rare.

Secondly, it is possible that as we move to large q new geodesics to the target unitary appear that cannot be generated as deformations of a q=1 geodesic. If this is the case then it may be difficult to deduce anything about the minimal geodesic by deforming.

Despite these caveats, we emphasize that any geodesic between the identity and the unitary gives an upper bound on the distance of that unitary from the origin and so is potentially interesting. For example, using the methods of [5], any geodesic in the large q limit can be well-approximated by a sequence of one- and two-qubit quantum gates, and it is plausible that gate sequences generated in this way may suggest algorithms for computing a family of unitaries of which the target unitary is a representative (cases of high symmetry would be natural candidates). Further study of the mathematical properties of the geodesic deformation procedure, including the conjectures mentioned above, is needed to provide more definitive answers as to its usefulness as a general technique for finding minimal curves. It is also desirable to compare to other techniques (e.g. [20]) which can be used to find geodesics in spaces of high dimension.

VI. WHAT CAN GEOMETRY TEACH US ABOUT QUANTUM COMPUTATION?

Motivated by its close connection to quantum gate complexity, in this paper we have developed a basic understanding of the geometry of the Riemannian metric defined by Equation (2). However, substantial further progress will be required to obtain either new quantum algorithms or to prove limits on computational complexity.

In this section we discuss some of the obstacles that need to be overcome for this to occur. We begin in Subsection VIA with a discussion of the Razborov-Rudich theorem, a result from classical computational complexity that illuminates the difficult of proving lower bounds in classical circuit complexity. We describe an analogous quantum result, and an interesting corollary, namely, that if good classical pseudorandom number generators exist, then the problem of determining distances on $SU(2^n)$ according to the standard metric is not (classically) soluble in time polynomial in 2^n . The Razborov-Rudich theorem thus poses a considerable barrier to any general program for understanding quantum gate complexity, including our geometric program.

In Subsection VIB we discuss a second obstacle to the use of geometry, namely that the bounds of Equation (3) apply only for circuits which do not make use of ancillary working qubits. While such circuits are of substantial interest, in general when computing a desired function f or unitary U, it may help to introduce extra ancillary working qubits. In this Subsection we explain how ancillas can be incorporated into the geometric point of view by using a canonical extension procedure for unitary operations.

A. The Razborov-Rudich theorem and the computational complexity of finding geodesics

The Razborov-Rudich theorem [21] is a result from classical computational complexity theory that poses a significant barrier to any general program for understanding gate complexity, either classical or quantum. In this section we briefly survey some implications the Razborov-Rudich theorem has for the geometric program. The discussion is in the nature of an informal outline, since our intent here is merely to outline the main ideas, rather than to give the rather extensive formal definitions which a full discussion would require. In general, the full formal details are easy to fill in by experts familiar with the Razborov-Rudich theorem.

In its simplest variant⁶, the Razborov-Rudich theorem shows that, loosely, if good pseudorandom generators exist, then it is impossible to efficiently distinguish hardand easy-to-compute Boolean functions.

This statement can be unpacked in three stages. First, a "good" pseudorandom generator is here taken in the Blum-Micali-Yao sense (see, e.g., Chapter 9 of [22]). Such generators can be show to exist if one-way functions exist. So, for example, if the factoring or discrete logarithm problems are difficult to solve on a classical computer, then such generators exist, and the conclusion of Razborov-Rudich holds. Second, by hard-to-compute we mean a Boolean function whose minimal (non-uniform) circuit complexity exceeds some threshold, e.g., $n^{\ln n}$. Easy-to-compute means the minimal circuit complexity is below that threshold. Note that the threshold can be varied somewhat, with the result still holding. Third, by an efficient procedure to distinguish hard- and easy-tocompute Boolean functions, we mean an efficient classical Turing machine which takes as input the truth table for the Boolean function, and determines whether it is hardor easy-to-compute. The criterion for efficiency is very relaxed: it is that the Turing machine operate in time polynomial in the size of the truth table, i.e., in time $2^{O(n)}$.

The idea behind the proof of the Razborov-Rudich theorem is easily stated. First, observe following Shannon [23] (c.f. problem 4.4.14 in [24]) that a randomly chosen Boolean function is with high probability hard to compute. Second, using a good pseudorandom number generator it is possible to construct pseudorandom function generators producing Boolean functions which appear pseudorandom, but which actually have small circuits. Any method for efficiently distinguishing easy-from hard-to-compute functions would therefore provide an efficient means of distinguishing random functions from pseudorandom functions, and this contradicts the definition of a pseudorandom generator. As a result, such

⁶ See [21] for full details. Our discussion in this paper is for a very simple type of natural proof system, in the language of [21].

a procedure cannot exist.

It is straightforward to generalize this reasoning to the quantum case. In particular, it can be shown that if good (classical) pseudorandom generators exist, then there is no efficient classical algorithm which can be used to distinguish unitary operations that can be synthesized using small quantum circuits, and those which require large quantum circuits.

A similar line of reasoning can be applied to the distance function d(I,U). In particular, suppose it were possible to efficiently distinguish unitaries U for which d(I,U) is large (i.e., exceeds a threshold like $n^{\ln n}$) from unitaries for which d(I,U) is small. Such a procedure could be used to distinguish a unitary chosen using a pseudorandom generator from one chosen truly at random, and this could be used to break the pseudorandom generator⁷. It follows that there must be no efficient procedure to evaluate the distance function d(I,U).

Theorem 2 Suppose classical pseudorandom generators exist. Let d(I,U) be the metric on $SU(2^n)$ induced by the standard metric of Equation (2), with $q > 4^n$. Then there is no classical algorithm running in time polynomial in 2^n and which produces an accurate approximation to d(I,U).

This result is particularly remarkable when one considers that when q = 1 it is possible to evaluate d(I, U) in polynomial time.

These results are, obviously, rather discouraging. It is worth emphasizing that analogous results apply to any general approach to quantum circuit complexity, and are not special to the geometric approach. In particular, any approach to the proof of lower bounds must necessarily contend with the Razborov-Rudich theorem.

Given these results, what is the best approach to finding unitary operations which can be analyzed using geometric techniques? We do not know the answer to this question. One possibility is to try to use symmetries to avoid the obstruction posed by Razborov-Rudich. Symmetries are often used to simplify the analysis of the geodesic equation, and may, in some cases, make it possible to analyze d(I,U) for those U satisfying the symmetries, without providing a general efficient procedure for determining d(I,U). This is currently under investigation.

B. Extending the geometric picture to take account of ancilla

A drawback of the results of [4, 5, 6] is that they apply only to the synthesis of unitary operations without the assistance of ancillary working qubits. We now develop a technique enabling the geometric approach to be applied to many (not all) unitary operations, even in the case of ancilla. In particular, this technique may be applied to unitary operations which compute a permutation function, $|x\rangle \to |f(x)\rangle$, or which are diagonal in the computational basis $|x\rangle \to e^{i\theta_x}|x\rangle$. The technique works by showing that quantum circuits using ancilla may be put into a standard canonical form which can then be analyzed geometrically.

To make the issue at stake more explicit, suppose we wish to synthesize a unitary operation, U, on some number, n, of qubits. To do this synthesis it may help to introduce m additional ancillary qubits, which start in a standard state. Without loss of generality we assume this state is the all $|0\rangle$ state, which we denote $|0\rangle$. We then attempt to synthesize a unitary operation V such that for all n-qubit states, $|\psi\rangle$,

$$V|\psi\rangle|0\rangle = (U|\psi\rangle)|A\rangle,$$
 (89)

where $|A\rangle$ is some ancilla state. Note that by linearity $|A\rangle$ cannot depend on $|\psi\rangle$. We call a V satisfying this relation an *extension* of U. Empirically it is found that sometimes the gate complexity of synthesizing such an extension may be strictly less than the gate complexity of synthesizing U without ancilla.

This situation presents a difficulty for the geometric approach, since it suggests that we need to evaluate the distance $d(I, \mathcal{U})$, where \mathcal{U} is the entire set of extensions of U. The set \mathcal{U} is rather complex, and it seems likely to be far more difficult to evaluate $d(I, \mathcal{U})$ than $d(I, \mathcal{U})$.

In this section we show how $d(I, \mathcal{U})$ can be accurately estimated using distances $d(I, \mathcal{U}')$, for a suitably chosen unitary U' = U'(U). This enables us to use distances to obtain bounds on the gate complexity of unitary operations, with ancilla allowed. The constructions we describe do not apply for all unitary operations, but they do apply for many unitaries of interest, including the unitaries that arise in the computation of classical functions.

To state our results more formally, let $G_{\infty}(U)$ be the minimal number of one- and two-qubit gates required to synthesize an extension of U, with an unbounded number of qubits allowed. We define a *special extension* of U to be an extension V such that the final state of the ancilla is the same as the initial state, $|A\rangle = |0\rangle$, i.e.,

$$V|\psi\rangle|0\rangle = (U|\psi\rangle)|0\rangle. \tag{90}$$

We say a special extension is an m-fold special extension if the number of ancilla qubits is m. We define $\tilde{G}_m(U)$ to be minimal exact gate complexity of an m-fold special extension of U, and $\tilde{G}_{\infty}(U)$ to be the minimal exact gate complexity of a special extension of U with an unbounded number of ancilla qubits.

We will show how to obtain bounds on $G_{\infty}(U)$ by showing that for suitable choice of m there is a single m+1-fold special extension U_m of U such that $G(U_m)$ can be used to bound $\tilde{G}_{\infty}(U)$. Furthermore, we will also

⁷ To make this description a little more precise, suppose we define U by $U|x\rangle \equiv (-1)^{f(x)}|x\rangle$, where f is a Boolean function that is either generated pseudorandomly, or truly at random.

show that for many interesting unitaries, including all those associated with the evaluation of classical functions, $G_{\infty}(U)$ and $\tilde{G}_{\infty}(U)$ behave in essentially the same way.

This allows us to reduce the study of the gate complexity of U with ancilla to the study of the complexity of a fixed unitary, U_m , without ancilla. This study can then be done through geometric methods, or using any other preferred method of analysis.

The bounds relating $\tilde{G}_{\infty}(U)$ to $G(U_m)$ and $d(I, U_m)$ go in one direction. Bounds in the other direction, analogous to the first inequality in (3), may be obtained by replacing $G_{\infty}(U)$ by an approximate analogue, $G_{\infty}(U, \epsilon)$.

In particular, we define $G_{\infty}(U,\epsilon)$ to be the minimal number of one- and two-qubit gates needed to synthesize a unitary operation V such that $\|\mathcal{V}-\mathcal{U}\| \leq \epsilon$, where \mathcal{U} and \mathcal{V} are the natural quantum operations on the n-qubit input space induced by U and V, and $\|\mathcal{E}\| \equiv \max_{\rho} \operatorname{tr}|\mathcal{E}(\rho)|$, with the maximization over density matrices ρ ; note that $\|\mathcal{V}-\mathcal{U}\| \leq \|U-V\|$.

Theorem 3 There exist positive constants c_1 and c_2 such that for any U and m we can construct an m+1-fold special extension U_m such that:

$$\min(m, c_1 G(U_m) - c_2 m) \leq \tilde{G}_{\infty}(U) \tag{91}$$

$$G_{\infty}(U,\epsilon) \leq G(U_m,\epsilon).$$
 (92)

Proof: Let V be any m-fold special extension of U. Consider the circuit:

$$|x\rangle \qquad /V \qquad V^{\dagger} \qquad (93)$$

$$|y\rangle \qquad /Z \qquad X$$

Note that the first wire represents the n qubits on which we desire to implement U, the second wire represents m ancilla qubits, and the third wire is a single qubit. Note that operations controlled on the second wire are only applied if all the qubits in the second wire are set to $|0\rangle$.

We claim that: (1) this circuit defines an m + 1-fold special extension of U; and (2) the action of this extension is *independent* of the choice of special extension, V, and is given by the operation U_m defined by the circuit:

$$U_m = \begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$
 (94)

We call U_m the *m'th canonical unitary extension* of U. Note that the fact that U_m is an m+1-fold unitary extension of U follows trivially from the form of this circuit, and so the true challenge here is to prove that the action of U_m is the same as the action of the circuit in Equation (93). To verify this it helps to consider separately the cases where $y = 0, y \neq 0$ and z = 0, z = 1. The three cases (i) y = 0, z = 0, (ii) y = 0, z = 1 and

(iii) $y \neq 0, z = 1$ all follow from straightforward circuit analysis.

The final case, $y \neq 0$, z = 0, requires more care. After the first gate is applied, the state is $(V|x\rangle|y\rangle)|0\rangle$. The critical claim, proved in the next paragraph, is that the state $V|x\rangle|y\rangle$ has zero overlap with any state of the form $|x'\rangle|0\rangle$. As a result, the second gate has no effect on the state of the system, and the third gate merely inverts the effect of the first. The final gate has no effect (since $y \neq 0$), and thus the net effect of the circuit is to transform $|x\rangle|y\rangle|0\rangle$ to $|x\rangle|y\rangle|0\rangle$, which matches the action of U_m . This completes the proof.

To see that $V|x\rangle|y\rangle$ has zero overlap with any state of the form $|x'\rangle|0\rangle$, observe that $|x'\rangle|0\rangle = V(U^{\dagger}|x'\rangle)|0\rangle$, and thus:

$$\langle x'|\langle 0|V|x\rangle|y\rangle = \langle x'|U\langle 0|V^{\dagger}V|x\rangle|y\rangle$$
 (95)

$$= \langle x'|U|x\rangle\langle 0|y\rangle, \tag{96}$$

which vanishes since $y \neq 0$.

The remainder of the proof of Theorem 3 is relatively straightforward. The proof that $G_{\infty}(U,\epsilon) \leq G(U_m,\epsilon)$ follows from the fact that any unitary which approximates U_m to accuracy ϵ necessarily approximates U to accuracy ϵ , using standard arguments about operator norms.

To prove the other inequality, note that without loss of generality we can assume that $m > \tilde{G}_{\infty}(U)$ (otherwise the inequality is trivially true). In this instance observe that $\tilde{G}_{\infty}(U) = \tilde{G}_m(U)$, since it cannot help to have more ancilla qubits than gates in a circuit. Let V be the optimal m-fold special extension of U, so $\tilde{G}_m(U) = G(V)$. Observe that U_m can be synthesized using the circuit in Equation (93). It follows that $G(U_m) \leq c_1 G(V) + c_2 m = c_1 \tilde{G}_m(U) + c_2 m$, where the term liner in G(V) is due the the controlled-V and V^{\dagger} , and the term linear in M is due to the multiply controlled operations. Rearranging this inequality gives the desired result. **QED**

The following corollary follows from the theorem and the results of Section II:

Corollary 1 There exist positive constants c_1 and c_2 such that for any U and m we can construct an m+1-fold special extension, U_m (the canonical extension), such that:

$$\min(m, c_1 d(I, U_m) - c_2 m) \le \tilde{G}_{\infty}(U) \tag{97}$$

$$\operatorname{poly}(G_{\infty}(U, \epsilon)) \leq d(I, U_m). \tag{98}$$

In order to apply the theorem and corollary, we need to find scenarios where $\tilde{G}_{\infty}(U)$ and $G_{\infty}(U)$ behave in essentially the same way. We now show that this is the case for Boolean functions, $f: B_n \to B$, where $B = \{0, 1\}$ is the set of states of a single bit, and B_n is the set of states of a string of n bits. An extension to more complex classical functions may be performed along similar lines.

We define $G_{\infty}(f)$ to be the minimal number of quantum gates required to exactly compute f(x). That is, it is

the minimal number of one- and two-qubit gates required to compute a unitary V such that:

$$V|x\rangle|0\rangle = |f(x)\rangle|A_x\rangle,\tag{99}$$

where $|A_x\rangle$ is some "junk" final state that will be ignored. We define $G^c_{\infty}(f)$ to be the minimal classical circuit complexity required to exactly compute f.

Suppose we define a unitary U_f by $U_f|x\rangle|z\rangle \equiv |x\rangle|z \oplus f(x)\rangle$, where addition is done modulo two, and a unitary V_f by $V_f|x\rangle \equiv (-1)^{f(x)}|x\rangle$. Then the following theorem shows that the quantum circuit complexity of f is essentially equal to $\tilde{G}(U_f)$ and $\tilde{G}(V_f)$. Thus, Theorem 3 and Corollary 1 may be applied to obtain insight into the quantum circuit complexity of Boolean functions.

Theorem 4

$$G_{\infty}^{c}(f) \ge G_{\infty}(f) = \Theta(\tilde{G}_{\infty}(U_f)) = \Theta(\tilde{G}_{\infty}(V_f))$$
 (100)

Proof: The first inequality is obvious. The first equality follows by standard techniques of reversible computation [25, 26]. In brief, note that by definition $G_{\infty}(f) \leq G_{\infty}(U_f) \leq \tilde{G}_{\infty}(U_f)$. Conversely, let V be the unitary of minimal gate complexity satisfying Equation (99). Then by applying V to the first and third register of $|x\rangle|z\rangle|0\rangle$ we obtain $|f(x)\rangle|z\rangle|A_x\rangle$. Adding the value of the first register to the second and then applying V^{\dagger} we obtain $|x\rangle|z\oplus f(x)\rangle|0\rangle$. It follows that $\tilde{G}_{\infty}(U_f)\leq 2G_{\infty}(f)+1$, and thus $G_{\infty}(f)=\Theta(\tilde{G}_{\infty}(f))$.

The second equality follows by standard techniques of phase estimation [27, 28]; see e.g., Section 5.2 of [3]. **QED**

To conclude this section, we give some examples of Theorem 3 and its consequences in action. We will focus on the behaviour of $\tilde{G}_{\infty}(U)$, assuming that we are working in a situation like that provided by Theorem 4, e.g., with a class of unitaries for which $\tilde{G}_{\infty}(U)$ and $G_{\infty}(U)$ behave similarly.

A simple example of the theorem is to suppose that U is an n-qubit unitary for which we can prove

$$d(I, U_{n^2}) \ge \left(\frac{c_2}{c_1} + \delta\right) n^2 \tag{101}$$

for some $\delta > 0$. It need not be that $d(I, U_{n^2})$ actually scales quadratically — it would be just as good if $d(I, U_{n^2}) = 2^n$, for example. Substituting $m = n^2$ into the theorem, it follows that:

$$\tilde{G}_{\infty}(U) \ge \min(1, \delta)n^2 = \Omega(n^2).$$
 (102)

Thus, if $G_{\infty}(U) \sim \tilde{G}_{\infty}(U)$, then we can prove that the number of gates required to synthesize U scales at least as $\Omega(n^2)$.

This conclusion perhaps appears somewhat surprising. After all, U_{n^2} involves n^2 qubits, and so surely we would expect $d(I, U_{n^2})$ to scale as in Equation (101), no matter what U is. The resolution is that it is only the excess

beyond $(c_2/c_1)n^2$ that contributes to the bound on the gate complexity. Fortunately, there are many situations where such an excess is likely to occur. To see this, recall from Equation (3) that

$$\frac{b_0 G(U, \epsilon)^{b_1} \epsilon^{b_2}}{n^{b_3}} \le d(I, U). \tag{103}$$

In the papers [4, 6] the constants found were $b_1 = 1/3, b_2 = 2/3$ and $b_3 = 2$; a value for b_0 was not calculated explicitly. It is now straightforward to prove that:

Proposition 1

$$\frac{b_0 G_{\infty}(U, \epsilon)^{b_1} \epsilon^{b_2}}{(n+m)^{b_3}} \le d(I, U_m). \tag{104}$$

Proof: Simply observe that $G_{\infty}(U, \epsilon) \leq G(U_m, \epsilon)$, and then apply (103). **QED**

This proposition shows that rapid scaling in $G_{\infty}(U,\epsilon)$ implies rapid scaling in $d(I,U_m)$. As a result, if U is difficult to approximate, then the geometric properties imply that U is difficult to compute exactly, even when ancilla are allowed. Needless to say, if U is difficult to approximate, then it is difficult to compute exactly. The significance of the Proposition is that it provides circumstances under which we can guarantee something about the behaviour of the geometry.

As an example, suppose we define $a \equiv (1+b_3)/b_1$, and that $G_{\infty}(U,1/10) = \Omega(n^{a+\delta})$ for some $\delta > 0$. Suppose we choose $\gamma > 0$ such that $\gamma < \delta/a$. Then applying the proposition we see with a little algebra that $d(I,U_{n^{1+\gamma}}) = \Omega(n^{1+\beta})$ for some $\beta > \gamma$. In such a situation, it follows from Theorem 3 that the geometric properties imply superlinear lower bounds on the exact gate complexity $\tilde{G}_{\infty}(U)$.

In a similar vein, if we have $G_{\infty}(U, 1/10) = \Omega(2^{c_1 n})$, and choose a positive value for c_2 such that $c_2 < c_1/a$ then we see from the proposition that $d(I, U_{2^{c_2 n}}) = \Omega(2^{c_3 n})$ for some $c_3 > c_2$, and thus by Theorem 3 the geometric properties imply exponential lower bounds on the exact gate complexity $\tilde{G}_{\infty}(U)$.

So, for example, if, as suspected by many people, it turns out that **NP**-hard problems require exponential size quantum circuits to approximate, then it will immediately follow that there are constants $0 < c_2 < c_3$ such that $d(I, U_{2^{c_2 n}}) = \Omega(2^{nc_3})$, and thus, by Theorem 3 the geometric properties imply exponential lower bounds on the exact gate complexity.

VII. CONCLUSION

We have explored the basic geometry of quantum computation, including the Levi-Civita connection, the geodesic equation and many solutions and invariants of the equation, as well as all the basic curvature quantities. We have also developed a geodesic deformation procedure which in many cases of interest allows us to find geodesics connecting the identity I to some desired unitary U. This gives a more or less complete picture of the basic geometry of quantum computation, and should provide a foundation for a more detailed understanding.

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APPENDIX A: CURVATURE

In this appendix we derive explicit expressions for the various quantities describing curvature. This includes the curvature tensor (Subsection A 1), the sectional curvature (Subsection A 2), the Ricci tensor (Subsection A 3), and the scalar curvature (Subsection A 4). Note that many of these quantities are presented for a general right-invariant metric in [29]. However, it is helpful to have explicit forms of these curvature quantities for the standard metric, Equation (2), and so we present detailed calculations.

1. Curvature tensor

In this section we compute the Riemann curvature tensor, R, which is a $\binom{0}{4}$ tensor field defined by $R(W,X,Y,Z) \equiv \langle \nabla_W \nabla_X Y - \nabla_X \nabla_W Y - \nabla_{i[W,X]} Y, Z \rangle$. We work with respect to a basis of right-invariant frame fields ρ, σ, τ, μ , corresponding to generalized Pauli matrices, and compute the corresponding components of the

curvature tensor,

$$R_{\rho\sigma\tau\mu} \equiv \langle \nabla_{\rho}\nabla_{\sigma}\tau - \nabla_{\sigma}\nabla_{\rho}\tau - \nabla_{i[\rho,\sigma]}\tau, \mu \rangle$$
(A1)
$$= \langle \nabla_{\rho}\tau, \nabla_{\sigma}\mu \rangle - \langle \nabla_{\sigma}\tau, \nabla_{\rho}\mu \rangle - \langle \nabla_{i[\rho,\sigma]}\tau, \mu \rangle,$$
(A2)

where in the second line we used the fact that $\langle X, \nabla_Y Z \rangle = -\langle \nabla_Y X, Z \rangle$ for any triple of right-invariant vector fields, X, Y and Z. Using the formula of Equation (25), we see that

$$\nabla_{\sigma}\tau = ic_{\sigma,\tau}[\sigma,\tau],\tag{A3}$$

where

$$c_{\sigma,\tau} \equiv \frac{1}{2} \left(1 + \frac{q_{\tau} - q_{\sigma}}{q_{[\sigma,\tau]}} \right). \tag{A4}$$

Note that we use q_{σ} to refer to the value of the penalty for the generalized Pauli matrix σ , i.e., $q_{\sigma} = 1$ if σ has weight zero, one or two, and otherwise $q_{\sigma} = q$. The notation $q_{[\sigma,\tau]}$ is the value of the penalty for the generalized Pauli matrix proportional to $[\sigma,\tau]$; in the trivial case when σ and τ commute, we arbitrarily assign $q_{[\sigma,\tau]} = 1$. We use a similar convention for expressions like $c_{[\rho,\sigma],\tau}$.

Substituting Equation (A3) into Equation (A2), we obtain

$$R_{\rho\sigma\tau\mu} = c_{\rho,\tau}c_{\sigma,\mu}\langle i[\rho,\tau], i[\sigma,\mu]\rangle -c_{\sigma,\tau}c_{\rho,\mu}\langle i[\sigma,\tau], i[\rho,\mu]\rangle -c_{[\rho,\sigma],\tau}\langle i[i[\rho,\sigma],\tau],\mu\rangle.$$
(A5)

We use this as our basic expression for the curvature tensor, and derive other curvature quantities starting from this point. In doing so we will often find it helpful to use the observation that $\langle \sigma, \tau \rangle = q_{\sigma} \delta_{\sigma\tau}$. Note that this expression has several symmetries in addition to those satisfied in general by the curvature tensor. In particular, it is easy to verify that to have $R_{\rho\sigma\tau\mu} \neq 0$ we must have $\rho\sigma\tau\mu$ proportional to the identity, and it must be possible to partition the indices into two pairs, e.g., (ρ, σ) and (τ, μ) , such that: (1) the pairs commute, i.e., $[\rho, \sigma] = [\tau, \mu] = 0$; and (2) all other pairs anticommute, i.e., $[\rho, \tau]_+ = [\rho, \mu]_+ = \ldots = 0$. Even when these conditions hold, individual terms in the expression (A5) may still vanish, e.g., the first term vanishes if ρ and τ commute, or if σ and μ commute.

2. Sectional curvature

The sectional curvature in the tangent plane spanned by orthonormal right-invariant vector fields X and Y is defined by

$$K(X,Y) \equiv R(X,Y,Y,X). \tag{A6}$$

Define a bilinear operation $\mathcal{B}(X,Y) \equiv \mathcal{F}(i[\mathcal{G}(X),Y])$. Observe that we have the identities $\langle X,i[Y,Z]\rangle =$ $\langle \mathcal{B}(X,Y),Z\rangle$ and $\nabla_X Y=\frac{1}{2}(i[X,Y]-\mathcal{B}(X,Y)-\mathcal{B}(Y,X))$. Using these facts and the cyclic property of trace a calculation shows that

$$K(X,Y) = -\frac{3}{4} \langle i[X,Y], i[X,Y] \rangle$$

$$+\frac{1}{4} \langle \mathcal{B}(X,Y) + \mathcal{B}(Y,X), \mathcal{B}(X,Y) + \mathcal{B}(Y,X) \rangle$$

$$+\frac{1}{2} \langle i[X,Y], \mathcal{B}(X,Y) - \mathcal{B}(Y,X) \rangle. \tag{A7}$$

For values of q of computational interest (indeed, for any q > 4/3) it is easily verified from this formula that the sectional curvature can be both positive and negative.

3. Ricci tensor

The Ricci tensor, $Rc_{\sigma\tau}$, is defined as the contraction of the raised form of the curvature tensor, $R_{\rho\sigma\tau}{}^{\mu}$, on the first and last indices,

$$Rc_{\sigma\tau} = R_{\rho\sigma\tau}^{\quad \rho}$$
 (A8)
= $g^{\rho\mu}R_{\rho\sigma\tau\mu}$. (A9)

Observing from Equation (16) that $g^{\rho\mu}$ is nonzero only when $\rho = \mu$, and that $R_{\rho\sigma\tau\mu}$ vanishes unless $\rho\sigma\tau\mu \propto I$, we see that $Rc_{\sigma\tau}$ must be diagonal, i.e., the components vanish unless $\sigma = \tau$.

To compute the diagonal entries in the Ricci tensor, we observe from Equation (16) that the diagonal entries of the metric $g^{\rho\tau}$ are equal to $1/q_{\rho}$. We thus obtain (no implied sum on repeated indices)

$$Rc_{\sigma\sigma} = \sum_{\rho} \frac{R_{\rho\sigma\sigma\rho}}{q_{\rho}}.$$
 (A10)

Using the expression of Equation (A5), the definition Equation (A4), and the observations $\langle i[\rho,\sigma],i[\rho,\sigma]\rangle=4q_{[\rho,\sigma]}$ and $\langle i[i[\rho,\sigma],\sigma],\rho\rangle=-4q_{\rho}$, we obtain after some algebra

$$Rc_{\sigma\sigma} = \sum_{\rho}' \left(2 + \frac{q_{\rho}^2 + q_{\sigma}^2 - 2q_{\rho}q_{\sigma} - 3q_{[\rho,\sigma]}^2 + 2q_{[\rho,\sigma]}q_{\sigma}}{q_{\rho}q_{[\rho,\sigma]}} \right), \tag{A11}$$

where the prime indicates that the sum is only over ρ which anticommute with σ . This sum may be further simplified by observing that up to proportionality factors ρ and $[\rho, \sigma]$ range over the same set of matrices, i.e., generalized Pauli matrices which anticommute with σ . Using this fact a change of variables may be used to show that the sum of the $-2q_{\rho}q_{\sigma}/q_{\rho}q_{[\rho,\sigma]}$ and $2q_{[\rho,\sigma]}q_{\sigma}/q_{\rho}q_{[\rho,\sigma]}$ terms cancel. For similar reasons, the $q_{\rho}^2/q_{\rho}q_{[\rho,\sigma]}$ and $-3q_{[\rho,\sigma]}^2/q_{\rho}q_{[\rho,\sigma]}$ terms partially cancel. Finally, provided $\sigma \neq I$, a simple counting argument shows that the number of ρ which anticommute with σ is $4^n/2$. Combining

all these observations, we obtain

$$Rc_{\sigma\sigma} = 4^n + \sum_{\rho}' \frac{q_{\sigma}^2 - 2q_{\rho}^2}{q_{\rho}q_{[\rho,\sigma]}}.$$
 (A12)

To evaluate this more explicitly, let us define $N_{\sigma}(\mathcal{P}, \mathcal{P})$ to be the number of generalized Pauli matrices ρ such that: (1) ρ anticommutes with σ ; (2) ρ is in \mathcal{P} , i.e., has only one- or two-body terms; and (3) $[\rho, \sigma]$ is also in \mathcal{P} . We make analogous definitions for $N_{\sigma}(\mathcal{P}, \mathcal{Q}), N_{\sigma}(\mathcal{Q}, \mathcal{P})$ and $N_{\sigma}(\mathcal{Q}, \mathcal{Q})$. Expressed in these terms we have:

$$Rc_{\sigma\sigma} = 4^{n} + q_{\sigma}^{2} \left(N_{\sigma}(\mathcal{P}, \mathcal{P}) + \frac{1}{q} N_{\sigma}(\mathcal{P}, \mathcal{Q}) + \frac{1}{q} N_{\sigma}(\mathcal{Q}, \mathcal{P}) + \frac{1}{q^{2}} N_{\sigma}(\mathcal{Q}, \mathcal{Q}) \right)$$

$$-2 \left(N_{\sigma}(\mathcal{P}, \mathcal{P}) + \frac{1}{q} N_{\sigma}(\mathcal{P}, \mathcal{Q}) + q N_{\sigma}(\mathcal{Q}, \mathcal{P}) + N_{\sigma}(\mathcal{P}, \mathcal{P}) \right). \tag{A13}$$

Elementary counting allows us to evaluate the factors $N_{\sigma}(\cdot,\cdot)$. It is most convenient to consider separately the cases where the weight w of σ is 1,2,3 and 4 or more. The corresponding values for $Rc_{\sigma\sigma}$ are

$$\operatorname{wt}(\sigma) = 1 : Rc_{\sigma\sigma} = 2(3n - 2) + \left(\frac{4^n}{2} - 2(3n - 2)\right) \frac{1}{q^2}$$

$$(A14)$$

$$\operatorname{wt}(\sigma) = 2 : Rc_{\sigma\sigma} = -24(n - 2)q + 8(6n - 11)$$

$$+ \left(\frac{4^n}{2} - 8(3n - 5)\right) \frac{1}{q^2}$$

$$(A15)$$

$$\operatorname{wt}(\sigma) = 3 : Rc_{\sigma\sigma} = 12q^2 + \frac{4^n}{2} + 36(n - 3)$$

$$- 12(3n - 8)\frac{1}{q}$$

$$(A16)$$

$$\operatorname{wt}(\sigma) = w \ge 4 : Rc_{\sigma\sigma} = \frac{4^n}{2} + 4w(3n - 2w)$$

$$- 4w(3n - 2w)\frac{1}{q}.$$

$$(A17)$$

The Ricci flow: In Section V we study the way geodesics deform when the metric is smoothly changed. A well-known method for changing the metric is the Ricci flow introduced by Hamilton [30] and recently used by Perelman [31, 32, 33] in the resolution of the Poincare conjecture. The normalized Ricci flow is an equation for the metric tensor defined in components by $\partial g_{\sigma\tau}/\partial s = -2R_{\sigma\tau} + 2Rg_{\sigma\tau}/(4^n - 1)$. This equation defines a smooth family g_s of metrics on the manifold. Although we do not seriously study the Ricci flow in this paper, we now briefly digress to note some interesting properties of the behaviour of the standard metric under the Ricci flow. Our numerical investigations suggest that the normalized Ricci flow takes the standard metric to the bi-invariant metric with q=1, up to an overall

scaling factor. This is interesting, and deserves further study, for the geodesics of the bi-invariant metric are well understood.

To understand the normalized Ricci flow, observe from Equation (A12) that if q_{σ} depends only on the weight of σ , then the resulting diagonal entries $Rc_{\sigma\sigma}$ in the Ricci tensor depend only on the weight of σ . As a result, under the Ricci flow we can assume that the metric tensor is always diagonal with entries that depend only on the weight.

To obtain an explicit expression for the metric under the Ricci flow, we define $N_{\sigma}(v, w)$ to be the number of ρ with weight v such that the commutator $[\sigma, \rho]$ is nonvanishing with weight w. Equation (A12) can be rewritten

$$Rc_{\sigma\sigma} = 4^n + \sum_{vv} N_{\sigma}(v, w) \frac{q_{\sigma}^2 - 2q_v^2}{q_v q_w},$$
 (A18)

where q_v is the penalty for Pauli matrices of weight v. To find a simple formula for $N_{\sigma}(v,w)$, we observe that $N_{\sigma}(v,w) = 3^v \binom{n}{v} p(w|\sigma,v)$, where $p(w|\sigma,v)$ is the conditional probability that a random Pauli of weight v will commute with σ to give a Pauli of weight w. This probability can be computed by conditioning on the size of the overlap between σ and the Pauli of weight v. The probability is zero unless wt $(\sigma) + v - w$ is an odd and positive number. If that is the case then

$$N_{\sigma}(v, w) = \frac{3^{v}}{2^{\operatorname{wt}(\sigma)+v-w}} \sum_{k} \left(\frac{4}{3}\right)^{k} {\operatorname{wt}(\sigma) \choose k} {n - \operatorname{wt}(\sigma) \choose v - k} \times {k \choose \operatorname{wt}(\sigma) + v - w - k}, \quad (A19)$$

where k runs over the possible sizes of the overlap region. A similar calculation can be done to obtain an expression for the scalar curvature. These provide elegant expressions for the Ricci tensor and scalar curvature in the cases when the metric is diagonal with entries depending only on the weight, and are useful in numerically simulating the normalized Ricci flow.

4. Scalar curvature

Returning to the study of the standard metric, the scalar curvature is obtained from the Ricci tensor via the contraction $R = Rc_{\sigma}^{\ \sigma} = \sum_{\sigma} Rc_{\sigma\sigma}/q_{\sigma}$. Using Equations (A14)-(A17) we obtain

$$R = -54n(n-1)(n-2)q + 6n(36n^2 - 99n + 64)$$

$$+ \left[\left(4^n - 1 + \frac{3n(3n-1)}{2} \right) \frac{4^n}{2} \right]$$

$$- 6n(45n^2 - 117n + 74) \frac{1}{q}$$

$$- \left[3n(3n-1)4^{n-1} - 6n(3n-4)(6n-7) \right] \frac{1}{q^2}$$
(A20)

For large n and fixed q the dominant terms in the scalar curvature are therefore

$$R \sim -54n^3q + 216n^3 + \frac{16^n}{2} \frac{1}{q} - 9n^2 4^{n-1} \frac{1}{q^2}$$
. (A21)

We see that provided $q \sim 4^n$, the scalar curvature is necessarily negative. Remarkably, the proof in [4] that Equation (5) holds also requires $q \sim 4^n$ (or larger), and thus entails negative scalar curvature. Whether a relationship like Equation (5) can be proved for smaller values of q (and thus for positive scalar curvature) remains an open question.

The scalar curvature can be shown to be the average of the sectional curvature,

$$R = (4^{n} - 1) \int d\mu(X, Y) K(X, Y),$$
 (A22)

where $\mu(X,Y)$ is the normalized measure induced by our metric on the space of orthonormal X and Y. Note that the constant of proportionality out the front is 4^n-1 if we are working on $U(2^n)$, and is 4^n-2 if we are working on $SU(2^n)$. This suggests (and Equation (A7) can be used to verify) that typical values of the sectional curvature are negative. It is well known that on manifolds with everywhere negative curvature, the dynamical system defined by the geodesic flow is ergodic and mixing; see Sections 10.5 and 10.6 of [19] for an overview and references. This suggests the conjecture that such ergodic and mixing behaviour may be seen at least on parts of our manifold. If true, this may have interesting implications for quantum computation.