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QUANTUM COMPUTATIONAL JACOBI FIELDS

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Abstract. In the Riemannian geometry of quantum computation, the quantum evolution is described in terms of the special unitary group of n-qubit unitary operators with unit determinant. To elaborate on several aspects of the methodology, the Riemannian curvature, geodesic equation, Jacobi equation, and lifted Jacobi equation on the group manifold are explicitly derived. This is important for investigations of the global characteristics of geodesic paths in the group manifold, and the determination of optimal quantum circuits for carrying out a quantum computation.

1. Introduction

A Riemannian metric can be chosen on the manifold of the Lie Group $SU(2^n)$ (special unitary group) of n-qubit unitary operators with unit determinant [8], [1]-[7], [15], [22]. The traceless Hamiltonian of a quantum computational system serves as a tangent vector to a point on the group manifold of the n-qubit unitary transformation U, describing the time evolution of the system. The Hamiltonian H is an element of the Lie algebra $su(2^n)$ of traceless $2^n \times 2^n$ Hermitian matrices [20], [5], [6] and is taken to be tangent to the evolutionary curve $e^{-iHt}U$ at $t = 0$. (Here and throughout, units are chosen such that Planck's constant divided by 2π is $\hbar = 1$.)

The Riemannian metric (inner product) $\langle.,.\rangle$ is taken to be a positive definite bilinear form $\langle H, J\rangle$ defined on tangent vectors (Hamiltonians) H and J. Following [8], the n-qubit Hamiltonian H can be divided into two parts $P(H)$ and

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$Q(H)$, where $P(H)$ contains only one and two-body terms, and $Q(H)$ contains more than two-body terms. Thus:

$$H = P(H) + Q(H), \tag{1.1}$$

in which P and Q are superoperators acting on H, and obey the following relations:

$$P + Q = I, \quad PQ = QP = 0, \quad P^2 = P, \quad Q^2 = Q, \tag{1.2}$$

where I is the identity.

The Hamiltonian can be expressed in terms of tensor products of the Pauli matrices. The Pauli matrices are given by [18]

$$\begin{aligned} \sigma_0 \equiv I \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 \equiv X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \\ \sigma_2 \equiv Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \; \sigma_3 \equiv Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \end{aligned} \tag{1.3}$$

They are Hermitian,

$$\sigma_i = \sigma_i^{\dagger} \;, i = 0, 1, 2, 3, \tag{1.4}$$

and, except for σ_0, they are traceless,

$$\mathrm{Tr}\sigma_i = 0, \quad i \neq 0. \tag{1.5}$$

Their products are given by

$$\sigma_i^2 = I, \tag{1.6}$$

and

$$\sigma_i \sigma_j = i\varepsilon_{ijk}\sigma_k, \quad i, j, k \neq 0, \tag{1.7}$$

expressed in terms of the totally antisymmetric Levi-Civita symbol with $\varepsilon_{123} = 1$.

An example of Eq. (1.1), in the case of a 3-qubit Hamiltonian, is

$$
\begin{aligned}
P(H) = {} & x_1\sigma_1 \otimes I \otimes I \\
& + x_2\sigma_2 \otimes I \otimes I + x_3\sigma_3 \otimes I \otimes I \\
& + x_4 I \otimes \sigma_1 \otimes I + x_5 I \otimes \sigma_2 \otimes I \\
& + x_6 I \otimes \sigma_3 \otimes I + x_7 I \otimes I \otimes \sigma_1 \\
& + x_8 I \otimes I \otimes \sigma_2 + x_9 I \otimes I \otimes \sigma_3 \\
& + x_{10}\sigma_1 \otimes \sigma_2 \otimes I + x_{11}\sigma_1 \otimes I \otimes \sigma_2 \\
& + x_{12} I \otimes \sigma_1 \otimes \sigma_2 + x_{13}\sigma_2 \otimes \sigma_1 \otimes I \\
& + x_{14}\sigma_2 \otimes I \otimes \sigma_1 + x_{15} I \otimes \sigma_2 \otimes \sigma_1 \\
& + x_{16}\sigma_1 \otimes \sigma_3 \otimes I + x_{17}\sigma_1 \otimes I \otimes \sigma_3 \\
& + x_{18} I \otimes \sigma_1 \otimes \sigma_3 + x_{19}\sigma_3 \otimes \sigma_1 \otimes I \\
& + x_{20}\sigma_3 \otimes I \otimes \sigma_1 + x_{21} I \otimes \sigma_3 \otimes \sigma_1 \\
& + x_{22}\sigma_2 \otimes \sigma_3 \otimes I + x_{23}\sigma_2 \otimes I \otimes \sigma_3 \\
& + x_{24} I \otimes \sigma_2 \otimes \sigma_3 + x_{25}\sigma_3 \otimes \sigma_2 \otimes I \\
& + x_{26}\sigma_3 \otimes I \otimes \sigma_2 + x_{27} I \otimes \sigma_3 \otimes \sigma_2 \\
& + x_{28}\sigma_1 \otimes \sigma_1 \otimes I + x_{29}\sigma_2 \otimes \sigma_2 \otimes I \\
& + x_{30}\sigma_3 \otimes \sigma_3 \otimes I + x_{31}\sigma_1 \otimes I \otimes \sigma_1 \\
& + x_{32}\sigma_2 \otimes I \otimes \sigma_2 + x_{33}\sigma_3 \otimes I \otimes \sigma_3 \\
& + x_{34} I \otimes \sigma_1 \otimes \sigma_1 + x_{35} I \otimes \sigma_2 \otimes \sigma_2 + x_{36} I \otimes \sigma_3 \otimes \sigma_3,
\end{aligned}
\tag{1.8}
$$

in which $\otimes$ denotes the tensor product, and

$$
\begin{aligned}
Q(H) = {} & x_{37}\sigma_1 \otimes \sigma_2 \otimes \sigma_3 + x_{38}\sigma_1 \otimes \sigma_3 \otimes \sigma_2 \\
& + x_{39}\sigma_2 \otimes \sigma_1 \otimes \sigma_3 + x_{40}\sigma_2 \otimes \sigma_3 \otimes \sigma_1 \\
& + x_{41}\sigma_3 \otimes \sigma_1 \otimes \sigma_2 + x_{42}\sigma_3 \otimes \sigma_2 \otimes \sigma_1 \\
& + x_{43}\sigma_1 \otimes \sigma_1 \otimes \sigma_2 + x_{44}\sigma_1 \otimes \sigma_2 \otimes \sigma_1 \\
& + x_{45}\sigma_2 \otimes \sigma_1 \otimes \sigma_1 + x_{46}\sigma_1 \otimes \sigma_1 \otimes \sigma_3 \\
& + x_{47}\sigma_1 \otimes \sigma_3 \otimes \sigma_1 + x_{48}\sigma_3 \otimes \sigma_1 \otimes \sigma_1 \\
& + x_{49}\sigma_2 \otimes \sigma_2 \otimes \sigma_1 + x_{50}\sigma_2 \otimes \sigma_1 \otimes \sigma_2 \\
& + x_{51}\sigma_1 \otimes \sigma_2 \otimes \sigma_2 + x_{52}\sigma_2 \otimes \sigma_2 \otimes \sigma_3 \\
& + x_{53}\sigma_2 \otimes \sigma_3 \otimes \sigma_2 + x_{54}\sigma_3 \otimes \sigma_2 \otimes \sigma_2 \\
& + x_{55}\sigma_3 \otimes \sigma_3 \otimes \sigma_1 + x_{56}\sigma_3 \otimes \sigma_1 \otimes \sigma_3 \\
& + x_{57}\sigma_1 \otimes \sigma_3 \otimes \sigma_3 + x_{58}\sigma_3 \otimes \sigma_3 \otimes \sigma_2 \\
& + x_{59}\sigma_3 \otimes \sigma_2 \otimes \sigma_3 + x_{60}\sigma_2 \otimes \sigma_3 \otimes \sigma_3 \\
& + x_{61}\sigma_1 \otimes \sigma_1 \otimes \sigma_1 + x_{62}\sigma_2 \otimes \sigma_2 \otimes \sigma_2 + x_{63}\sigma_3 \otimes \sigma_3 \otimes \sigma_3.
\end{aligned}
\tag{1.9}
$$

Here, all possible tensor products of one and two-qubit Pauli matrix operators on three qubits appear in $P(H)$, and analogously, all possible tensor products of three-qubit operators appear in $Q(H)$. Tensor products including only the identity are excluded because the Hamiltonian is taken to be traceless. Each of the terms in Eqs. (1.8) and (1.9) is an 8×8 matrix. The various tensor products of Pauli matrices such as those appearing in Eqs. (1.8) and (1.9) are referred to as generalized Pauli matrices. In the case of an n-qubit Hamiltonian, there are 4^n-1 possible tensor products (corresponding to the dimension of $SU(2^n)$), and each term is a 2^nx2^n matrix.

The right-invariant [22], [5]–[7], [13] Riemannian metric for tangent vectors H and J is given by [8]

$$\langle H, J\rangle \equiv \frac{1}{2^n}\mathrm{Tr}\left[HP(J)+qHQ(J)\right]. \tag{1.10}$$

Here q is a large penalty parameter which taxes more than two-body terms. The length l of an evolutionary path on the $SU(2^n)$ manifold is given by the integral over time t from an initial time t_i to a final time t_f, namely,

$$l=\int_{t_i}^{t_f} dt\,\left(\langle H(t), H(t)\rangle\right)^{1/2}, \tag{1.11}$$

and is a measure of the cost, in terms of quantum circuit complexity, of applying a control Hamiltonian $H(t)$ along the path [8].

2. Covariant derivative

In order to obtain the Levi-Civita connection, one exploits the Lie algebra $su(2^n)$ associated with the group $SU(2^n)$. Because of the right-invariance of the metric, if the connection is calculated at the origin, the same expression applies everywhere on the manifold. Following [8], consider the unitary transformation

$$U=e^{-iX} \tag{2.1}$$

in the neighborhood of the identity $I\subset SU(2^n)$ with

$$X=x\cdot\sigma\equiv\sum_\sigma x_\sigma\sigma, \tag{2.2}$$

which expresses symbolically terms like those in Eqs. (1.8) and (1.9) generalized to 2^n dimensions. In Eqs. (2.1) and (2.2), X is defined using the standard branch of the logarithm with a cut along the negative real axis. In Eq. (2.2), for the general case of n qubits, x represents the set of real (4^n-1) coefficients of the generalized Pauli matrices σ which represent all of the n-fold tensor products. It follows from Eq. (2.2) that the factor x^σ multiplying a particular term σ is given by

$$x^\sigma=\frac{1}{2^n}\mathrm{Tr}(X\sigma). \tag{2.3}$$

Next, the right-invariant metric, Eq. (1.10), in the so-called Hamiltonian representation can be written as

$$\langle H, J\rangle = \frac{1}{2^n}\mathrm{Tr}[HG(J)], \tag{2.4}$$

in which the positive self-adjoint superoperator G is given by

$$G = P + qQ. \tag{2.5}$$

Using Eqs. (1..2) and (2.5), it follows that

$$F \equiv G^{-1} = P + q^{-1}Q. \tag{2.6}$$

A vector Y in the group tangent space can be written as

$$Y = \sum_{\sigma} y^{\sigma}\sigma \tag{2.7}$$

with so-called Pauli coordinates y^{σ}. Here σ, as an index, is used to refer to a particular tensor product appearing in the generalized Pauli matrix σ. This index notation, used throughout, is a convenient abbreviation for the actual numerical indices (e.g. in Eq. (1.8), the number 31 appearing in x_{31}, the coefficient of $\sigma_1 \otimes I \otimes \sigma_1$).

Next consider a curve passing through the origin with tangent vector Y with components $y^{\sigma} = dx^{\sigma}/dt$. It can be shown that the covariant derivative of a right-invariant vector field Z along the curve in the Hamiltonian representation is given by [8],[4]

$$(\nabla_Y Z) = \frac{i}{2}\{[Y, Z] + F([Y, G(Z)] + [Z, G(Y)])\}, \tag{2.8}$$

which, because of the right-invariance of the metric, is true everywhere on the manifold.

3. Riemann curvature

For a right-invariant vector field Z, one has after substituting

$$Z = \sum_{\tau} z^{\tau}\tau, \quad Y = \sum_{\sigma} y^{\sigma}\sigma \tag{3.1}$$

in Eq. (2.8),

$$\nabla_{\sigma}\tau = \frac{i}{2}\left([\sigma, \tau] + F([\sigma, G(\tau)] + [\tau, G(\sigma)])\right). \tag{3.2}$$

Next, denoting S_0 as the set containing only tensor products of the identity, and S_{12} as the set of terms in the Hamiltonian containing only one and two body terms, that is

$$S_0 \equiv \{I \otimes I \otimes ...\}, \tag{3.3}$$

and

$$S_{12} = \{I \otimes I \otimes ...\sigma_i \otimes I.., ..\}$$

$$\cup\{I \otimes I \otimes ...\sigma_i \otimes I..\sigma_j \otimes I..,..\}, \tag{3.4}$$

then evidently,

$$[\sigma, G(\tau)] = \begin{cases} [\sigma,\tau], & \tau \in S_{12} \cup S_0 \\ q[\sigma,\tau], & \tau \notin S_{12} \cup S_0 \end{cases}, \tag{3.5}$$

and therefore

$$F\left([\sigma, G(\tau)]\right) = \begin{cases} F([\sigma,\tau]), & \tau \in S_{12} \cup S_0 \\ qF([\sigma,\tau]), & \tau \notin S_{12} \cup S_0 \end{cases}. \tag{3.6}$$

Using Eq. (2.6) in Eq. (3.6), one obtains

$$F\left([\sigma, G(\tau)]\right) = \begin{cases} \frac{1}{q_{[\sigma,\tau]}}[\sigma,\tau], & \tau \in S_{12} \cup S_0 \\ \frac{q}{q_{[\sigma,\tau]}}[\sigma,\tau], & \tau \notin S_{12} \cup S_0 \end{cases}, \tag{3.7}$$

where

$$q_{[\sigma,\tau]} = 1 \text{ if } [\sigma,\tau] = 0, \quad q_{[\sigma,\tau]} = q_\lambda \text{ if } [\sigma,\tau] \propto \lambda, \text{ and } q_{[\sigma,\tau]} = q_{[\tau,\sigma]}, \tag{3.8}$$

and q_λ is defined by

$$q_\sigma \equiv \begin{cases} 0, & \sigma \in S_0 \\ 1, & \sigma \in S_{12} \\ q, & \sigma \notin S_0 \cup S_{12} \end{cases}. \tag{3.9}$$

Equation (3.7) can be written as

$$F\left([\sigma, G(\tau)]\right) = \frac{q_\tau}{q_{[\sigma,\tau]}}[\sigma,\tau]. \tag{3.10}$$

Next substituting Eq. (3.10) in Eq. (3.2), and using Eq. (3.8), one obtains

$$\nabla_\sigma \tau = ic_{\sigma,\tau}[\sigma,\tau], \tag{3.11}$$

where

$$c_{\sigma,\tau} = \frac{1}{2}\left(1 + \frac{q_\tau - q_\sigma}{q_{[\sigma,\tau]}}\right). \tag{3.12}$$

The Riemann curvature tensor with the inner-product (metric) Eq. (2.4) is given by [16]

$$R(W,X,Y,Z) = \left\langle \nabla_W \nabla_X Y - \nabla_X \nabla_W Y - \nabla_{i[W,X]} Y, Z \right\rangle, \tag{3.13}$$

and after substituting the vector fields,

$$W = \sum_\sigma w^\rho \rho, \quad X = \sum_\sigma z^\sigma \sigma, \quad Y = \sum_\tau y^\tau \tau, \quad Z = \sum_\mu z^\mu \mu, \tag{3.14}$$

Eq. (3.13) becomes

$$R_{\rho\sigma\tau\mu} = \left\langle \nabla_\rho \nabla_\sigma \tau - \nabla_\sigma \nabla_\rho \tau - \nabla_{i[\rho,\sigma]} \tau, \mu \right\rangle. \tag{3.15}$$

Next, for three right-invariant vector fields X, Y, and Z, one has

$$0 = \nabla_Y \langle X, Z\rangle = \langle X, \nabla_Y Z\rangle + \langle \nabla_Y X, Z\rangle, \tag{3.16}$$

or

$$\langle X, \nabla_Y Z\rangle = -\langle \nabla_Y X, Z\rangle\,, \tag{3.17}$$

and substituting Eqs. (3.14) in Eq. (3.17), one then has

$$\langle \sigma, \nabla_\tau \mu\rangle = -\langle \nabla_\tau \sigma, \mu\rangle\,. \tag{3.18}$$

Therefore

$$\langle \nabla_\rho \nabla_\sigma \tau, \mu\rangle = -\langle \nabla_\sigma \tau, \nabla_\rho \mu\rangle\,, \tag{3.19}$$

and

$$\langle \nabla_\sigma \nabla_\rho \tau, \mu\rangle = -\langle \nabla_\rho \tau, \nabla_\sigma \mu\rangle\,. \tag{3.20}$$

Then substituting Eqs. (3.19) and (3.20) in Eq. (3.15), and interchanging the first and second terms, one obtains

$$R_{\rho\sigma\tau\mu} = \langle \nabla_\rho \tau, \nabla_\sigma \mu\rangle - \langle \nabla_\sigma \tau, \nabla_\rho \mu\rangle - \left\langle \nabla_{i[\rho,\sigma]} \tau, \mu\right\rangle\,. \tag{3.21}$$

Also clearly

$$\nabla_{iY} Z = i\nabla_Y Z, \tag{3.22}$$

so Eq. (3.21) can also be written as

$$R_{\rho\sigma\tau\mu} = \langle \nabla_\rho \tau, \nabla_\sigma \mu\rangle - \langle \nabla_\sigma \tau, \nabla_\rho \mu\rangle - i\left\langle \nabla_{[\rho,\sigma]} \tau, \mu\right\rangle\,. \tag{3.23}$$

Next substituting Eq. (3.11) in Eq. (3.23), one obtains the following useful form for the Riemann curvature tensor [8]:

$$\begin{aligned} R_{\rho\sigma\tau\mu} &= c_{\rho,\tau} c_{\sigma,\mu} \langle i[\rho,\tau], i[\sigma,\mu]\rangle \\ &\quad - c_{\sigma,\tau} c_{\rho,\mu} \langle i[\sigma,\tau], i[\rho,\mu]\rangle \\ &\quad - c_{[\rho,\sigma],\tau} \langle i[i[\rho,\sigma],\tau], \mu\rangle\,. \end{aligned} \tag{3.24}$$

4. Geodesic equation

Next consider a curve passing through the origin with tangent vector Y having components $y^\sigma = dx^\sigma/dt$. The covariant derivative along the curve in the Hamiltonian representation is given by [8], [4].

$$(D_t Z) \equiv (\nabla_Y Z) = \frac{dZ}{dt} + \frac{i}{2}\left([Y,Z] + F\left([Y,G(Z)] + [Z,G(Y)]\right)\right). \tag{4.1}$$

(Note that the term $\frac{dZ}{dt}$ in Eq. (4.1) does not appear in Eq. (2.8) because there the vector field Z is taken to be right invariant, in which case $\frac{dZ}{dt} = 0$.) Because of the right-invariance of the metric, Eq. (4.1) is true on the entire manifold. Furthermore, a geodesic in $SU(2^n)$ is a curve $U(t)$ with tangent vector $H(t)$ parallel transported along the curve, namely,

$$D_t H = 0. \tag{4.2}$$

However, according to Eq. (4.1) with $Y = Z = H$, one has

$$D_t H = \frac{dH}{dt} + \frac{i}{2}([H,H] + F([H,G(H)] + [H,G(H)])), \tag{4.3}$$

which when substituting Eq. (4.2) becomes [8]

$$\frac{dH}{dt} = -iF([H,G(H)]). \tag{4.4}$$

One can rewrite Eq. (4.4) using the dual [8], [4],

$$L \equiv G(H) = F^{-1}(H), \tag{4.5}$$

and then noting that

$$\frac{dL}{dt} = \frac{d}{dt}\left(F^{-1}(H)\right) = F^{-1}\left(\frac{dH}{dt}\right). \tag{4.6}$$

Thus substituting Eq. (4.4) in Eq. (4.6), one obtains

$$\frac{dL}{dt} = -iF^{-1}(F([H,G(H)])), \tag{4.7}$$

or

$$\frac{dL}{dt} = -i[H,G(H)], \tag{4.8}$$

and again using Eq. (4.5), Eq. (4.8) becomes

$$\frac{dL}{dt} = -i[H,L] = i[L,H]. \tag{4.9}$$

Furthermore, again using Eq. (4.5) in Eq. (4.9), one obtains the sought geodesic equation [8]:

$$\frac{dL}{dt} = i[L,F(L)]. \tag{4.10}$$

Equation (4.10) is a Lax equation, a well-known nonlinear differential matrix equation, and L and $iF(L)$ are Lax pairs [12], [26] [27].

5. Jacobi fields

Consider a one-parameter family of geodesics

$$x^j = x^j(s,t), \tag{5.1}$$

in which the parameter s distinguishes a particular geodesic in the family, and t is the usual curve parameter which can be taken to be time. The Riemannian geodesic equation in a coordinate representation is given by [13]

$$\frac{\partial^2 x^j}{\partial t^2} + \Gamma^j_{kl}(s)\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} = 0, \tag{5.2}$$

in which the Levi Civita connection is given by,

$$\Gamma^j_{kl}(s) = \frac{1}{2}g^{jm}(s)(g_{km,l}(s) + g_{lm,k}(s) - g_{kl,m}(s)), \tag{5.3}$$

for metric $g_{ij}(x(s,t)) \equiv g_{ij}(s)$. (Note, the geodesic equation, Eq. (4.10), on the $SU(2^n)$ group manifold can be shown to follow from Eq. (5.2) [8], [4].)

Let $x^j(0,t)$ be the base geodesic, and define the lifted Jacobi field along the base geodesic by [8]

$$J^j(t) = \frac{\partial}{\partial s} x^j(s,t)_{|s=0}, \tag{5.4}$$

describing how the base geodesic changes as the parameter s is varied. Using a Taylor series expansion, one has for small Δs in the neighborhood of the base geodesic,

$$x^j(\Delta s, t) = x^j(0,t) + \Delta s J^j(t) + O(\Delta s^2). \tag{5.5}$$

Here $x^j(\Delta s, t)$ satisfies the geodesic equation with the metric $g_{ij}(\Delta s)$. Operating on the geodesic equation, Eq. (5.2) with $\partial_s \equiv \frac{\partial}{\partial s}$ and substituting Eqs. (5.4) and (5.5), one obtains for $\Delta s \to 0$,

$$\begin{aligned} 0 = {} & \frac{\partial^2}{\partial t^2} \operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^j(t)}{\Delta s} \\ & + \Gamma^j_{kl,m}(s)_{|s=0} \operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^m(t)}{\Delta s} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} + \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} \\ & + \Gamma^j_{kl}(0) \left\{ \frac{\partial}{\partial t} \left(\operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^k(t)}{\Delta s} \right) \frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t} \frac{\partial}{\partial t} \operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^l(t)}{\Delta s} \right\}, \end{aligned} \tag{5.6}$$

in which $g_{ij}(0) \equiv g_{ij}$ is the base metric and $\Gamma^j_{kl}(0) \equiv \Gamma^j_{kl}$ is the base connection. Equation (5.6) then becomes

$$\begin{aligned} 0 = {} & \frac{\partial^2 J^j(t)}{\partial t^2} + \Gamma^j_{kl,m}(s)_{|s=0} J^m(t) \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} \\ & + \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} + \Gamma^j_{kl} \left(\frac{\partial J^k}{\partial t} \frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t} \frac{\partial J^l}{\partial t} \right). \end{aligned} \tag{5.7}$$

Taking account of dummy indices summed over, it is clearly true that

$$-\Gamma^j_{lq} \Gamma^q_{ik} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k + \Gamma^j_{kp} \Gamma^p_{mn} \frac{\partial x^k}{\partial t} \frac{\partial x^m}{\partial t} J^n = 0. \tag{5.8}$$

One also has

$$-\Gamma^j_{ik,l} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k + \Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t} J^p = 0. \tag{5.9}$$

Also, using the geodesic equation, Eq. (5.2), one has

$$\Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} J^p = -\Gamma^j_{kp} \Gamma^k_{iq} \frac{\partial x^i}{\partial t} \frac{\partial x^q}{\partial t} J^p, \tag{5.10}$$

or renaming dummy indices on the right hand side, it follows that

$$\Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} J^p + \Gamma^j_{qk} \Gamma^q_{il} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k = 0. \tag{5.11}$$

Next adding Eqs. (5.7)-(5.9) and (5.11), one obtains

$$
\begin{aligned}
0 = {} & \frac{\partial^2 J^j(t)}{\partial t^2} + \ \Gamma^j_{kl,m} J^m(t) \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} \\
& + \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} + \Gamma^j_{kl} \left(\frac{\partial J^k}{\partial t} \frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t} \frac{\partial J^l}{\partial t} \right) \\
& - \Gamma^j_{lq} \Gamma^q_{lk} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k + \Gamma^j_{kp} \Gamma^p_{mn} \frac{\partial x^k}{\partial t} \frac{\partial x^m}{\partial t} J^n \\
& - \Gamma^j_{ik,l} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k + \Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t} J^p \\
& + \Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} J^p + \Gamma^j_{qk} \Gamma^q_{il} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k,
\end{aligned} \tag{5.12}
$$

or equivalently,

$$
\begin{aligned}
\frac{\partial^2 J^j(t)}{\partial t^2} = {} & - \Gamma^j_{kl,m} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} J^m + \Gamma^j_{lq} \Gamma^q_{ik} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k \\
& - \Gamma^j_{kp} \Gamma^p_{mn} \frac{\partial x^k}{\partial t} \frac{\partial x^m}{\partial t} J^n - \Gamma^j_{qk} \Gamma^q_{il} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k \\
& + \Gamma^j_{ik,l} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k - \Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} J^p \\
& - \Gamma^j_{kl} \left(\frac{\partial J^k}{\partial t} \frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t} \frac{\partial J^l}{\partial t} \right) \\
& - \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} - \Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t} J^p.
\end{aligned} \tag{5.13}
$$

Rearranging terms, then

$$
\begin{aligned}
\frac{\partial^2 J^j(t)}{\partial t^2} = {} & \Gamma^j_{ik,l} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k - \ \Gamma^j_{kl,m} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} J^m + \Gamma^j_{lq} \Gamma^q_{ik} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k \\
& - \Gamma^j_{kp} \Gamma^p_{mn} \frac{\partial x^k}{\partial t} \frac{\partial x^m}{\partial t} J^n - \Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t} J^p - \Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} J^p \\
& - \Gamma^j_{kl} \frac{\partial x^k}{\partial t} \frac{\partial J^l}{\partial t} - \Gamma^j_{kl} \frac{\partial x^l}{\partial t} \frac{\partial J^k}{\partial t} \\
& - \Gamma^j_{qk} \Gamma^q_{il} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k - \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t}.
\end{aligned} \tag{5.14}
$$

Noting that for the Levi-Civita connection, one has

$$
\Gamma^j_{qp} = \Gamma^j_{pq}, \tag{5.15}
$$

and renaming dummy indices, Eq. (5.14) becomes

$$\begin{aligned}\frac{\partial^2 J^j}{\partial t^2} &= \left(\Gamma^j_{ik,l} - \Gamma^j_{il,k} + \Gamma^j_{lq}\Gamma^q_{ik} - \Gamma^j_{kp}\Gamma^p_{li}\right)\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k \\ &\quad - \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p - \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p - \Gamma^j_{kl}\frac{\partial x^k}{\partial t}\frac{\partial J^l}{\partial t} \\ &\quad - \Gamma^j_{pk}\frac{\partial x^k}{\partial t}\left(\frac{\partial J^p}{\partial t} + \Gamma^p_{mn}\frac{\partial x^m}{\partial t}J^n\right) - \partial_s\Gamma^j_{kl}(s)_{|s=0}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}.\end{aligned} \tag{5.16}$$

Next, using the expression for the covariant derivative, one has

$$\begin{aligned}\frac{D^2 J^j}{Dt^2} &= \frac{\partial}{\partial t}\left(\frac{DJ^j}{Dt}\right) + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{DJ^p}{Dt} \\ &= \frac{\partial}{\partial t}\left(\frac{\partial J^j}{\partial t} + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}J^p\right) + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{DJ^p}{Dt},\end{aligned} \tag{5.17}$$

or

$$\begin{aligned}\frac{D^2 J^j}{Dt^2} &= \frac{\partial^2 J^j}{\partial t^2} + \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p + \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{\partial J^p}{\partial t} \\ &\quad + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\left(\frac{\partial J^p}{\partial t} + \Gamma^p_{mn}\frac{\partial x^m}{\partial t}J^n\right).\end{aligned} \tag{5.18}$$

Also it is known that the Riemann curvature tensor is given by [16]

$$R^j_{ikl} = \Gamma^j_{il,k} - \Gamma^j_{ik,l} + \Gamma^j_{kp}\Gamma^p_{li} - \Gamma^j_{lq}\Gamma^q_{ik}. \tag{5.19}$$

Substituting Eqs. (5.16) and (5.19) in Eq. (5.18), one obtains the so-called lifted Jacobi equation [8],

$$\frac{D^2 J^j}{Dt^2} + R^j_{ikl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \partial_s\Gamma^j_{kl}(s)_{|s=0}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} = 0. \tag{5.20}$$

This equation is useful for investigations of the global behavior of geodesics and their extrapolation to nonvanishing values of the parameter s [8].

For g_{ij} independent of s, one has

$$\partial_s\Gamma^j_{kl}(s)_{|s=0} = 0, \tag{5.21}$$

the last term of Eq. (5.20) is then vanishing, and one obtains the standard Jacobi equation for the Jacobi vector J^j [13],

$$\frac{D^2 J^j}{Dt^2} + R^j_{ikl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k = 0. \tag{5.22}$$

Equation (5.22) is also known as the equation of geodesic deviation [24],[16], measuring the local convergence or divergence of neighboring geodesics, and it is useful in the determination of possible geodesic conjugate points [13], [8].

Next consider the factor in the last term of the lifted Jacobi equation, Eq. (5.20),

$$L^j_{kl} \equiv \partial_s\Gamma^j_{kl}(s)_{|s=0}. \tag{5.23}$$

Substituting Eq. (5.3) in Eq. (5.23), one has

$$L^j_{kl} \equiv \left\{\partial_s \left[\frac{1}{2} g^{jm}(s)(g_{km,l}(s) + g_{lm,k}(s) - g_{kl,m}(s)\right]\right\}_{|s=0}, \tag{5.24}$$

or equivalently,

$$L^j_{kl} \equiv \frac{\partial g^{jm}(s)}{\partial s}_{|s=0} \Gamma_{mkl} + \frac{1}{2} g^{jm}(g'_{km,l} + g'_{lm,k} - g'_{kl,m}), \tag{5.25}$$

in which

$$g'_{km} \equiv \partial_s g_{km}(s)_{|s=0}. \tag{5.26}$$

Next, the covariant derivative of g'_{km} is given by [16]

$$g'_{km;l} = g'_{km,l} - g'_{ki}\Gamma^i_{ml} - g'_{mi}\Gamma^i_{kl}. \tag{5.27}$$

Then substituting Eq. (5.27) in Eq. (5.25) and using Eq. (5.15), one obtains

$$\begin{aligned} L^j_{kl} \equiv \frac{\partial g^{jm}(s)}{\partial s}_{|s=0} &\Gamma_{mkl} + \frac{1}{2} g^{jm}(g'_{km;l} + g'_{ki}\Gamma^i_{ml} + g'_{mi}\Gamma^i_{kl} \\ &+ g'_{lm;k} + g'_{li}\Gamma^i_{mk} + g'_{mi}\Gamma^i_{kl} \\ &- g'_{kl;m} - g'_{ki}\Gamma^i_{lm} - g'_{li}\Gamma^i_{km}), \end{aligned} \tag{5.28}$$

or

$$\begin{aligned} L^j_{kl} \equiv &\frac{1}{2} g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m}) \\ &+ \frac{\partial g^{jm}(s)}{\partial s}_{|s=0} \Gamma_{mkl} + g^{jm} g'_{mi}\Gamma^i_{kl}. \end{aligned} \tag{5.29}$$

Next, one notes that

$$(g^{jm} g_{mi})' = (\delta^j_i)' = 0, \tag{5.30}$$

and therefore

$$g^{jm}(0) \left(\frac{\partial}{\partial s} g_{mi}(s)\right)_{|s=0} = -\left(\frac{\partial g^{jm}(s)}{\partial s}\right)_{|s=0} g_{mi}(0). \tag{5.31}$$

Multiplying both sides of Eq. (5.31) by Γ^i_{kl}, one obtains

$$g^{jm} g'_{mi}\Gamma^i_{kl} = -\left(\frac{\partial g^{jm}(s)}{\partial s}\right)_{|s=0} \Gamma_{mkl}, \tag{5.32}$$

so that Eq. (5.29) reduces to

$$L^j_{kl} \equiv \frac{1}{2} g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m}). \tag{5.33}$$

Finally then combining Eqs. (5.20), (5.23) and (5.33), one obtains

$$\frac{D^2 J^j}{Dt^2} + R^j_{ikl} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k + \frac{1}{2} g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m}) \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t} = 0. \tag{5.34}$$

Next define the vector field,

$$C^j \equiv \frac{1}{2} g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m}) \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t}, \tag{5.35}$$

which is independent of the Jacobi field J^j. Equivalently, by symmetry, Eq. (5.35) can also be written as

$$C^j \equiv \frac{1}{2} g^{jm}(2g'_{km;l} - g'_{kl;m}) \frac{\partial x^k}{\partial t} \frac{\partial x^l}{\partial t}. \tag{5.36}$$

Substituting Eq. (5.35) in Eq. (5.34), one obtains the second-order differential equation,

$$\frac{D^2 J^j}{Dt^2} + R^j_{ikl} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k + C^j = 0, \tag{5.37}$$

the so-called 'lifted Jacobi equation' [8]. Nielsen and Dowling used the lifted Jacobi equation, Eq. (5.37), to deform geodesics from the value $q = 1$ for the penalty parameter to much larger values, and this enabled them to define a so-called 'geodesic derivative' and to deform a geodesic as the penalty parameter is varied without changing the fixed values $U = 1$ and $U = U_f$ of the initial and final unitary transformation corresponding to a quantum computation [8].

Proceeding to solve the lifted Jacobi equation, Eq. (5.37), one first rewrites Eq. (5.18) as

$$\begin{aligned} \frac{D^2 J^j}{Dt^2} = {} & \frac{\partial^2 J^j}{\partial t^2} + 2\Gamma^j_{kp} \frac{\partial x^k}{\partial t} \frac{\partial J^p}{\partial t} + \Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t} J^p + \Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} J^p \\ & + \Gamma^j_{kp} \frac{\partial x^k}{\partial t} \Gamma^p_{mn} \frac{\partial x^m}{\partial t} J^n, \end{aligned} \tag{5.38}$$

and renaming dummy indices in the last term, then

$$\begin{aligned} \frac{D^2 J^j}{Dt^2} = {} & \frac{\partial^2 J^j}{\partial t^2} + \left(2\Gamma^j_{kp} \frac{\partial x^k}{\partial t} \right) \frac{\partial J^p}{\partial t} \\ & + \left(\Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t} + \Gamma^j_{kp} \frac{\partial^2 x^k}{\partial t^2} + \Gamma^j_{kq} \frac{\partial x^k}{\partial t} \Gamma^q_{mp} \frac{\partial x^m}{\partial t} \right) J^p, \end{aligned} \tag{5.39}$$

or equivalently

$$\frac{D^2 J^j}{Dt^2} = \frac{\partial^2 J^j}{\partial t^2} + A^j_p \frac{\partial J^p}{\partial t} + \left(\sum_{n=1}^{3} {}^{(n)}B^j_p \right) J^p \tag{5.40}$$

where

$$A^j_p \equiv \left(2\Gamma^j_{kp} \frac{\partial x^k}{\partial t} \right), \tag{5.41}$$

and

$${}^{(1)}B^j_p \equiv \Gamma^j_{kp,m} \frac{\partial x^m}{\partial t} \frac{\partial x^k}{\partial t}, \tag{5.42}$$

$$^{(2)}B^j_p \equiv \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}, \tag{5.43}$$

$$^{(3)}B^j_p \equiv \Gamma^j_{kq}\frac{\partial x^k}{\partial t}\Gamma^q_{mp}\frac{\partial x^m}{\partial t}. \tag{5.44}$$

Next Eq. (5.37) can written as

$$\frac{D^2 J^j}{Dt^2} + {}^{(4)}B^j_p J^p + C^j = 0, \tag{5.45}$$

where

$$^{(4)}B^j_p \equiv R^j_{ipl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}. \tag{5.46}$$

Next substituting Eq. (5.45) in Eq. (5.40), one obtains

$$\frac{\partial^2 J^j}{\partial t^2} + A^j_p\frac{\partial J^p}{\partial t} + B^j_p J^p + C^j = 0, \tag{5.47}$$

where

$$B^j_p = \sum_{n=1}^{4} {}^{(n)}B^j_p. \tag{5.48}$$

Next define the column vectors

$$J \equiv \left[J^j\right], \tag{5.49}$$

$$C \equiv \left[C^j\right], \tag{5.50}$$

and the matrices

$$A \equiv \left[A^j_p\right], \tag{5.51}$$

$$B \equiv \left[B^j_p\right] = \left[\sum_{n=1}^{4} {}^{(n)}B^j_p.\right]. \tag{5.52}$$

Then Eq. (5.47) becomes

$$\frac{\partial^2 J}{\partial t^2} + A\frac{\partial J}{\partial t} + BJ + C = 0. \tag{5.53}$$

Next defining the column vector

$$K \equiv \begin{bmatrix} J_1 \\ J_2 \end{bmatrix} \equiv \begin{bmatrix} J \\ \frac{\partial J}{\partial t} \end{bmatrix}, \tag{5.54}$$

then Eq. (5.53) is equivalent to

$$\frac{\partial K}{\partial t} \equiv \begin{bmatrix} 0 & I \\ -B & -A \end{bmatrix} K - \begin{bmatrix} 0 \\ C \end{bmatrix}. \tag{5.55}$$

The homogeneous part of Eq. (5.55) with $C = 0$ is equivaalent to the Jacobi equation, Eq. (5.22), and is given by

$$\frac{\partial K_0}{\partial t} \equiv M K_0, \tag{5.56}$$

where the matrix M is given by

$$M \equiv \begin{bmatrix} 0 & I \\ -B(t) & -A(t) \end{bmatrix}, \tag{5.57}$$

in which the time dependence of A and B is indicated explicitly. The solution to the Jacobi equation, Eq. (5.56), is given in terms of the time-ordered exponential [9],[25] namely,

$$K_0(t) = \left(I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 .. \int_0^{t} dt_n T(M(t_1)...M(t_n)) \right) K_0(0), \tag{5.58}$$

in which T denotes the time ordering operator. Thus, Eq. (5.58) gives the Jacobi field and can be expressed formally as

$$K_0(t) = T \exp \left(\int_0^t dt' M(t') \right) K_0(0), \tag{5.59}$$

or defining the operator

$$E_t \equiv T \exp \left(\int_0^t dt' M(t') \right) = I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 .. \int_0^t dt_n T(M(t_1)...M(t_n)), \tag{5.60}$$

Eq. (5.59) can be written as

$$K_0(t) = E_t K_0(0), \tag{5.61}$$

Also, it follows from Eq. (5.60) that

$$\begin{aligned} \frac{\partial E_t}{\partial t} &= M(t) + \sum_{n=2}^{\infty} \frac{1}{n!} n \int_0^t dt_1 .. \int_0^t dt_{n-1} T(M(t_1)...M(t_{n-1})M(t)) \\ &= M(t) + M(t) \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \int_0^t dt_1 .. \int_0^t dt_{n-1} T(M(t_1)...M(t_{n-1})) \\ &= M(t) \left(I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 .. \int_0^t dt_n T(M(t_1)...M(t_n)) \right), \end{aligned} \tag{5.62}$$

or equivalently then substituting Eq. (5.60), one obtains

$$\frac{\partial E_t}{\partial t} = M(t) E_t. \tag{5.63}$$

Next, it follows that the solution to the inhomogeneous equation, Eq. (5.55) is given by

$$K(t) = E_t K(0) - E_t \int_0^t dr E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix}, \tag{5.64}$$

This is the lifted Jacobi field. To see that Eq, (5.64) solves the inhomogeneous equation, Eq. (5.55), note that using Eqs. (5.64) and (5.63) one has

$$\begin{aligned} \frac{\partial K(t)}{\partial t} &= \frac{\partial E_t}{\partial t} K(0) - \frac{\partial E_t}{\partial t} \int_0^t dr E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix} - E_t E_t^{-1} \begin{bmatrix} 0 \\ C(t) \end{bmatrix} \\ &= M(t) E_t K(0) - M(t) E_t \int_0^t dr E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix} - \begin{bmatrix} 0 \\ C(t) \end{bmatrix}. \end{aligned} \tag{5.65}$$

Next substituting Eqs. (5.61), (5.64) and (5.57) in Eq. (5.65), then

$$\begin{aligned} \frac{\partial K(t)}{\partial t} &= M(t) E_t K(0) + M(t) K(t) - M(t) E_t K(0) - \begin{bmatrix} 0 \\ C(t) \end{bmatrix} \\ &= \begin{bmatrix} 0 & I \\ -B(t) & -A(t) \end{bmatrix} K(t) - \begin{bmatrix} 0 \\ C(t) \end{bmatrix}, \end{aligned} \tag{5.66}$$

and thus Eq. (5.55) is in fact satisfied by Eq. (5.64).

6. Conclusion

In this expository work, the Riemann curvature, geodesic equation, and lifted Jacobi equation on the manifold of the $SU(2^n)$ group of n-qubit unitary operators with unit determinant were explicitly derived using the Lie algebra $su(2^n)$. The Riemann curvature is given by Eqs. (3.24), (3.12), (3.8), and (3.9). The geodesic equation is given by Eqs. (4.10) and (4.5). The Jacobi equation and its solution are given by Eqs. (5.22) and (5.58), respectively. The lifted Jacobi equation is given by Eqs. (5.37), (5.36), and (3.24), and the solution is given by Eq. (5.64) together with the supporting equations, Eqs. (5.57), (5.60), (5.49)-(5.52), (5.54), (5.36), (5.41), (5.48), (5.42)-(5.44), and (5.46).These equations are germane to investigations of the global characteristics of geodesic paths [3], [13] and minimal complexity quantum circuits [8], [18], [4].

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