The Local C-Numerical Range: Examples, Conjectures, and Numerical Algorithms

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Abstract—Motivated by applications in quantum computing and quantum control, we consider the task of maximizing the trace function $\operatorname{Re}(\operatorname{tr}(C^{\dagger}UAU^{\dagger}))$ on the Lie group of Nfold tensor products of special unitary (2×2) -transformations. In order to approach this highly non-convex optimization problem, a new object, the local C-numerical range $W_{loc}(C, A)$, is introduced and its geometry is studied. We first present examples that illustrate the rather complex geometric structure of the local C-numerical range. It is shown that, in contrast to the ordinary C-numerical range, $W_{loc}(C, A)$ is in general neither star-shaped nor simply connected. The equivalence of finding bounds on the size of $W_{loc}(C, A)$ and maximizing the above trace function is derived. We then describe and analyse two intrinsic optimization methods to tackle these problems: (a) a gradient flow with an Euler step discretization scheme and (b) a Jacobi-type algorithm. Explicit step size selections are given for which the gradient algorithm converges to the set of critical points. Finally, numerical experiments are presented.

Index Terms—*C*-Numerical Range, Quantum Control, Quantum Computing, Optimization on Lie Groups.

I. INTRODUCTION

Before describing in more precise terms the specific optimization task which will be studied in this paper, we first recall some basic facts from quantum mechanics. The state of a closed quantum system is represented by a normalized element ψ , the state vector, in a complex Hilbert space \mathbb{H} . Similarly, the state of an ensemble of a finite number of identical and non-interacting quantum subsystems requires a representation by a positive semidefinite selfadjoint operator A on \mathbb{H} , normalized to tr (A) = 1. It is called the density operator of the ensemble. Moreover, an observable is represented by a selfadjoint linear operator on \mathbb{H} . The time evolution of the state is governed by the associated unitary propagator U(t) in the sense

$$\psi(t) = U(t)\psi$$
 and $A(t) = U(t)AU(t)^{\dagger}$, (1)

respectively, where $U^{\dagger} := \overline{U}^{\top}$ denotes conjugate transpose. The dynamics of the unitary operator U(t) is in turn described by the corresponding Schrödinger equation, i.e.

$$\dot{U} = -\mathrm{i}HU, \quad U(0) = \mathrm{Id}_{\mathbb{H}}.$$
(2)

Here the Hermitian operator H is called the joint Hamiltonian. In this paper, we focus on ensembles of N coupled spin- $\frac{1}{2}$ particles or N-qubits. In this specific case, the joint

Hilbert state space is formed by the N-fold tensor product over all single spin- $\frac{1}{2}$ particle spaces, i.e.

$$\mathbb{H}=\mathbb{C}^2\otimes\mathbb{C}^2\otimes\cdots\otimes\mathbb{C}^2\cong\mathbb{C}^{2^N},$$

endowed with its natural Hermitian inner product. Moreover, we assume that the Hamiltonian operator H decomposes as

$$H = H_d + \sum_{k=1}^{2N} v_k(t) H_k,$$
(3)

where $H_d := \sum_{k < l} J_{kl} \sigma_{k,z} \sigma_{l,z}$,

$$H_k := \begin{cases} \sigma_{k,x} & \text{for } k = 1, \dots, N \\ \\ \sigma_{(k-N),y} & \text{for } k = N+1, \dots, 2N \end{cases}$$

and $\sigma_{k,\alpha}$ denotes the N-fold Kronecker product

$$\sigma_{k,\alpha} := I_2 \otimes \cdots \otimes I_2 \otimes \sigma_\alpha \otimes I_2 \otimes \cdots \otimes I_2,$$

$$k = 1, \dots, N, \quad \alpha \in \{x, y, z\}$$

with the Pauli matrices

$$\sigma_x := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y := \begin{bmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{bmatrix}, \quad \sigma_z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

appearing at the k-th position. Such Hamiltonians describe a sufficiently rich class of physically relevant situations. The time-dependent real-valued functions v_k define the controls that are accessible to the experimenter, while the operator H_d describes the spin-spin interactions, e.g. of Ising-type. Thus, we refer to H_d and H_k as drift and control Hamiltonians, respectively. The real scalars J_{kl} denote the weak coupling constants. Summarizing, the Schrödinger equation (2) in our situation of interest has the explicit form

$$\dot{U} = -i\left(H_d + \sum_{k=1}^{2N} v_k(t)H_k\right)U, \quad U(0) = I_{2^N}.$$
 (4)

The solutions U(t) thus evolve on the compact Lie group $SU(2^N)$ of unitary $(2^N \times 2^N)$ -matrices with determinant $\det U = 1$.

In a quantum ensemble, whose state evolution is represented by a density operator $A(t) = U(t)AU(t)^{\dagger}$, the expectation value of an observable C is determined by the trace function $\operatorname{Re}(\operatorname{tr}(C^{\dagger}U(t)AU(t)^{\dagger}))$. In other settings, C may denote a desired target operator, whose best approximation by $A(t) = U(t)AU(t)^{\dagger}$ is sought for. For instance, in coherent ensemble spectroscopy, the maximum signal intensity that is experimentally achievable by transferring an initial operator A = A(0) to a target operator C is bounded from above by the maximal value of $\operatorname{Re}(\operatorname{tr}(C^{\dagger}U(t)AU(t)^{\dagger}))$. Note, that in such applications, the matrices C, A are no longer confined to be Hermitian. For further details on quantum mechanics of coupled spin systems and coherent ensemble spectroscopy see e.g. [5].

Recall, that the reachable set \mathcal{R} of (4) is precisely the union of all trajectories of (4), i.e. $\mathcal{R} := \{U(T) \mid T \ge 0\}$, where U(t) is a solution of (4). Thus, the above optimal control problem can be reformulated as an optimization task on the closure $\overline{\mathcal{R}}$ of the reachable set of (4):

$$\max f(U) := \operatorname{Re}(\operatorname{tr}(C^{\dagger}UAU^{\dagger})),$$

subject to: $U \in \overline{\mathcal{R}}.$ (5)

It is a well-known fact from nonlinear control theory [10], that the closure of the reachable sets of the Schrödinger equation (4) are closed Lie subgroups of $SU(2^N)$. Thus, the above optimization problem is equivalent to maximizing the function $f(U) = \text{Re}(\text{tr}(C^{\dagger}UAU^{\dagger}))$ over a closed Lie subgroup of $SU(2^N)$. In [14] it is shown that the Schrödinger equation (4) is controllable for spin systems, whose interactions form a connected graph, e.g. Ising-type couplings. Problem (5) then corresponds to maximizing $\text{Re}(\text{tr}(C^{\dagger}UAU^{\dagger}) \text{ over the full unitary group } SU(2^N)$. For a detailed discussion of this case and a study of gradient algorithms see [7], [8].

In this paper we focus on the other extreme case when all couplings vanish and one is left with so-called local controls, i.e. $H_d = 0$ in (4). Here, the reachable set of (4) is easily characterized as the Lie subgroup generated by the one-parameter subgroups $t \mapsto \exp(-itH_k)$, $k = 1, \ldots, 2N$. As these span the N-fold Kronecker product of special unitary (2 × 2)-matrices, the reachable set is equal to the Lie subgroup

$$SU_{\text{loc}}(2^N) := \{U_1 \otimes \cdots \otimes U_N \mid U_k \in SU(2)\}.$$

Following standard terminology from quantum computing we refer to $SU_{loc}(2^N)$ as the Lie subgroup of *local* unitary operations. Problem (5) for local unitary operations can thus be stated as the

Local Subgroup Optimization Problem (LSOP)

$$\max f(U) := \operatorname{Re}(\operatorname{tr}(C^{\dagger}UAU^{\dagger})),$$

subject to: $U \in SU_{\operatorname{loc}}(2^{N})$ (6)

The LSOP is of considerable interest in areas such as quantum control. In particular, in coherent ensemble spectroscopy – as we mentioned earlier – it is equivalent to the task of maximizing the experimentally achievable signal intensity using only local unitary operations. Moreover, the Euclidean distance between C and UAU^{\dagger} is

$$||C - UAU^{\dagger}||^2 = ||C||^2 + ||A||^2 - 2\operatorname{Re}(\operatorname{tr}(C^{\dagger}UAU^{\dagger})),$$
(7)

where in the sequel $\|\cdot\|$ always denotes the Frobenius norm, i.e., $\|C\| = \sqrt{\operatorname{tr}(CC^{\dagger})}$. Thus minimizing the distance between C and UAU^{\dagger} is the same as maximizing the trace function f. Therefore, the LSOP is also closely related to the task of computing entanglement measures in quantum information theory, which are induced by the Euclidean distance.

In the subsequent sections the LSOP is related to the geometry of the *C*-numerical range of *A* and two numerical algorithms for solving it are presented: (a) a gradient method and (b) a Jacobi-type algorithm. Finally, in Section IV some numerical experiments are discussed. For a similar approach applying a conjugate gradient method and a Newton-type algorithm we refer to [4].

II. THE LOCAL C-NUMERICAL RANGE

An object that arises naturally in the study of the LSOP is the *local* C-numerical range of A

$$W_{\rm loc}(C,A) := \left\{ \operatorname{tr} \left(C^{\dagger} U A U^{\dagger} \right) \middle| U \in SU_{\rm loc}(2^N) \right\}, \quad (8)$$

defined for arbitrary complex matrices $C, A \in \mathbb{C}^{2^N \times 2^N}$. Natural measures of the size of $W_{\text{loc}}(C, A)$ are the so-called *local C-numerical radius* of A defined by

$$r_{\rm loc}(C,A) := \tag{9}$$
$$\max\left\{ \left| \operatorname{tr} \left(C^{\dagger} U A U^{\dagger} \right) \right| \mid U \in SU_{\rm loc}(2^N) \right\}.$$

or the local C-numerical abszissa of A defined by

$$\alpha_{\text{loc}}^{\pm}(C, A) :=$$

$$\max \left\{ \pm \operatorname{Re}(\operatorname{tr}(C^{\dagger}UAU^{\dagger})) \mid U \in SU_{\text{loc}}(2^{N}) \right\}.$$
(10)

Thus $r_{\rm loc}(C, A)$ is the radius of smallest disk centered at the origin and containing $W_{\rm loc}(C, A)$, whereas $\alpha_{\rm loc}^{\pm}(C, A)$ and $\alpha_{\rm loc}^{\pm}(C, iA)$ specify the side lengths of the smallest rectangle containing $W_{\rm loc}(C, A)$. Observe, that the determination of $\alpha_{\rm loc}^{\pm}(C, A)$ is completely equivalent to the LSOP (6).

By definition, $W_{\rm loc}(C,A)$ is a subset of the ordinary C-numerical range of A

$$W(C,A) := \left\{ \operatorname{tr} \left(C^{\dagger} U A U^{\dagger} \right) \mid U \in SU(2^{N}) \right\}.$$
(11)

Thus estimates of the C-numerical range provide bounds for the size of $W_{\text{loc}}(C, A)$. However, such bounds turn out to be too coarse and therefore require a deeper investigation of the geometry of $W_{\text{loc}}(C, A)$. Quite a bit is known already about the geometry of the ordinary C-numerical range. For example, W(C, A) is always a star-shaped, and hence a simply-connected, compact subset of \mathbb{C} , cf. [3]. Moreover, Li and Tsing [12] have shown that W(C, A) is a circular disk centered at the origin for any complex matrix C, if and only if A is unitarily similar to a block-shift matrix in canonical form, i.e. unitarily similar to a nilpotent matrix whose only nonzero entries occur on lower subdiagonal blocks.

To the best of our knowledge, the geometry of $W_{\rm loc}(C, A)$ has not been studied in any systematic way. From (8) it is easily seen that $W_{\rm loc}(C, A)$ is invariant under special unitary similarities of A or C by elements of $SU_{\rm loc}(2^N)$. Furthermore, $W_{\rm loc}(C, A)$ is the continuous image of the

compact and connected set $SU_{\text{loc}}(2^N)$ and therefore itself compact and connected. However, in contrast to the ordinary C-numerical range, $W_{\text{loc}}(C, A)$ is neither star-shaped nor simply connected. The following two examples illustrate this new phenomenon. In the first example, W(C, A) is convex while $W_{\text{loc}}(C, A)$ is non-convex (but star-shaped). The second example shows that $W_{\text{loc}}(C, A)$ can even be nonsimply connected, while this never happens for W(C, A).

Example 2.1: The matrices C and A are given by

 $C = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \ A = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes \begin{bmatrix} 1+i & 0 \\ 0 & 1-i \end{bmatrix}.$

The local C-numerical range of A is plotted in Fig. 1.



Fig. 1. The local C-numerical range of A with A, C as in example 2.1.

Example 2.2: The matrices C and A are given by

$$\begin{split} C &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\ A &= \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2}{3}i\pi} \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2}{3}i\pi} \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2}{3}i\pi} \end{bmatrix} \end{split}$$

The local C-numerical range of A is plotted in Fig. 2. In both examples the boundary of $W_{\rm loc}(C, A)$ has been analytically computed and added for a better visualization.

A complete analogue to the Li-Tsing circular disc characterization for W(C, A) is unknown. Part of their characterization shows that rotational invariance of the *C*-numerical range is equivalent to being circular. This is not surprising, as being star-shaped and rotationally invariant obviously implies that W(C, A) is circular. However, for the local *C*-numerical range this argument fails. Nevertheless, it can be shown to hold even in the local case.

Theorem 2.1: $W_{\text{loc}}(C, A)$ is rotationally invariant for any $C \in \mathbb{C}^{2^N \times 2^N}$ if and only if for all $C \in \mathbb{C}^{2^N \times 2^N}$ it is a circular disc in the complex plane, centered at the origin.

The proof is in preparation and out of the scope of this paper. Regarding the characterization of rotational symmetry of $W_{\text{loc}}(C, A)$ we give the following conjecture.



Fig. 2. The local C-numerical range of A with A, C as in example 2.2.

Conjecture 2.1: If $W_{\text{loc}}(C, A)$ is rotationally invariant for any $C \in \mathbb{C}^{2^N \times 2^N}$ with $N \ge 2$, then A is similar to a blockshift matrix in canonical form via a special unitary transformation of the form U = VP, where $V \in SU_{\text{loc}}(2^N)$ and P is contained in the subgroup generated by permutations of the form

$$I_2 \otimes \dots \otimes I_2 \otimes \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \otimes I_2 \otimes \dots \otimes I_2.$$
(12)

However, concerning sharp estimates for $W_{\text{loc}}(C, A)$, the circular and even the hermitian case, which is well understood if U is allowed to range over the entire special unitary group, cf. [1], [7], are both completely unknown. Thus, the LSOP seems to be a very difficult problem, much harder than the C-numerical range analog. Therefore, we recourse to numerical methods in order to find such bounds for $W_{\text{loc}}(C, A)$, which is the subject of the next section.

III. GEOMETRIC OPTIMIZATION METHODS

Here we present two different geometric approaches to solve the LSOP. The first one amounts to an intrinsic Euler step discretization of the gradient flow of f on the Lie group $SU_{loc}(2^N)$. Explicit choices of step sizes are given such that the algorithm converges from any initial point to the set of critical points. We then discuss a variant of the Jacobi method where the control directions of (3) serve as search directions. Both algorithms are linearly convergent.

A. Preliminaries

Recall that the set $SU(2^N)$ of unitary $(2^N \times 2^N)$ -matrices of determinant one is a compact connected Lie group of real dimension $2^{2N} - 1$. The tangent space of $SU(2^N)$ at an element U is

$$T_U SU(2^N) = \{ \Omega U \mid \Omega^{\dagger} = -\Omega, \operatorname{tr} \Omega = 0 \}.$$
 (13)

In particular, the tangent space of $SU(2^N)$ at the identity element I_{2^N} is the Lie algebra

$$\mathfrak{su}(2^N) := \{ \Omega \mid \Omega^{\dagger} = -\Omega, \operatorname{tr} \Omega = 0 \}$$
(14)

of all traceless skew-Hermitian matrices. Our main interest will be in the compact, connected, 3N-dimensional Lie subgroup

$$SU_{\text{loc}}(2^N) :=$$

$$\{U_1 \otimes \dots \otimes U_N \mid U_k \in SU(2)\} \subset SU(2^N),$$
(15)

known in quantum information theory as the subgroup of *local* unitary operations. The Lie algebra of $SU_{loc}(2^N)$ is

$$\mathfrak{su}(2)\widehat{\otimes}\cdots\widehat{\otimes}\mathfrak{su}(2):=\{\Omega_1\widehat{\otimes}\cdots\widehat{\otimes}\Omega_N \mid \Omega_j\in\mathfrak{su}(2)\},$$
 (16)

where the $(2^N \times 2^N)$ -matrix $\Omega_1 \widehat{\otimes} \cdots \widehat{\otimes} \Omega_N$ is defined as

$$\Omega_1 \widehat{\otimes} \cdots \widehat{\otimes} \Omega_N :=$$

$$\sum_{k=1}^N I_2 \otimes \cdots \otimes I_2 \otimes \Omega_k \otimes I_2 \otimes \cdots \otimes I_2.$$
(17)

Here, the term $\Omega_k \in \mathfrak{su}(2)$ appears at the k-th position of the Kronecker product and I_2 denotes the (2×2) -identity matrix. Moreover, the tangent space of $SU_{\text{loc}}(2^N)$ at an element U is given by

$$T_U SU_{loc}(2^N) = \{ \Omega U \mid \Omega \in \mathfrak{su}(2)\widehat{\otimes} \cdots \widehat{\otimes} \mathfrak{su}(2) \}.$$
(18)

In the sequel, we will endow $SU_{loc}(2^N)$ with the bi-invariant Riemannian metric induced by $SU(2^N)$, i.e.

$$\langle \Omega U, \Xi U \rangle := \operatorname{tr} \left(\Omega^{\dagger} \Xi \right)$$
 (19)

for $\Omega U, \Xi U \in T_U SU_{loc}(2^N)$. Thus, for two Lie algebra elements $\Omega_1 \widehat{\otimes} \cdots \widehat{\otimes} \Omega_N$ and $\Xi_1 \widehat{\otimes} \cdots \widehat{\otimes} \Xi_N$ we have

$$\langle \Omega_1 \widehat{\otimes} \cdots \widehat{\otimes} \Omega_N, \Xi_1 \widehat{\otimes} \cdots \widehat{\otimes} \Xi_N \rangle = 2^{N-1} \sum_{k=1}^N \operatorname{tr} \left(\Omega_k^{\dagger} \Xi_k \right).$$
(20)

Furthermore, we will use for any element $\Omega \in \mathfrak{su}(2)$ and $k = 1, \dots, N$ the following short cut notation. Let

$$\widehat{\Omega}^k := I_2 \otimes \cdots \otimes I_2 \otimes \Omega \otimes I_2 \otimes \cdots \otimes I_2, \qquad (21)$$

where the term Ω appears at the *k*-th position of the Kronecker product. In particular, for $j \neq k$ then $\widehat{\Omega}^k$ and $\widehat{\Xi}^l$ are orthogonal, for arbitrary elements $\Omega, \Xi \in \mathfrak{su}(2)$. Therefore the map

$$(\Omega_1, \cdots, \Omega_N) \mapsto \Omega_1 \widehat{\otimes} \cdots \widehat{\otimes} \Omega_N \tag{22}$$

is injective, as the summands are mutually orthogonal. This proves

Lemma 3.1: The map

$$\begin{aligned} \mathfrak{su}(2) \times \cdots \times \mathfrak{su}(2) &\to \quad \mathfrak{su}(2) \widehat{\otimes} \cdots \widehat{\otimes} \mathfrak{su}(2), \\ (\Omega_1, \cdots, \Omega_N) &\mapsto \quad \Omega_1 \widehat{\otimes} \cdots \widehat{\otimes} \Omega_N \end{aligned}$$

is a Lie algebra isomorphism.

Finally, let

$$X := \begin{bmatrix} 0 & \mathbf{i} \\ \mathbf{i} & 0 \end{bmatrix}, \quad Y := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad Z := \begin{bmatrix} \mathbf{i} & 0 \\ 0 & -\mathbf{i} \end{bmatrix}$$
(23)

denote the Pauli matrices which form a basis of $\mathfrak{su}(2)$. From the above we see that

$$\pi: \mathbb{C}^{2^N \times 2^N} \to \mathfrak{su}(2)\widehat{\otimes} \cdots \widehat{\otimes} \mathfrak{su}(2)$$
(24)

defined by

$$\pi(A) := \frac{1}{2^N} \sum_{k=1}^N \left(\operatorname{Re}(\operatorname{tr}(A^{\dagger} \widehat{X}^k)) \widehat{X}^k + \operatorname{Re}(\operatorname{tr}(A^{\dagger} \widehat{Y}^k)) \widehat{Y}^k + \operatorname{Re}(\operatorname{tr}(A^{\dagger} \widehat{Z}^k)) \widehat{Z}^k \right)$$

is the orthogonal projection onto the Lie algebra $\mathfrak{su}(2)\widehat{\otimes}\cdots\widehat{\otimes}\mathfrak{su}(2).$

B. The Gradient Flow and the Hessian

Now, we are prepared to determine the gradient flow of f on $SU_{\rm loc}(2^N)$ and its Hessian. The latter will be important for specifying a suitable step size for the discretization of the gradient flow. In the following, let

$$[A,B] := AB - BA \tag{25}$$

denote the commutator for arbitrary $A, B \in \mathbb{C}^{2^N \times 2^N}$.

Theorem 3.1: Let $f : SU_{loc}(2^N) \to \mathbb{R}$ be defined as in (6). The gradient of f with respect to the bi-invariant Riemannian metric (19) and the corresponding flow is given by

$$\operatorname{grad} f(U) = \pi([C^{\dagger}, UAU^{\dagger}])U \tag{26}$$

and

$$\dot{U} = \pi([C^{\dagger}, UAU^{\dagger}])U, \qquad (27)$$

respectively. More explicitly, (27) is equivalent to a system of N coupled equations

$$\dot{U}_k = \Omega_k U_k, \quad k = 1, \cdots, N \tag{28}$$

on SU(2), where

$$\Omega_k = \frac{1}{2^N} \Big(\operatorname{Re}(\operatorname{tr}([C^{\dagger}, UAU^{\dagger}]^{\dagger}\widehat{X}^k)) X \\ + \operatorname{Re}(\operatorname{tr}([C^{\dagger}, UAU^{\dagger}]^{\dagger}\widehat{Y}^k)) Y \\ + \operatorname{Re}(\operatorname{tr}([C^{\dagger}, UAU^{\dagger}]^{\dagger}\widehat{Z}^k)) Z \Big).$$

Every solution of (28) exists for all $t \in \mathbb{R}$ and converges for $t \to \pm \infty$ to a critical point. The critical points of f are characterized by

$$\pi([C^{\dagger}, UAU^{\dagger}]) = 0.$$
⁽²⁹⁾

Proof. The Fréchet derivative of f at $U \in SU_{loc}(2^N)$ is the linear map on the tangent space $T_U SU_{loc}(2^N)$ defined by

$$Df(U)(\Omega U) = \operatorname{Re}(\operatorname{tr}(C^{\dagger}[\Omega, UAU^{\dagger}]))$$

=
$$\operatorname{Re}(\operatorname{tr}([UAU^{\dagger}, C^{\dagger}]\Omega)) \qquad (30)$$

=
$$\operatorname{tr}(\pi([C^{\dagger}, UAU^{\dagger}])^{\dagger}\Omega)$$

and therefore the gradient of f is

$$\operatorname{grad} f(U) = \pi([C^{\dagger}, UAU^{\dagger}])U.$$
(31)

By compactness of $SU_{loc}(2^N)$ the solutions of (27) exist for all $t \in \mathbb{R}$ and converge to the set of critical points. Since grad f is a real analytic gradient vector field the pointwise convergence of (27) follows from a result by Łojasiewicz [13]. Thus, the theorem is proved.

Moreover, if $C = C_1 \otimes \cdots \otimes C_N$ and $A = A_1 \otimes \cdots \otimes A_N$ are Kronecker products of Hermitian matrices C_k and A_k , then the gradient flow simplifies to

$$U_k = \Omega_k U_k, \quad k = 1, \cdots, N$$
 (32)

with

$$\Omega_k = \frac{1}{2^N} \prod_{i \neq j} \operatorname{tr}(C_i U_j A_j U_j^{\dagger}) \cdot \left(\operatorname{tr}([C_k, X] U_k A_k U_k^{\dagger}) X + \operatorname{tr}([C_k, Y] U_k A_k U_k^{\dagger}) Y + \operatorname{tr}([C_k, Z] U_k A_k U_k^{\dagger}) Z \right).$$

In this case the critical points are characterized by

$$\prod_{i \neq j} \operatorname{tr}(C_i^{\dagger} U_j A_j U_j^{\dagger}) \cdot [C_k, U_k A_k U_k^{\dagger}] = 0, \quad k = 1, \dots, N$$

because $[C_k, U_k A_k U_k^{\dagger}]$ is skew-Hermitian.

By construction, the gradient flow (27) tends to maximize the trace function $f: SU_{loc}(2^N) \to \mathbb{R}$. Hence its discretizations will lead to optimization methods for the LSOP, see Section III-C.

Moreover, the stability analysis of the critical points as well as suitable step size selections of (27) require knowledge of the Hessian of f. To compute the Hessian we note that the geodesics of $U \in SU_{loc}(2^N)$ with respect to the biinvariant metric are just the one-parameter groups $\alpha(t) =$ $\exp(t\Omega)U$, where Ω denotes an arbitrary Lie algebra element of $\mathfrak{su}(2)\widehat{\otimes}\cdots\widehat{\otimes}\mathfrak{su}(2)$. Therefore, the Hessian of f at U is determined by evaluating the second derivative of $\varphi := f \circ$ α at t = 0, for any geodesic α . This yields the Hessian quadratic form

$$\operatorname{Hess}_{f}(U)(\Omega U, \Omega U) := (f \circ \alpha)''(0). \tag{33}$$

The Hessian operator $H_f(U)$ then is obtained by the standard polarization process from this quadratic form. Explicitly, the second derivative of

$$\varphi(t) = \operatorname{Re}(\operatorname{tr}\left(C^{\dagger} \mathrm{e}^{t\Omega} U A U^{\dagger} \mathrm{e}^{-t\Omega}\right)) \tag{34}$$

at t = 0 for arbitrary $\Omega \in \mathfrak{su}(2)\widehat{\otimes} \cdots \widehat{\otimes} \mathfrak{su}(2)$ is

$$\varphi''(0) = \operatorname{Re}\left(\operatorname{tr}\left(C^{\dagger}[\Omega, [\Omega, UAU^{\dagger}]]\right)\right), \quad (35)$$

implying for the Hessian quadratic form

$$\operatorname{Hess}_{f}(U)(\Omega U, \Omega U) = \operatorname{Re}\left(\operatorname{tr}\left(C^{\dagger}[\Omega, [\Omega, UAU^{\dagger}]]\right)\right)$$
$$= \operatorname{Re}\left(\operatorname{tr}\left(\left[C^{\dagger}, \Omega\right] \cdot [\Omega, UAU^{\dagger}]\right)\right).$$

This yields the following result.

Theorem 3.2: Let $f : SU_{loc}(2^N) \to \mathbb{R}$ be defined as in (6). Then the Hessian operator of f at U is given by the selfadjoint linear map

$$\begin{aligned} \mathbf{H}_{f}(U) &: \mathbf{T}_{U}SU_{\mathrm{loc}}(2^{N}) &\to & \mathbf{T}_{U}SU_{\mathrm{loc}}(2^{N}), \\ \mathbf{H}_{f}(U)\Omega U &= & S(\Omega)U \end{aligned}$$

where $\Omega \in \mathfrak{su}(2)\widehat{\otimes} \cdots \widehat{\otimes} \mathfrak{su}(2)$ and

$$S(\Omega) := \frac{1}{2}\pi \Big([[\Omega, UAU^{\dagger}], C^{\dagger}] + [[\Omega, C^{\dagger}], UAU^{\dagger}] \Big)$$
$$= \frac{1}{2}\pi \Big([[\Omega, UAU^{\dagger}], C^{\dagger}] + [[\Omega, C], UA^{\dagger}U^{\dagger}] \Big).$$

C. Euler Step Discretization of the Gradient Flow

We now aim at a suitable step size selection to derive an implementable numerical integration scheme for (27). Standard numerical integration methods for unconstrained ODEs are not useful here as they do not preserve the unitary nature of the solution. The discretization we propose is similar as in [6]

$$U_{k+1} := \exp\left(\alpha_k \pi([C^{\dagger}, U_k A U_k^{\dagger}])\right) U_k \tag{36}$$

yet with a specific step size $\alpha_k \ge 0$ to be determined. See also [2], [7] for related step size selection schemes in different contexts.

Theorem 3.3: Let

$$\alpha_k := \frac{\left\| \pi\left([C^{\dagger}, U_k A U_k^{\dagger}] \right) \right\|^2}{\left\| \left[C^{\dagger}, \pi\left([C^{\dagger}, U_k A U_k^{\dagger}] \right) \right] \right\| \cdot \left\| \left[U_k A U_k^{\dagger}, \pi\left([C^{\dagger}, U_k A U_k^{\dagger}] \right) \right] \right\|}.$$
 (37)

Then (36) converges to the set of critical points of f.

Proof. For
$$\Omega := \pi([C^{\dagger}, B])$$
 and $B := U_k A U_k^{\dagger}$ let
 $\varphi(t) := \operatorname{Re}(\operatorname{tr}(C^{\dagger} e^{t\Omega} B e^{-t\Omega})).$ (38)

The derivative of φ is

$$\varphi'(t) = \operatorname{Re}(\operatorname{tr}\left([\mathrm{e}^{t\Omega}B\mathrm{e}^{-t\Omega}, C^{\dagger}]\Omega\right))$$
(39)

with

$$\varphi'(0) = \operatorname{Re}(\operatorname{tr}([B, C^{\dagger}]\Omega))$$

= $\|\pi([C^{\dagger}, B])\|^{2} \ge 0$ (40)

and $\varphi'(0) = 0$ if and only if U_k is a critical point of f. Moreover,

$$\varphi''(t) = \operatorname{Re}(\operatorname{tr}([C^{\dagger}, \Omega][\Omega, e^{t\Omega}Be^{-t\Omega}])).$$
(41)

Therefore, since $e^{t\Omega}$ is unitary, we have

$$\begin{aligned} |\varphi''(t)| &\leq \left\| [C^{\dagger}, \Omega] \right\| \cdot \left\| [\Omega, e^{t\Omega} B e^{-t\Omega}] \right\| \\ &= \left\| [C^{\dagger}, \Omega] \right\| \cdot \left\| e^{t\Omega} [\Omega, B] e^{-t\Omega} \right\| \\ &= \left\| [C^{\dagger}, \Omega] \right\| \cdot \left\| [\Omega, B] \right\|. \end{aligned}$$
(42)

By the Mean Value Theorem this implies

$$|\varphi'(t) - \varphi'(0)| \le \sup_{0 \le \tau \le t} |\varphi''(\tau)| \cdot t \tag{43}$$

for $t \ge 0$. That is, for

$$t \le \alpha_k := \frac{\|\Omega\|^2}{\left\| [C^{\dagger}, \Omega] \right\| \cdot \left\| [\Omega, B] \right\|}$$
(44)

we obtain by (42)

$$\begin{aligned} |\varphi'(t) - \varphi'(0)| &\leq \left\| [C^{\dagger}, \Omega] \right\| \cdot \left\| [\Omega, B] \right\| \cdot t \\ &\leq \|\Omega\|^2 = \varphi'(0) \end{aligned}$$
(45)

for all $t \in [0, \alpha_k]$. This shows that

$$\varphi'(t) \ge 0 \quad \text{for} \quad t \in [0, \alpha_k]$$
(46)

and therefore φ is monotonically increasing on $[0, \alpha_k]$. Since $SU_{loc}(2^N)$ is compact, the result now follows from a familiar Lyapunov-type argument, as explained in section 2.3 of [7]. \Box

In particular, the above result holds for all step sizes $0 < \alpha \le \alpha_k$. Thus, upper bounds on the denominator in (44) lead to more conservative step size selection schemes.

Corollary 3.1: Convergence of (36) to the set of critical points holds for the step size

$$\alpha_k^* := \frac{\left\| \pi\left([C^{\dagger}, U_k A U_k^{\dagger}] \right) \right\|}{2\|A\| \cdot \left\| \left[C^{\dagger}, \pi\left([C^{\dagger}, U_k A U_k^{\dagger}] \right) \right] \right\|}$$
(47)

and in particular for the constant step size

$$\alpha_k^{**} = \frac{1}{4\|A\| \cdot \|C\|}.$$
(48)

Proof. From

$$\left\| [B,\Omega] \right\| \le 2\|B\| \cdot \|\Omega\| = 2\|A\| \cdot \|\Omega\|$$
(49)

we obtain

$$\alpha_k^* = \frac{\|\Omega\|}{2\|A\| \cdot \left\| [C^{\dagger}, \Omega] \right\|} \le \frac{\|\Omega\|^2}{\left\| [C^{\dagger}, \Omega] \right\| \cdot \left\| [\Omega, B] \right\|} = \alpha_k$$

and similarly

$$\alpha_k^{**} \le \alpha_k^*. \tag{50}$$

D. The Jacobi Algorithm

The Jacobi-type method proposed here uses the directions $\widehat{X}^k, \widehat{Y}^k$ and \widehat{Z}^k to maximize the trace function. The obtained step-sizes yield controls for steering system (4) to a maximum. The underlying idea is the following. Let \mathcal{B} be the ordered basis

$$(\widehat{X}^k, \widehat{Y}^k, \widehat{Z}^k), \quad k = 1, \dots, N$$

of the Lie algebra of $SU_{\rm loc}(2^N)$. Then, for given $C, A \in \mathbb{C}^{2^N \times 2^N}$, consider the first basis element $\Omega_1 = \widehat{X}^1 \in \mathcal{B}$ and maximize

$$t \longmapsto \operatorname{Re}(\operatorname{tr}(C^{\dagger} \mathrm{e}^{t\Omega_1} A \mathrm{e}^{-t\Omega_1})).$$
 (51)

Note, that by the special form of the Ω_i 's, this maximization task results in maximizing a polynomial of degree two in

 $\cos t$ and $\sin t$ and hence is not expensive. Let $t_*^{(1)}$ denote the local maximum that is nearest to 0 and set

$$A_1 := e^{t_*^{(1)}\Omega_1} A e^{-t_*^{(1)}\Omega_1}.$$

Now consider the next basis element $\Omega_2 = \widehat{Y}^1 \in \mathcal{B}$ and maximize

$$t \longmapsto \operatorname{Re}(\operatorname{tr}(C^{\dagger} \mathrm{e}^{t\Omega_2} A_1 \mathrm{e}^{-t\Omega_2}))$$
(52)

to obtain in an analogous way $t_*^{(2)}$ and $A_2 := e^{t_*^{(2)}\Omega_2}A_1e^{-t_*^{(2)}\Omega_2}$, and so forth. More precisely, we implement a cyclic Jacobi sweep as follows. Let

$$t^{(i)}_*(A) := \mathop{\mathrm{arg\,max}}_{t \in \mathbb{R}} \operatorname{Re}(\operatorname{tr}\left(C^\dagger \mathrm{e}^{t\Omega_i} A \mathrm{e}^{-t\Omega_i}\right))$$

be a local maximum of the function $\operatorname{Retr} (C^{\dagger} e^{t\Omega_i} A e^{-t\Omega_i})$. We choose $t_*^{(i)}$ to have minimal absolute value. Let A_k be given and set

$$\begin{array}{rcl}
A_{k}^{(1)} &:= & \mathrm{e}^{t_{*}^{(1)}(A_{k})\Omega_{1}}A_{k}\mathrm{e}^{-t_{*}^{(1)}(A_{k})\Omega_{1}} \\
A_{k}^{(2)} &:= & \mathrm{e}^{t_{*}^{(2)}(A_{k}^{(1)})\Omega_{2}}A_{k}^{(1)}\mathrm{e}^{-t_{*}^{(2)}(A_{k}^{(1)})\Omega_{2}} \\
& \vdots \\
& & \vdots \\
& & & & \\
\end{array}$$
(53)

$$A_{k}^{(3N)} := e^{t_{*}^{(3N)}(A_{k}^{(3N-1)})\Omega_{3N}} A_{k}^{(3N-1)} e^{-t_{*}^{(3N)}(A_{k}^{(3N-1)})\Omega_{3N}}$$

The Jacobi algorithm itself consists of iterating sweeps.

1. Let $A_0, A_1, ..., A_k$ be given for some $k \in \mathbb{N}$.

- 2. Define the sequence $A_k^{(1)}, \dots, A_k^{(3N)}$ as in (53).
- 3. Set $A_{k+1} := A_k^{(3N)}$ and continue with the next sweep.

The Jacobi algorithm generates a sequence of elementary unitary matrices $\theta_k \in SU_{\text{loc}}(2^N), k \in \mathbb{N}$, converging – supported by numerical experiments – to a local maximum $U := \prod_{k=1}^{\infty} \theta_k$ of the trace function.

Orthogonality of the maximizing directions Ω_i with respect to the Hessian of f at a local maximum would lead to local quadratic convergence of the algorithm, see [9], [11]. In our case, this is unfortunately not guaranteed and therefore the Jacobi algorithm converges in general only linearly. We leave it as an open problem to find a clever choice of basis vectors $\{\Omega_1, \dots, \Omega_{3N}\}$ that are orthogonal with respect to the Hessian.

IV. NUMERICAL EXPERIMENTS

In this section we present a few numerical experiments. A comparison of the Euler step discretization of the gradient flow and the Jacobi-type method is presented. The former one is visualized in Fig. 3 for example 2.2.

Both algorithms have been implemented in MATHEMAT-ICA 5.2. The partial maximization steps, cf. (53), have been done using the MATHEMATICA-command FindMaximum with initial condition t = 0. In Fig. 4, N = 5 and C has (1,1)-entry equal to 1 and zeros elsewhere. The matrix A is Hermitian and diagonalizable by local transformations. Its eigenvalues are randomly chosen integers ranged between -10 and 30. In Fig. 5, again N = 5 and the entries of the real as well as of the imaginary part of A and C are realizations of a standard normal distributed random variable. Note, that for a visualization of the Jacobi method, one step corresponds to one single step within a sweep, i.e. in the above cases, one sweep consists of 32 steps.

Unfortunately, both algorithms occasionally get stuck in points that are not global maxima. We take that as an indication that the trace function possesses local maxima that are not global ones.



Fig. 3. The gradient flow for Example 2.2.



Fig. 4. N = 5, C is non-zero only in (1, 1)-entry, where $C_{11} = 1$; A diagonalizable by fast transformations; solid line = Jacobi-type method; dashed line = Euler step discretization of the gradient flow.

V. CONCLUSIONS

We have introduced a new mathematical object, the *local* C-numerical range $W_{\text{loc}}(C, A)$. It has been shown that $W_{\text{loc}}(C, A)$ has a rather complex geometry. Two intrinsic numerical algorithms have been proposed to obtain sharp bounds on the size of $W_{\text{loc}}(C, A)$. Moreover, the second one additionally yields a local unitary propagator solving an underlying quantum control problem. Numerical experiments have indicated that both methods apparently can get stuck in local maxima. This gives rise to future work.

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Fig. 5. N = 5, C, A randomly chosen; solid line = Jacobi-type method; dashed line = Euler step discretization of the gradient flow.

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