Computational complexity of quantum optimal control landscapes

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We study the Hamiltonian-independent contribution to the complexity of quantum optimal control problems. The optimization of controls that steer quantum systems to desired objectives can itself be considered a classical dynamical system that executes an analog computation. The system-independent component of the equations of motion of this dynamical system can be integrated analytically for various classes of discrete quantum control problems. For the maximization of observable expectation values from an initial pure state and the maximization of the fidelity of quantum gates, the time complexity of the corresponding computation belongs to the class continuous log (CLOG), the lowest analog complexity class, equivalent to the discrete complexity class NC. The simple scaling of the Hamiltonian-independent contribution to these problems with quantum system dimension indicates that with appropriately designed search algorithms, quantum optimal control can be rendered efficient even for large systems.

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I. INTRODUCTION

In recent years the methodology of optimal control theory has been applied to achieve various objectives in quantum systems. The two most common objectives are the maximization of the expectation value of an observable, and the maximization of the fidelity of a unitary transformation of the wavefunction. Whereas the maximization of observable expectation values has met with widespread success in experimental and computational incarnations [1], the achievement of high fidelity unitary transformations has proven more challenging [2], especially for large systems. However, it is not clear whether these apparent distinctions are specific to the algorithms employed, or whether they are indicative of universal and inherent features of the quantum optimization problems.

Given the computational expense of propagating the Schrödinger equation, the scaling with system size of the expense of executing a search over the space of control fields – referred to as the problem’s computational complexity – plays an essential role in determining the feasibility and efficiency of control optimizations in large quantum systems. The complexity of control optimization for quantum gates is of particular interest, as it corresponds to the classical complexity associated with the physical implementation of quantum logical operations. Recent studies have addressed the computational complexity (and related, the critical topology) of several associated problems in quantum information science, including quantum state and process identification [3]. In contrast to these tasks, the variational problem of quantum control optimization occurs on an infinite-dimensional parameter space. However, for discrete quantum systems, both the complexity and critical topology of quantum control problems can be divided into finite- and infinite-dimensional contributions, simplifying their study.

Consider first the critical topology of quantum control variational problems. Denoting the cost functional by $J$ and the control field by $\varepsilon(t)$, we have according to the chain rule

$$\frac{\delta J}{\delta \varepsilon(t)} = \frac{dJ}{dU(T)} \cdot \frac{\delta U(T)}{\delta \varepsilon(t)},$$

where $U(T)$ is the dynamical propagator resulting from application of the control $\varepsilon(t)$ over the time interval $0 \leq t \leq T$. As such, the critical points of quantum control problems fall into two classes. The first type of minimizer corresponds to those control Hamiltonians that are critical points of the control objective functional, but are not critical points of the map between control fields and associated dynamical propagators (i.e., points at which $\frac{dJ}{dU(T)} = 0$, while the Frechet derivative mapping from the control variation $\delta \varepsilon(t)$ to $\delta U(T)$ at $t = T$ is surjective). These critical points are called normal extremal controls. The second type of minimizer corresponds to critical points of the latter map (i.e., points at which the mapping from $\delta \varepsilon(t)$ to $\delta U(T)$ is not locally surjective). These latter points are referred to as abnormal extremal controls. For several low-dimensional quantum control problems, it has been shown that abnormal extremals are particularly scarce [4, 5, 6], suggesting that the normal extremal controls dominate the critical point topology of these problems.

As such, attention has focused on characterizing the system-independent (or kinematic) contribution to the critical topology of quantum optimal control problems [2, 3, 4]. For a given quantum system, several different classes of quantum control problems may be envisioned, each of which has its own associated kinematic critical topology. Besides the distinction between quantum gate and observable control, observable control itself may be subdivided into several qualitatively distinct optimization problems, depending on the initial state (density...
II. CONTROL OPTIMIZATION AS A DYNAMICAL SYSTEM

A universal quantum optimal control cost functional can be written as:

\[
J = \Phi(U(T), T) - \text{Re} \text{Tr} \left[ \int_0^T \left\{ \left( \frac{dU(t)}{dt} + \frac{i}{\hbar} H(\varepsilon(t))U(t) \right) B(t) \right\} dt \right] - \lambda \int_0^T \frac{1}{s(t)} |\varepsilon(t)|^2 dt
\]

where \( B(t) \) is a Lagrange multiplier constraining the quantum system dynamics to obey the Schrödinger equation, \( \varepsilon(t) \) denotes the time-dependent control field, \( s(t) \) denotes the pulse envelope, and \( \Lambda \) weights the importance of the penalty on the total field fluence. Solutions to the optimal control problem correspond to \( \frac{\delta J}{\delta \varepsilon(t)} = 0 \).

The problem of maximizing the expectation value of an observable corresponds to:

\[
\Phi_1(U) = \text{Tr}(U(T) \rho_0 U^\dagger(T) \Theta)
\]

where \( \rho_0 \) is the initial density matrix of the system and \( \Theta \) is an arbitrary observable operator, and the problem of maximizing the fidelity of a dynamical transformation \( W \) then corresponds to [2]:

\[
\Phi_2(U) = \text{Re} \text{Tr}(AW^\dagger U(T))
\]

where \( W \) is the target unitary transformation and \( A \) is any Hermitian matrix. In the present study, we ignore the fluence penalty term because its effect is system-specific and not revealing with respect to the universal complexity of quantum control problems.

We are interested in the convergence to the global optimum of the gradient flow trajectories of the objective functions, which are the solutions to the differential equations

\[
\frac{d\varepsilon(s, t)}{ds} = \nabla \Phi(\varepsilon(t)) = \alpha \frac{\delta \Phi_1(\varepsilon, s, t)}{\delta \varepsilon(s, t)}
\]

where \( s \) is a continuous variable parametrizing the algorithmic time evolution of the search trajectory and \( \alpha \) is an arbitrary scalar that we will set to 1. The complexity of quantum control optimization is associated with the scaling with system size of the rate of convergence of the function

\[
\Phi_1(s, T) - \Phi_1(\infty, T) = \alpha \int_0^T ds \int_0^T dt \left[ \frac{\delta \Phi_1(s', t)}{\delta \varepsilon(s', t)} \right]^2
\]

to zero. The gradients \( \frac{\delta \Phi_1}{\delta \varepsilon(t)} \) can be shown to be, respectively [10, 11, 12]:

\[
\frac{\delta \Phi_1}{\delta \varepsilon(t)} = \text{Tr}(\{\Theta(T), \rho_0\} \mu(t)),
\]

and

\[
\frac{\delta \Phi_2}{\delta \varepsilon(t)} = \text{Tr} \left( (AA^\dagger W^\dagger U - U^\dagger W A^\dagger) \mu(t) \right),
\]

within the electric dipole approximation, where \( \mu(t) = -\frac{i}{\hbar} U(t, 0) \mu_0 U(t, 0) \) is the time-evolved dipole operator of the quantum system and we have adopted the shorthand notation \( U \equiv U(T) \).

The gradient on \( \varepsilon(t) \) is related to the gradient on \( U(N) \) through

\[
\frac{\delta \Phi_1}{\delta \varepsilon(t)} = \sum_{ij} \frac{\delta U_{ij}}{\delta \varepsilon(t)} \frac{d\Phi_1}{dU_{ij}}
\]

Now suppose that we have the gradient flow of \( \varepsilon(s, t) \) that follows [1] and let \( U(s) \), the system propagator at time \( T \) driven by \( \varepsilon(s, t) \), be the projected trajectory on the unitary group \( U(N) \). The (algorithmic) time derivative of \( U(s) \) is then

\[
\frac{dU_{ij}(s)}{ds} = \int_0^T \frac{dU_{ij}(s)}{dt} \frac{\delta \varepsilon(s, t)}{\delta \varepsilon(s, t)} dt
\]

which, combined with [11] and [7], gives

\[
\frac{dU_{ij}(s)}{ds} = \int_0^T \frac{dU_{ij}(s)}{dt} \sum_{p,q} \frac{\delta U_{pq}(s)}{\delta \varepsilon(s, t)} \frac{d\Phi_1}{dU_{pq}} dt.
\]

It is convenient to write this equation in vector form, replacing the \( N \times N \) matrix \( U(s) \) with the \( N^2 \) dimensional vector \( u(s) \):

\[
\frac{du(s)}{ds} = \left[ \int_0^T \frac{d\varepsilon(s, t)}{\delta \varepsilon(s, t)} \frac{d\varepsilon(s, t)}{\delta \varepsilon(s, t)} dt \right] \nabla \Phi [u(s)]
\]

\[
\equiv G[\varepsilon(s, t)] \nabla \Phi [u(s)]
\]

where the superscript \( T \) denotes the transpose. This relation implies that the variation of the propagator in \( U(N) \) caused by the natural gradient flow in the space of control fields is Hamiltonian-dependent, where the influence of the Hamiltonian is contained in the \( N^2 \)-dimensional symmetric matrix \( G[\varepsilon(s, t)] \). Within the electric dipole approximation, \( G \) is given by

\[
G_{ij,pq}(s) = \int_0^T \mu_{ij}(s, t) \mu_{pq}(s, t) dt.
\]
As we will discuss below, it is possible to eliminate \( G \) in this differential equation, and hence to explicitly follow the \( U(T) \) gradient flow, by adopting an alternative algorithmic step on \( \varepsilon(t) \). Importantly, the properties of the map \( \varepsilon(t) \rightarrow U(T) \) for finite-dimensional quantum systems render this fairly simple to achieve across many diverse systems, albeit with an error that is Hamiltonian-dependent. For the present purpose, we can effectively ignore \( G \) because we are interested in comparing the complexity scalings of the flow trajectories for gate and observable control problems on the same quantum system. Averaged over many initial conditions, the time required for convergence of the \( U(T) \) gradient flows will determine this comparative scaling.

Because the kinematic gradient flows associated with these differential equations evolve on the continuous space of a Lie group (for \( \Phi_2 \)) or its adjoint orbit of skew-Hermitian matrices (for \( \Phi_1 \)), the optimization processes can be considered to be analog rather than discrete computations. In prior work [12], we demonstrated that these flow trajectories can in fact be viewed as dynamical systems whose equations of motion guide the algorithmic time evolution of gradient-based algorithms. We showed that although the infinite-dimensional gradient flow equations do not admit analytical solutions, the equations of motion for the gradient flow lines on the unitary group domain, namely

\[
\begin{align*}
\left( \frac{dU}{ds} \right)_1 &= -U[\rho_0, U^\dagger \Theta U], \\
\left( \frac{dU}{ds} \right)_2 &= A^\dagger - UAU
\end{align*}
\]

can in principle be exactly solved and explicitly integrated them for specific cases of interest. The solutions to the optimal control problem are the critical points of the flow, i.e., \( \nabla \Phi(U) = 0 \), or equivalently, the equilibria of the dynamical system. In this work, we use the integrated gradient flow equations to derive upper bounds on the time for convergence to the solutions of these problems and thereby assign the problems to computational complexity classes.

The possible outputs of the dynamical system executing the analog computation are the attracting fixed points of the gradient flow of the control objective functional. Just as a discrete computation can be assigned a measure of time complexity, i.e., the scaling with system size (e.g., polynomial or exponential) of the time required to solve the problem, analog computations can be assigned time complexities, which correspond to the scaling with system size of the time required for the dynamical system to converge to a vicinity of the optimal fixed point. Time complexity of an analog computation can be analytically determined for systems that are completely integrable; i.e., for those systems whose equations of motion can be exactly solved. For this purpose, we apply the recently developed theory of complexity for continuous time dynamics [13, 14].

For \( \Phi_1 \), the gradient flow evolves on a polytope whose dimension varies depending on the spectrum of \( \rho_0 \). Since the flow is cubic in \( U \), many trajectories \( U_1(s) \) correspond to the same function \( J(s) \). Rewriting the gradient flow as a quadratic function on the domain of Hermitian operators \( \rho_T = U(T)\rho_0 U^\dagger(T) [12] \), one can solve explicitly for a unique solution \( \rho_T(s) \) corresponding to \( J(s) \). In the case that \( \rho_0 \) has only one nonzero eigenvalue, corresponding to an initial pure state, we showed that under the change of variables \( \rho_T(s) \rightarrow |\psi(s)\rangle \langle \psi(s)| \), \( \rho_T(s) = (c_1(s), \cdots, c_N(s)) \), \( x(s) \equiv (|c_1(s)|^2, \cdots, |c_N(s)|^2) \), the gradient flow can be explicitly integrated to give [12]:

\[
x(s) = \frac{e^{2s\theta} \cdot (|c_1(0)|^2, \cdots, |c_N(0)|^2)}{\sum_{i=1}^N |c_i(0)|^2 e^{2s\lambda_i}} \]

\[
= \frac{e^{2s\lambda_1} |c_1(0)|^2, \cdots, e^{2s\lambda_N} |c_N(0)|^2}{\sum_{i=1}^N |c_i(0)|^2 e^{2s\lambda_i}}
\]

where \( \lambda_1, \cdots, \lambda_N \) denote the eigenvalues of \( \Theta \). The explicit solution for the gradient trajectory of objective functional \( \Phi_2 \) was shown to be

\[
W^\dagger U(s) = (\sinh(As) + \cosh(As)W^\dagger U_0) \cdot (\cosh(As) + \sinh(As)W^\dagger U_0)^{-1}
\]

where the initial condition is \( U_0 = U(0) [12] \).

In the case of objective functional \( \Phi_1 \), the input for the computation may be viewed as being the eigenvalues of the observable operator, while the initial density matrix determines the initial condition. For the purpose of assigning a complexity class to the problem, the latter is generally taken as fixed. The time complexity is then expressed as a function of the eigenvalues of \( \Theta \). However, as discussed below, the complexity of the optimal control problem can vary sharply as a function of the initial state as well. For objective functional \( \Phi_2 \), we consider the input for the computation to be the target unitary transformation \( W \). The time complexity is expressed in terms of the eigenvalues of \( W \). Again, time complexity can be modulated by varying the initial condition of the search away from the identity matrix \( I \).

It is possible to assess the convergence of the optimal control search in terms of the difference in objective function values \( \Phi(s) - \Phi(\infty) \), but because of the degeneracy of solutions corresponding to a given value of \( \Phi \), a more precise assessment of complexity can be achieved in terms of the convergence of the distance between the current guess and the global solution to the problem. As mentioned, the distance \( ||E(s) - E(\infty)||^2 = \int_0^T E(s,t)E(\infty,t)dt \) is not an appropriate measure because it is highly system-specific (precluding uniform behavior as a function of system size) and obscures the underlying geometry of convergence since \( \Phi \) is not explicitly a function of \( E(t) \). The most appropriate choice is a distance on the space of solutions that displays the lowest degeneracy for a given value of \( \Phi \), while remaining independent of the system Hamiltonian. For \( \Phi_1 \),
this distance is \( |U(s) - U(\infty)|^2 \), whereas for \( \Phi_2 \), it is the Euclidean distance on the polytope wherein the flow evolves.

The attracting region \( R \) of an attracting fixed point is the subset of phase space wherein the distance to the point is monotonically decreasing with time. We consider the quantum control optimization problem to be solved to a desired precision, and the computation halted, if the gradient flow trajectory enters within an \( \epsilon_p \)-radius of the global optimum and is also within its attracting region. This definition ensures that for inputs on which the \( \epsilon_p \)-vicinity of the attractor is larger than the attracting region, entrance into the attracting region is required for halting of the computation. The computational complexity of the control optimization algorithm is then defined as the scaling with system size of the convergence time \( t_c(H) = \max [t_c(e), t_c(R)] \) to the intersection of the attracting region and the ball of radius \( \epsilon_p \), starting from a given initial condition.

### III. ANALOG COMPLEXITY OF QUANTUM CONTROL OPTIMIZATION

#### A. Quantum observable maximization

For optimization of \( \Phi_1 \) starting from an initial pure state, we can establish a bound on \( t_c(e) \) as follows. We assume without loss of generality that the eigenvalues of \( \Theta \) are arranged such that \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_N \). For nondegenerate \( \Theta \), the global optimum is then the unit vector \( e_{i^*} = e_1 \) and the distance of the current point \( x(s) \) on the search trajectory to the global optimum can be written:

\[
||x(s) - x(\infty)||^2 = \nonumber \]

\[
||x(s)||^2 - 2 \frac{e^{2s\lambda_1} |c_1(0)|^2 \cdots e^{2s\lambda_N} |c_N(0)|^2 \cdot e_1}{\sum_{i=1}^N |c_i(0)|^2 e^{2s\lambda_i}} + 1 \leq 2 - 2 \frac{e^{2s\lambda_1} |c_1(0)|^2}{\sum_{i=1}^N e^{2s\lambda_i} |c_i(0)|^2} \tag{14}
\]

since \( \sum_{i=1}^N x_i = \sum_{i=1}^N c_i^2 \equiv 1 \) and therefore \( \sum_{i=1}^N x_i^2 = \sum_{i=1}^N c_i^2 \leq 1 \). Defining \( \mu \equiv \lambda_1 - \lambda_2 \), we then have

\[
\sum_{i=1}^N e^{2s(\lambda_i - \lambda_1)} |c_i(0)|^2 \leq e^{-2\mu s} + |c_1(0)|^2
\]

such that the bound on the distance to the solution becomes

\[
||x(s) - x(\infty)||^2 \leq 2 - 2(1 + e^{-2\mu s} |c_1(0)|^{-2})^{-1}.
\]

For simplicity, we choose the identity vector \( \frac{1}{\sqrt{N}}(1,\ldots,1) \) as the initial state. More generally, \( x_{i^*}(0) \) will scale inversely with \( N \) for randomly chosen initial conditions on the interior of the simplex. We then obtain the following bound on the convergence time to the global optimum:

\[
t_c(e) \leq \frac{\ln(\frac{2(c_1(0)^2)}{2\mu})}{2\mu} = \frac{1}{2\mu} \ln \left( \frac{2N}{\epsilon^2} \right)\nonumber
\]

for \( \epsilon \) small. Note that the time scale for convergence to the global optimum (the linearization of the coefficient in the exponential) is given by \( \mu \). This is equal to the lowest eigenvalue of the Hessian of the objective function, \( \mathcal{H}_A(\rho(\infty)) = -\sum_{j \neq 1} (\alpha_j^2 + |\beta_j|^2)(\lambda_j - \lambda_1) \), where \( \alpha_{jk}, \beta_{jk} \) are the real, complex parts of an arbitrary Hermitian matrix \( A \), obtained in [12]. If the maximum eigenvalue of \( \Theta \) is degenerate with multiplicity \( k \), such that \( \lambda_1 = \lambda_2 = \cdots = \lambda_k \), and \( \lambda_k > \lambda_j, \ j = k + 1, \cdots, N \), then the dynamics converges to the point \( \frac{1}{k}(1, \cdots, 1, 0, \cdots, 0) \) [12]. In this case, the distance to the global optimum becomes

\[
||x(s) - \frac{1}{k}(1, \cdots, 1, 0, \cdots, 0)||^2 \leq 2 - 2 \frac{e^{2s\lambda_1} \sum_{i=1}^k |c_i(0)|^2}{\sum_{j=1}^N e^{2s\lambda_j} |c_j(0)|^2} \tag{15}
\]

corresponding to

\[
t_c(e) \leq \frac{1}{2\mu} \ln \left( \frac{2Nk}{\epsilon^2} \right).
\]

A bound on the convergence time to the attracting region of the solution, \( t_c(R) \), can be derived as follows for the general case of a \( k \)-fold degenerate maximal eigenvalue of \( \Theta \). Again, without loss of generality, we assume \( \lambda_1 = \cdots = \lambda_k > \lambda_{k+1} > \cdots > \lambda_N \). In the present case, \( t_c(R) = t_c \) such that for all \( s > t_c \):

\[
\frac{\partial}{\partial s} ||x(s) - x(\infty)||^2 = \nonumber
\]

\[
e^{2s\lambda_1} \sum_{i=1}^k |c_i(0)|^2 \sum_{j=1}^N ((\lambda(1) - \lambda_j)e^{2s\lambda_j}|c_j(0)|^2) < 0.
\]

This corresponds to the condition \( \dot{x}_i < 0 \) for \( i > k \) [12]. This condition holds iff \( \sum_{j=1}^N \lambda_j x_j > \lambda_i, \ i = k + 1, \cdots, N \). Insertion of the analytical solution above gives

\[
\sum_{j=1}^N \lambda_j |c_j(0)|^2 e^{\lambda_j s} > \lambda_{k+1} \sum_{j=1}^N |c_j(0)|^2 e^{\lambda_j s}.
\]

For the purposes of obtaining a bound on \( t_c \), we can rewrite this

\[
\sum_{i=1}^k (\lambda(1)|c_i(0)|^2 - \lambda_{k+1}|c_{k+1}(0)|^2)e^{\lambda(1)t_c} > (N - k - 2)\lambda_{k+1}|c_{k+1}(0)|^2 e^{\lambda_{k+1}t_c}, \tag{17}
\]

1 It can be shown that the expression derived in [8] for \( \mathcal{H}_A(\mathcal{U}(\infty)) \) is equivalent to that for \( \mathcal{H}_A(\rho(\infty)) \).
which can be solved for \( t_c(R) \) to give:

\[
t_{c,1}(R) \leq \frac{1}{\lambda(1) - \lambda_{k+1}} \ln \left\{ \frac{(N - k - 2)\lambda_{k+1}|c_{k+1}(0)|^2}{\sum_{i=1}^{k} |\lambda(1)c_{i}(0)|^2 - \lambda_{k+1}|c_{k+1}(0)|^2} \right\}. \tag{18}
\]

Therefore, the attracting region of the solution \( x(\infty) = \frac{1}{2}(1, \cdots, 1, 0, \cdots, 0) \) does not cover the entire domain. Again taking the initial condition \( \frac{1}{2}(1, \cdots, 1, 0) \), this bound becomes \( t_{c,1}(R) \leq \frac{1}{\mu} \ln \left( \frac{(N-k-2)\lambda_{k+1}}{k(\lambda_{k+1} - \lambda_{k+1})} \right) \). The upper bound on the computation time of the problem is then given by

\[
t_{c,1}(H) = \max \{ t_{c,1}(\epsilon), t_{c,1}(R) \} \leq \frac{1}{2\mu} \ln \left( \frac{2Nk}{\epsilon^2} \right) + 2 \ln \left( \frac{(N - k - 2)\lambda_{k+1}}{k(\lambda(1) - \lambda_{k+1})} \right). \tag{19}
\]

### B. Quantum gate control

For objective function \( \Phi_2 \), the control optimization is generally initiated with \( U_0 \) at or near the identity transformation \( I_N \), such that \( W^\dagger U_0 = W^\dagger \). Writing \( U'(s) \equiv W^\dagger U(s) \), the solution to the problem then corresponds to \( U'(\infty) = I_N \). We consider the special case where the Hermitian matrix \( A = I \):

\[
U'(s) = (\sinh(sI) + \cosh(sI)W^\dagger)(\cosh(sI) + \sinh(sI)W^\dagger)^{-1}
\]

For \( \Phi_2 \), the natural distance measure for assessment of convergence is given by the Frobenius matrix norm between the current transformation \( U'(s) \) and the solution \( I_N \):

\[
||U'(s) - U'(\infty)||_F^2 = \text{Tr}[(U'(s) - I_N)^\dagger(U'(s) - I_N)]
\]

Diagonalizing \( W \) via the unitary transformation \( V \), we have

\[
W = V^\dagger AV
\]

where \( \Lambda \) is the matrix of eigenvalues of \( W \),

\[
\Lambda = \begin{pmatrix}
e^{-i\theta_1} & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
e^{-i\theta_N} & \cdot & \cdot
\end{pmatrix}
\]

We previously showed \[12\] that this transformation allows the expression above to be simplified as

\[
||U'(s) - I_N||^2 = \sum_{k=1}^{N} \left| \frac{\tanh s + e^{-i\theta_k} - 1}{1 + e^{-i\theta_k} \tanh s} \right|^2 = \sum_{k=1}^{N} \frac{2(1 - \cos \theta_k)}{1 + 2 \tanh s \cos \theta_k + \tanh^2 s} (1 - \tanh s)^2 \tag{21}
\]

The partial derivative of each term in this expression with respect to \( \cos \theta_k \) monotonically decreases with \( \cos \theta_k \), so the greatest term in the sum will correspond to the lowest value of \( \cos \theta_k \), denoted \( \cos \theta_0 \). Therefore, the sum is bounded from above by \( N \)-times the term corresponding to \( \theta_0 \),

\[
||U'(s) - I_N||^2 \leq N \frac{2(1 - \cos \theta_0)}{1 + 2 \tanh s \cos \theta_0 + \tanh^2 s} (1 - \tanh s)^2
\]

Under the change of variables \( x = \tanh s \), the condition for entering an \( \epsilon \)-vicinity of the solution is

\[
N \frac{2(1 - \cos \theta_0)}{1 + 2x \cos \theta_0 + x^2 (1 - x)^2} < \epsilon.
\]

To derive tight upper bounds on \( x_c \) and hence \( t_c \), we must therefore solve the quadratic equation \( (2N - 2N \cos \theta_0 - \epsilon)x_c^2 + (4N \cos \theta_0 - 4N - 2 \epsilon \cos \theta_0)x_{c,\text{max}} + (2N - 2N \cos \theta_0 - \epsilon) = 0 \). The solutions to this equation are:

\[
x_{c,\text{max}} = \tanh t_{c,\text{max}} = \frac{4N - 4N \cos \theta_0 + 2\epsilon \cos \theta_0 \pm \sqrt{(\epsilon^2 - 4N \epsilon)(\cos^2 \theta_0 - 1)}}{4N - 4N \cos \theta_0 - 2\epsilon}.
\]

One solution gives identically \( x_{c,\text{max},+} = 1 \), corresponding to \( t_{c,\text{max},+} = \infty \), which only provides an upper bound on the convergence time. The other solution gives \( x_{c,\text{max},-} \leq 1 \), \( t_{c,\text{max},-} \leq \infty \). In order to study the scaling of \( t_{c,\text{max},-} \) with the dimension of the system, we consider the deviation of \( x_{c,\text{max},-} \) from 1:

\[
\delta \equiv 1 - x_{c,\text{max},-} = \frac{2\epsilon(1 - \cos \theta_0) + \sqrt{(\epsilon^2 - 4N \epsilon)(\cos^2 \theta_0 - 1)}}{4N(1 - \cos \theta_0) + 2\epsilon} \approx \frac{\sin \theta_0}{1 - \cos \theta_0} \sqrt{\frac{\epsilon}{N}} = a \sqrt{\frac{\epsilon}{N}} \tag{22}
\]
for small $\epsilon$. This corresponds to

$$t_c(\epsilon) \leq t_{c,\text{max,}-}(\epsilon) = \ln \left( \frac{1 + x_{c,\text{max,}-}}{1 - x_{c,\text{max,}-}} \right) = \ln \left( \frac{2 - \delta}{\delta} \right) \approx \ln \left( \frac{2 - a\sqrt{c_0}}{a\sqrt{c_0}} \right) = \frac{1}{2} \ln \left( \frac{4N}{a^2\epsilon} \right) \quad (23)$$

For $\Phi_2$, the distance to the solution $U'(T) = I_N, U(T) = W^\dagger$ is a monotonically decreasing function of algorithmic time $s$ [12], and hence in this case, the attracting region of the solution covers the entire manifold $U(N)$ and $t_c(R) = 0$. Thus, an upper bound on the computation time for the problem is

$$t_{c,2}(H) = t_{c,2}(\epsilon) \leq \frac{1}{2} \ln \left( \frac{4N}{a^2\epsilon} \right) \quad (24)$$

for small $\epsilon$.

C. Assignment to complexity classes

A continuous time problem is said to be in the complexity class CLOG (continuous log) if it has a polynomial number of variables (here, the system dimension) and a logarithmic time complexity. Kinematic optimization of objective functions $\Phi_1$ and $\Phi_2$ therefore belong to the complexity class CLOG. CLOG is the analog counterpart of the classical complexity class NC$_1$, the class of problems that can be efficiently solved on a discrete parallel computer, meaning problems that are decidable in polylogarithmic time on a parallel computer with a polynomial number of processors. It is the lowest time complexity class, lying immediately below P (polynomial time complexity). For real control optimization algorithms evolving in discrete time, the kinematic component of these problems will have NC$_1$ complexity.

Quantum optimal control problems aimed at maximizing the expectation value of any observable operator starting from a pure state of the system all belong to the same analog time complexity class. However, their characteristic time scale for exponential convergence, when the optimization algorithm follows the gradient flow trajectories as faithfully as possible, differs in a predictable fashion. Specifically, the characteristic time scale for exponential convergence is given by $\min_{j \neq 1} |\lambda_j - \lambda_1|$, i.e., the magnitude of the difference between the largest and second largest eigenvalue of the observable operator. This corresponds to the magnitude of the smallest Hessian eigenvalue of the objective functional near the solution. As such, the rate of convergence for the problem of driving a pure initial state to a pure final state - which corresponds to $\lambda_1 = 1, \lambda_i = 0 \; \forall i > 1$ above - is the greatest, such that this problem has the lowest computational complexity of all observable maximization problems. The complexity classes corresponding to observable maximization problems starting from general mixed states may differ and are expected to be higher, as evidenced by 1) the factorial (vs exponential) scaling of the number of critical manifolds [8] and 2) the fact that the gradient flow evolves on a higher dimensional polytope [11, 12].

Similarly, the kinematic component of the problem of optimizing controls for the implementation of a quantum gate belongs to the complexity class CLOG irrespective of the identity of the target gate $W$. In contrast to observable expectation value maximization, however, the characteristic time scale for exponential convergence to the solution of quantum gate optimization does not vary directly as a function of the particular incarnation of the problem embodied in the choice of $W$, since the eigenvalues of the Hessian matrix do not vary as a function of the eigenvalues of $W$ [9]. Nonetheless, the eigenvalue spectrum of $W$ does affect the convergence time indirectly in conjunction with the initial guess $U_0$.

Although the problems belong to the same complexity class with respect to the scaling of the number of iterations required as a function of system size, they display distinct behavior in other regards. In particular, it can be shown [12] that for both problems, there exists a set of initial conditions from which the flow does not converge to the solution. For $\Phi_2$, this corresponds to the case where $\cos \theta_0 = -1$, resulting in $x_{c,-} = 1, t_{c,-} = \infty$. Thus, if $W$ has at least one eigenvalue equal to $-1$, the optimization does not converge if $U_0$ is chosen as $I$, since $U'(0) = WU_0 = W^\dagger$. For $\Phi_1$, initial conditions where $c_\ast = 0$ (i.e., where the initial state resides on the so-called basin boundary of the simplex) do not converge. The scaling of the convergence time as a function of the distance to this pathological initial condition differs for the two problems [12]. In these cases, the initial guess $U_0$ should be modulated to facilitate the convergence of gradient algorithms.

The complexity of optimal control landscapes for the optimization of quantum gates scales linearly with the number of qubits. If the problem size is measured in qubits, optimization of $\Phi_2$ belongs to the complexity class CP (continuous P), the set of problems with a polynomial number of variables and polynomial time complexity on a continuous variable computer. CP is the analog counterpart of the discrete complexity class P. In previous work aimed at optimizing quantum gates through OCT, the scaling of the number of control field iterations was reported to be exponential in the number of qubits [13]. In these studies, the gradient flow was not followed directly by the optimization algorithm. The results here suggest that exponential speedup should in principle be possible for the implementation of quantum gates through the use of algorithms that follow the gradient flow on the unitary group.

As such, a central issue concerns the accessibility of these lower bounds on scaling through the design of gradient-based algorithms in both the laboratory and in simulations. These continuous time complexities represent lower bounds on the complexities actually achieved by discretized Euclidean search algorithms that do not precisely follow the Riemannian curvature of the gradi-
ent flow trajectories. The increase in complexity induced by (Euclidean) discretization depends on the curvature of the trajectory. A quantitative analysis is beyond the scope of the current work, but the path length of the gradient flow trajectory offers insight into its geometry. On the unitary group $U(N)$, the path length of the gradient flow trajectory is given by

$$\int_0^{t_c} \sqrt{\text{Tr}(\dot{U}(s)\dot{U}(s))} ds,$$

where the Riemannian metric on the unitary group is defined as $(A, B) = \text{Tr}(A^\dagger B)$. For the optimization $\Phi_2$, this integral can be shown to be

$$L(U_0, t_c) = 2 \int_0^{t_c} \sqrt{N - \text{Re} \text{Tr} [(W^\dagger U)^2]} ds,$$

which can be expressed as a sum of $N$ scalars:

$$L(U_0, t_c) = 2 \int_0^{t_c} ds \left( \sum_{k=1}^{N} \frac{2 \sin^2 \theta_k (1 - \tanh^2 s)^2}{(1 + \tanh^2 s)^2 + 4 \tanh s \cos \theta_k} \right).$$

Again setting $x = \tanh t$, the integrand can be further simplified using the relation

$$\sqrt{\frac{2N \sin^2 \theta_k (1 - x^2)^2}{(1 + x^2)^2 + 4x [\cos \theta_k + (1 + x^2) \cos \theta_k]}},$$

which can be expressed as a sum of $N$ scalars:

$$\sqrt{\frac{2N \sin^2 \theta_k (1 - x^2)^2}{(1 + x^2)^2 (1 - x)}},$$

Then we have

$$L(U_0, t_c) \leq \sqrt{2N |\sin \theta|} \int_0^{x_c} \frac{(1 - x^2)}{(1 + x^2)\sqrt{1 - x}} d\ln \left( \frac{1 + x}{1 - x} \right)$$

$$= 2\sqrt{2N |\sin \theta|} \int_0^{x_c} \frac{dx}{(1 + x^2)\sqrt{1 - x}}$$

$$< 2\sqrt{2N |\sin \theta|} \int_0^{x_c} \frac{dx}{1 + x^2}$$

$$= 2\sqrt{2N |\sin \theta|} \arctan x_c$$

$$< \pi \sqrt{2N |\sin \theta|} \frac{1}{\sqrt{1 - x_c}} \sim |\sin \theta|^{-1/4} N^{3/4}.$$

Therefore, we see that the path length - which unlike the convergence time, does not depend directly on the magnitude of the gradient and hence is less sensitive to the effects of discretization - scales approximately linearly with $N$, roughly consistent with the scaling observed in kinematic simulations of this objective [16].

**IV. DISCUSSION**

The complexity results derived herein are based on analysis of the kinematic contribution to optimal control gradient flows, and have neglected the dynamical contribution of the $\varepsilon(t) \rightarrow U(T)$ map to the scaling of search effort. For an arbitrary Hamiltonian, if one averages over many initial conditions and target gates/states, the relative convergence times of gate and state control optimization should correspond to those of the kinematic gradient flows [12]. However, since the Hamiltonian, and hence the properties of the $\varepsilon(t) \rightarrow U(T)$ map must change with system dimension, the absolute scaling for either problem may in principle deviate from that predicted here. The primary importance of the above results is that the relative complexity scaling of these two problems will nonetheless be identical, since the contributions of the functional derivatives $\frac{\delta U(T)}{\delta \varepsilon(T)}$ to scaling, averaged over initial conditions and target gates, will be the same for each. As such, quantum pure state and gate control problems do belong to the same complexity class.

From a practical perspective, since the kinematic complexity of these problems is as low as possible, the scaling of control search effort should not prohibit the efficient application of gradient-based algorithms to high-dimensional systems. For state-to-state coherence transfer problems, this prediction is borne out by both simulations and experimental evidence [10]. However, the reported scaling of gate optimization simulations [2] is worse than that predicted according to the present theory, suggesting that a reexamination of current quantum gate control algorithms is warranted. For control problems whose kinematic complexity class exceeds CLOG, it may be advantageous to apply matrix tracking algorithms (below) rather than gradient-based algorithms in order to achieve the above lower bounds. Evidence suggests that observable maximization problems starting from an initial nondegenerate mixed state belong to this category [17].

For general $\rho_0$ and $\Theta$, the gradient flow for objective function $\Phi_1$ is an "isospectral" flow [13, 19, 20]. In $N$ dimensions, this flow has $N$ integrals of the motion that are in involution, which is the classical definition of complete integrability for a dynamical system. From the point of view of the modern theory of integrable systems, the
double bracket flow can be shown to represent a type of Lax pair, a general form that can be adopted by all completely integrable dynamical systems [21]. As such, the system-independent complexity of all discrete quantum observable maximization problems can in principle be analytically determined [12]. In contrast, the kinematic gradient flows of the gate and observable control problems in classical mechanics [4, 22] are not integrable, and hence cannot be assigned to analytic complexity classes.

In the present work, we have focused attention on the complexity of optimizations that employ local gradient search algorithms. The favorable scaling of the convergence times for kinematic gradient flows, and the scarcity of abnormal extremals in discrete quantum control problems [4] motivate a rigorous definition of the universal complexity of quantum control problems in terms of the scaling of the expense of tracking such kinematic paths through elimination of the Hamiltonian-dependent matrix $G$ in the algorithmic step (10). These global algorithms require an additional computational overhead of $N^4$ in order to invert the matrix $G$, as well as overhead for statistical estimation of the states or dynamical propagators based on experimental observations [4]. Assignment of quantum control problems to complexity classes based on the convergence of such global algorithms, which involves extensive sampling over Hamiltonian space, is the subject of a separate work [23].

[1] M. Shapiro and P. Brumer, Phys. Rep. 425, 195 (2006).
[2] Palao and R. Kosloff, Phys. Rev. Lett. 89, 1883011 (2002).
[3] M. Mohseni, A. T. Rezakhani, and D. A. Lidar, eprint quant-ph/0702131 (2007).
[4] R. Chakrabarti and H. Rabitz, Int. Rev. Phys. Chem. 26 (2007).
[5] R. Wu and H. Rabitz, in preparation (2007).
[6] D. D’Alessandro and M. Dahleh, IEEE Trans. Autom. Control 46, 866 (2001).
[7] H. Rabitz, M. Hsieh, and C. Rosenthal, Science 303, 1998 (2004).
[8] M. Hsieh, R. Wu, and H. Rabitz, J. Chem. Phys. 51, 204107 (2006).
[9] H. Rabitz, M. Hsieh, and C. Rosenthal, Phys. Rev. A 72, 052337 (2005).
[10] T. Ho and H. Rabitz, J. Photochem. Photobiol. A 180, 226 (2006).
[11] T. Ho, In preparation (2007).
[12] R. Chakrabarti, R. Wu, and H. A. Rabitz, eprint arXiv:0708.3384 (2007).
[13] H. Siegelmann, A. Ben-Hur, and S. Fishman, Phys. Rev. Lett. 83, 1463 (1999).
[14] A. Ben-Hur, H. Siegelmann, and S. Fishman, J. Complexity 18, 51 (2002).
[15] J. Palao and R. Kosloff, Phys. Rev. A 68, 062308 (2003).
[16] K. Moore, M. Hsieh, and H. Rabitz, To be submitted (2007).
[17] G. Rivillo, M. Hsieh, and H. Rabitz (2007).
[18] L. Faybusovich, Physica D 23, 309 (1991).
[19] A. Bloch, Contemp. Math. 114, 77 (1990).
[20] A. Bloch, *Hamiltonian and Gradient Flows, Algorithms and Control*, vol. 3 of Fields Institute Communications (Oxford University Press, Oxford, 1995).
[21] O. Babelon, D. Bernard, and M. Talon, *Introduction to classical integrable systems*, vol. 60 of Cambridge Monographs on Mathematical Physics (Cambridge, Cambridge, 2003).
[22] R. Wu, R. Chakrabarti, and H. Rabitz, eprint arXiv:0708.2118 (2007).
[23] R. Chakrabarti and H. Rabitz, In preparation (2007).