Forcing a unitary transformation by an external field: comparing two approaches based on optimal control theory.

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Abstract

A quantum gate is realized by specific unitary transformations operating on states representing qubits. Considering a quantum system employed as an element in a quantum computing scheme, the task is therefore to enforce the pre-specified unitary transformation. This task is carried out by an external time dependent field. Optimal control theory has been suggested as a method to compute the external field which alters the evolution of the system such that it performs the desired unitary transformation. This study compares two recent implementations of optimal control theory to find the field that induces a quantum gate. The first approach is based on the equation of motion of the unitary transformation. The second approach generalizes the state to state formulation of optimal control theory. This work highlights the formal relation between the two approaches.

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I. INTRODUCTION.

Quantum computation is based on implementing selected unitary transformations representing algorithms [1]. In many physical implementations the unitary transformation is generated using an external driving field. This driving field has to perform the quantum gate between, for example, two qubits, without altering the other levels which represent additional qubits. This means that the specific unitary transformation has to address a set of levels in an environment where other energy levels are present. An approach to correct this undesired coupling to other levels has been suggested for specific cases [2] but a general solution is not known.

The presence of a large number of levels coupled to the external driving field is specially relevant in the implementation of quantum computing in molecular systems [3, 4, 5]. Tesch et al. [5] proposed the use of optimal control theory (OCT) as a possible remedy. OCT [6] is a well developed approach that allows to obtain the driving field which induces a desired transition between preselected initial and final states. However, the dependence on the particular transitions (characterized by the initial and final states) makes the traditional formulation of OCT inappropriate for that purpose. For example, if the unitary transformation relates the initial states $\varphi_{ik}$ with the final states $\varphi_{fk}$ (the index $k$ denotes all the relevant states involved in the transformation), the traditional OCT approach derives an optimal field $\epsilon_k$ for each pair $\{\varphi_{ik}, \varphi_{fk}\}$. But the fields $\epsilon_k$ obtained are in general different, and then the transition induced by $\epsilon_k$ for the initial state $\varphi_{ik'}$ won’t necessarily give the right final state $\varphi_{fk'}$. To implement a given unitary transformation a single field $\epsilon$ that relates all the relevant pairs $\{\varphi_{ik}, \varphi_{fk}\}$ is needed.

An approach to overcome this problem was suggested in [7, 8]. The idea is to generalize OCT to deal directly with the evolution operator. Recently, a different approach using simultaneous optimization of several state to state transitions has been suggested by Tesch and Vivie-Riedle [9]. The purpose of this work is to compare the two approaches and two point the similarities and differences between them. This comparison has led to new insight into the use of optimal control theory for quantum systems.

Unitary transformation optimization can be formulated in the following way. We consider a quantum system with a Hilbert space of dimension $M$, expanded by an orthonormal basis of states $\{|k\rangle\}$ ($k = 1, ..., M$). In the following we will assume that the $k$ states
correspond to the free Hamiltonian proper states. The selected unitary transformation is imposed on the subspace of the first \( N \) energy levels of the system \((N \leq M)\). For example, the \( N \) levels could correspond to the physical implementation of the qubit(s) embedded in a larger system. The additional levels \((k = N + 1, \ldots, M)\) are not directly involved in the target unitary transformation and they are generally considered as “spurious levels” coupled to the field. However, it is not always the case: an example is the proposal of implementing quantum computation using rovibronic molecular levels. In the simplest description two electronic surfaces are considered. Two rovibronic states of one of the electronic surfaces are chosen as the implementation of a qubit (in this case \( N = 2 \)) and the unitary transformation is implemented using field induced transitions between the electronic surfaces. Out of the relevant subspace \((k = 3, \ldots, M)\) there are levels residing on both electronic surfaces, spurious in the sense that any leakage to them would destroy the desired final result, but at intermediate times they are used as intermediate storage which allow to carry out the desired unitary transformation [8, 10].

The optimization objective is to implement a selected unitary transformation in the relevant subspace at a final time \( T \). The target unitary transformation is represented by an operator in the system Hilbert space and denoted by \( \hat{\mathcal{O}} \). For \( N < M \), the matrix representation of \( \hat{\mathcal{O}} \) in the basis \( \{ |k\rangle \} \) has two blocks of dimension \( N \times N \) and \((M - N) \times (M - N)\). The elements connecting these blocks are zero. This structure means that population at the target time is not transferred between the two subspaces. Only the \( N \times N \) block is relevant for the optimization procedure, and the other block remains arbitrary.

The dynamics of the system is generated by the Hamiltonian \( \hat{\mathcal{H}} \),

\[
\hat{\mathcal{H}}(t; \epsilon) = \hat{\mathcal{H}}_0 - \hat{\mu} \epsilon(t),
\]

where \( \hat{\mathcal{H}}_0 \) is the free Hamiltonian, \( \epsilon(t) \) is the driving field and \( \hat{\mu} \) is a system operator describing the coupling (transition dipole operator in molecular systems). Eq. (1) can be generalized to more than one independent driving field, for example, controlling separately the two components of the polarization of an electro-magnetic field [11]. The dynamics of the system at time \( t \) is fully specified by the evolution operator \( \hat{\mathcal{U}}(t, 0; \epsilon) \). An optimal field \( \epsilon_{opt} \) induces the target unitary transformation \( \hat{\mathcal{O}} \) on the system, at time \( T \) if

\[
\hat{\mathcal{U}}(T, 0; \epsilon_{opt}) = e^{-i\phi(T)} \hat{\mathcal{O}}.
\]
Eq. (2) implies a condition only on the $N \times N$ block of the matrix representation of $\hat{U}$. The phase $\phi(T)$ is introduced to point out that in some cases the target unitary transformation $\hat{O}$ can be implemented up to an arbitrary global phase. The phase $\phi$ can be decomposed into two terms, $\phi_1(T) + \phi_2(T)$. The term $\phi_1$ originates from the arbitrary choice of the origin of the energy levels which formally means that a term proportional to the identity operator can always be added to the Hamiltonian. The phase $\phi_1$ is given by,

$$\phi_1(T) = \frac{\sum_{k=1}^{M} E_k T}{M \hbar},$$

where $E_k$ is the energy of the level $k$. By $\phi_2$ we denoted other contributions to the global phase due to the structure of the unitary transformation and its arbitrariness for the levels $k = N + 1, \ldots, M$.

II. EVOLUTION EQUATION APPROACH.

The optimization approach proposed in [7, 8] is based on Eq. (2) by defining a complex parameter $\tau$ as

$$\tau(\hat{O}; T; \epsilon) = \sum_{k=1}^{N} \langle k | \hat{O}^{\dagger} \hat{U}(T, 0; \epsilon) | k \rangle.$$

As $\hat{O}$ is a unitary transformation in the relevant subspace, $\tau$ is a complex number inside a circle of radius $N$. Its modulus is equal to $N$ only when the unitary transformation generated by the field $\hat{U}$ is equal to the target unitary transformation in the relevant subspace, except for a possible global phase. The modulus of $\tau$ is a measurement of the fidelity of the target unitary transformation implementation by the field [8]. For $N = M$, the sum in Eq. (4) is the trace of the operator product.

In [7, 8] the optimization of the real part of $\tau$, or the imaginary part, or a linear combination of both was suggested as a method to find the optimal field. For simplicity we will consider the real case. The maximization of $\text{Re}[\tau]$ can be formulated as a functional optimization. In this work we use the following form

$$J(\hat{U}, \hat{B}, \Delta \epsilon) = \text{Re} \left[ \sum_{k=1}^{N} \langle k | \hat{O}^{\dagger} \hat{U}(T, 0; \epsilon_0 + \Delta \epsilon) | k \rangle \right] - \lambda \int_{0}^{T} |\Delta \epsilon|^2 dt \quad - \quad \text{Re} \left[ \sum_{k=1}^{N} \int_{0}^{T} \langle k | \hat{B} \left( \frac{\partial}{\partial t} + i \frac{\hbar}{\hbar} \hat{H}(t; \epsilon_0 + \Delta \epsilon) \right) \hat{U} | k \rangle dt \right],$$

(5)
where $\hat{U}$, $\hat{B}$, $\epsilon_0$, and $\Delta \epsilon$ depends on $t$. The first term in the right-hand-side is the original objective. In our formulation, the other two terms are constrains depending on a reference field $\epsilon_0$ and a field correction $\Delta \epsilon$. The term including $|\Delta \epsilon|^2$ minimizes the total energy of the correction. The last term introduces the dynamics of the system under the field $\epsilon_0 + \Delta \epsilon$. $\hat{B}$ is an operator Lagrange multiplier and $\lambda$ a scalar Lagrange multiplier \[8\]. The common OCT form for the functional \[6\] is recuperated setting $\epsilon_0 = 0$ and interpreting $\Delta \epsilon$ as the driving field. However, Eq. \(5\) offers some advantages in the interpretation of the equations derived from the functional. More elaborated constrains are possible \[12, 13\], but they are not relevant for the following discussion.

Applying the calculus of variations, $\delta \bar{J} = 0$, with respect to $\hat{B}$, the Schrödinger equation for the evolution operator of the system is obtained,

$$\frac{\partial \hat{U}}{\partial t} = -\frac{i}{\hbar} \hat{H}(t; \epsilon_0 + \Delta \epsilon) \hat{U},$$  \hspace{1cm} (6)

with the condition $\hat{U}(0,0; \epsilon_0 + \Delta \epsilon) = 1$. The variation of $\hat{U}$ give the Schrödinger evolution equation for the operator $\hat{B}$,

$$\frac{\partial \hat{B}^\dagger}{\partial t} = -\frac{i}{\hbar} \hat{H}(t; \epsilon_0 + \Delta \epsilon) \hat{B}^\dagger,$$  \hspace{1cm} (7)

with the condition $\hat{B}^\dagger(T,T; \epsilon_0 + \Delta \epsilon) = \hat{O}$. $\hat{B}^\dagger$ can be interpreted as the backwards propagation in time of the target unitary transformation $\hat{O}$. It is related to $\hat{U}$ by

$$\hat{B}^\dagger(t,T; \epsilon) = \hat{U}(t,T; \epsilon) \hat{O}. \hspace{1cm} (8)$$

Eq. \(6\) and \(7\) represent the propagation forward and backwards in time of the boundary conditions of the problems, that is, the identity, $\mathbb{1}$, at time $t = 0$ and the target unitary transformation, $\hat{O}$, at time $t = T$. The variation of $\Delta \epsilon$ leads to an equation for the correction to the field,

$$\Delta \epsilon(t) = -\frac{1}{2 \lambda \hbar} \text{Im} \left[ \sum_{k=1}^{N} \langle k | \hat{B}(t,T; \epsilon_0 + \Delta \epsilon) \hat{\mu} \hat{U}(t,0; \epsilon_0 + \Delta \epsilon) | k \rangle \right].$$  \hspace{1cm} (9)

Eq. \(9\), more than Eq. \(5\), is the central result of the optimal control procedure and constitutes the starting point of the iterative algorithms devoted to determine the optimal field \[8\]. When an optimal field $\epsilon_{opt}$ is found $\Delta \epsilon = 0$, and from Eq. \(8\) and Eq. \(9\),

$$\text{Im} \left[ \sum_{k=1}^{N} \langle k | \hat{O}^\dagger \hat{U}^\dagger(t,T; \epsilon_{opt}) \hat{\mu} \hat{U}(t,0; \epsilon_{opt}) | k \rangle \right] = 0. \hspace{1cm} (10)$$
Eq. (10) constitutes a condition for the optimal fields for the first approach. It is the base for the following analysis. Let us denoted by \( \tilde{\epsilon} \) a field that generated the target unitary transformation up to a global phase, \( \hat{U}(T, 0; \tilde{\epsilon}) = e^{-i\phi} \hat{O} \). Using
\[
\hat{U}(t, 0, \epsilon) = \hat{U}(t, T, \epsilon) \hat{U}(T, 0, \epsilon),
\]
the diagonal block structure of the matrix representation of \( \hat{O} \) in the basis \( \{|k\rangle\} \), and the relation \( \langle k|\hat{\mu}|k\rangle = 0 \), it is found that the left-hand-side of Eq. (10) gives
\[
\text{Im} \left[ \sum_{k=1}^{N} e^{-i\phi} \langle k| \hat{U}(t, T; \tilde{\epsilon}) \hat{O} \hat{O}^\dagger \hat{U}^\dagger(t, T; \tilde{\epsilon}) \hat{\mu} |k\rangle \right] = 0.
\]
This result implies that any field inducing the target unitary transformation up to a global phase is a possible optimal solution of the optimization algorithm based on Eq. (9). The convergence to such a solution will depend on the particular numerical implementation. It must be remarked that Eq. (10) is a necessary but not a sufficient condition for the optimal field. For example, let us consider a target unitary transformation diagonal in the basis \( \{|k\rangle\} \) denoted by \( \hat{O}_D \). The unitary transformation generated by the free Hamiltonian \( \hat{U}(t_1, t_2; \epsilon = 0) \) is also diagonal in that basis, and then,
\[
\text{Im} \left[ \sum_{k=1}^{N} \langle k| \hat{O}_D^\dagger \hat{U}^\dagger(t, \epsilon = 0) \hat{\mu} \hat{U}(t, 0; \epsilon = 0) |k\rangle \right] = 0.
\]
However, in general \( \hat{U}(T, 0; \epsilon = 0) \) is not equal to the target \( \hat{O}_D \). These spurious solutions to the optimization can be avoided with a different choice of the initial guess for the algorithm.

In optimization procedures based on Eq. (9) the full operator propagation in Eqs. (6) and (7) is not needed since only the action of \( \hat{U} \) and \( \hat{O} \) on the states \(|k\rangle\) in the relevant subspace \((k = 1, ..., N)\) appears. Then only the first \( N \) rows of the matrix operator representations are propagated. Denoting by \( U^k_j \) \((B^\dagger)^k_j\) the \( k \) row of the matrix representation of \( \hat{U} \) \((\hat{B}^\dagger) \) in the basis \( \{|k\rangle\} \), and being \( U^k_j \) \((B^\dagger)^k_j\) the \( j \) element of the row \((j = 1, ..., M)\), the evolution equations (6) and (7) take the form,
\[
\frac{\partial U^k(t)}{\partial t} = -\frac{i}{\hbar} H(t) U^k(t),
\]
\[
\frac{\partial (B^\dagger)^k(t)}{\partial t} = -\frac{i}{\hbar} H(t) (B^\dagger)^k(t),
\]
with the conditions \( U^k_j(t = 0) = \delta_{jk} \) and \((B^\dagger)^k_j(t = T) = O^k_j\) respectively, being \( O^k_j \) the matrix elements of the target unitary transformation \( \hat{O} \) and \( H(t) \) the matrix representation.
of $\hat{H}$. The $2N$ evolution equations ($k = 1, \ldots, N$) are equivalent to the propagation of $2N$ states of the system. The advantage is that in this case only $2(N \times M)$ elements are propagated instead of the $2(M \times M)$ in Eq. (6) and Eq. (7).

III. STATE TO STATE APPROACH.

The state to state approach [9] is based on the simultaneous optimization of $N$ transitions between pairs of initial and final states. These pairs of states $\{\varphi_{il}, \varphi_{fl}\}$, ($l = 1, \ldots, N$) are related by the target unitary transformation, $|\varphi_{fl}\rangle = \hat{O} |\varphi_{il}\rangle$. The objective is formulated as

$$\eta(\hat{O}; T; \epsilon) = \sum_{l=1}^{N} |\langle \psi_{il}(T; \epsilon) | \varphi_{fl}\rangle|^2,$$

(15)

where $\psi_{il}(T; \epsilon)$ is the state at the target time that evolves with the driving field $\epsilon(t)$ and the initial condition $\psi_{il}(t = 0) = \varphi_{il}$. $\eta$ is a positive real number and its maximum value $\eta = N$ is reached when all the initial states $\varphi_{il}$ are driven by the field to the correct final states $\varphi_{fl}$. The task of obtaining the optimal field is equivalent to the maximization of $\eta$. The set of initial states $\varphi_{il}$ must be chosen carefully. In order to account for all the possible transitions the states $\varphi_{il}$ have to represent the relevant subspace. However, the choice of an orthonormal basis could produce undesired results. Let us denoted by $\{\tilde{\varphi}_{il}\}$ an orthonormal basis of the relevant subspace and by $\hat{D}$ an arbitrary unitary transformation diagonal in that basis. The product $\hat{O} \hat{D}$ is also a unitary transformation. If $\epsilon_O$ and $\epsilon_{OD}$ are fields that generate $\hat{O}$ and $\hat{O} \hat{D}$ at time $T$ respectively, it is found that the same optimization objective is obtained,

$$\eta_{\perp}(\hat{O}; T; \epsilon_O) = \eta_{\perp}(\hat{O}; T; \epsilon_{OD}),$$

(16)

where $\perp$ denotes that $\eta$ was evaluated using an orthonormal basis. Then any algorithm based on $\eta$ and using an orthonormal basis would find the optimal field corresponding to any of the possible targets $\hat{O} \hat{D}$ ($\hat{O}$ is a particular case when $\hat{D}$ is the identity operator). The reason is that $\eta$ is sensitive to the modulus of the projection of each pair $\{\varphi_{il}, \varphi_{fl}\}$ but not to the relative phases between them. The phase problem can be overcome with a careful choice of the states $\varphi_{il}$. Keeping the first $N - 1$ states of the basis and substituting the $N$ state by $\sum_{l=1}^{N} \tilde{\varphi}_{il}/\sqrt{N}$, the maximum condition is achieved only when the field induces the target unitary transformation up to a possible global phase.
The optimization is formulated as the maximization of the functional

\[
\hat{K}(\psi_{ik}, \psi_{fk}, \Delta \epsilon) = \sum_{l=1}^{N} |\langle \psi_{il}(T; \epsilon_0 + \Delta \epsilon) | \varphi_{fl} \rangle|^2 - \lambda \int_{0}^{T} |\Delta \epsilon(t)|^2 dt
- 2 \text{Re} \left[ \sum_{l=1}^{N} \langle \psi_{il}(T; \epsilon_0 + \Delta \epsilon) | \varphi_{fl} \rangle \int_{0}^{T} \langle \psi_{fl} | \left( \frac{\partial}{\partial t} + i \hbar \hat{H}(t; \epsilon_0 + \Delta \epsilon) \right) | \psi_{il} \rangle dt \right],
\]

(17)

where \( \psi_{il}, \psi_{fl}, \epsilon_0 \) and \( \Delta \epsilon \) depend on time. The form in Ref. [9] is recuperated setting \( \epsilon_0 = 0 \) and interpreting \( \Delta \epsilon \) as the driving field.

The variations with respect to \( \psi_{li} \) and \( \psi_{lf} \) lead to the following \( 2N \) equations

\[
\frac{\partial}{\partial t} | \psi_{il} \rangle = -i \frac{\hbar}{\lambda} \hat{H}(t; \epsilon_0 + \Delta \epsilon) | \psi_{il} \rangle,
\]

(18)

with the condition \( | \psi_{il}(t = 0) \rangle = | \varphi_{il} \rangle \), and

\[
\frac{\partial}{\partial t} | \psi_{lf} \rangle = -i \frac{\hbar}{\lambda} \hat{H}(t; \epsilon_0 + \Delta \epsilon) | \psi_{lf} \rangle,
\]

(19)

with the condition \( | \psi_{fk}(t = T) \rangle = | \varphi_{fk} \rangle \). The variation respect to \( \Delta \epsilon \) leads to the equation for the correction to the field,

\[
\Delta \epsilon_{ss}(t) = -\frac{1}{\lambda \hbar} \text{Im} \left[ \sum_{l=1}^{N} \langle \psi_{fl}(T; \epsilon_0 + \Delta \epsilon) | \varphi_{fl} \rangle \langle \psi_{fl}(t; \epsilon_0 + \Delta \epsilon) | \hat{\mu} | \psi_{il}(t; \epsilon_0 + \Delta \epsilon) \rangle \right].
\]

(20)

Eq. (18) and (19) are formally equivalent to Eq. (14), propagating forward or backward on time the boundary conditions of the problem. Then the main difference between the two approaches is found in the expression for the correction to the field, Eq. (9) and Eq. (20).

The connection between the two expressions is established by rewriting the states \( \varphi \) and \( \psi \) as

\[
| \varphi_{il} \rangle \rightarrow | l \rangle,
| \varphi_{fl} \rangle \rightarrow \hat{O} | l \rangle,
| \psi_{il}(t; \epsilon) \rangle \rightarrow \hat{U}(t, 0; \epsilon) | l \rangle,
| \psi_{fl}(t; \epsilon) \rangle \rightarrow \hat{B}^{\dagger}(t, T; \epsilon) | l \rangle
\]

(21)

and Eq. (20) as,

\[
\Delta \epsilon_{ss}(t) = -\frac{1}{\lambda \hbar} \text{Im} \left[ \sum_{l=1}^{N} \langle l | \hat{U}^{\dagger}(T, 0; \epsilon_0 + \Delta \epsilon) \hat{O} | l \rangle \langle l | \hat{B}(t, T; \epsilon_0 + \Delta \epsilon) \hat{\mu} \hat{U}(t, 0; \epsilon_0 + \Delta \epsilon) | l \rangle \right].
\]

(22)
This expression is formally equivalent to Eq. (9) except for the factor \( \langle l| \hat{U}^\dagger(T, 0, \epsilon_0 + \Delta \epsilon) \hat{O}|l \rangle \). (The different factor \( 1/2 \) can be removed with a redefinition of \( \lambda \)). Omitting this factor the two approaches would be completely equivalent: in that case the careful choice of the initial state set wouldn’t be necessary and the two approaches would lead to the same set of equations. In general the equivalence is only formal due to the additional factor and the different set of states \( \{|k\rangle\} \) and \( \{|l\rangle\} \). In the following we will chose \( |l\rangle = |k\rangle \) for \( l = 1, ..., N - 1 \) and \( |l\rangle = N \rangle = \frac{\sum_{k=1}^{N} |k\rangle}{\sqrt{N}} \). The condition for the optimal field (\( \Delta \epsilon = 0 \)) is obtained using Eq. (20) and (8),

\[
\text{Im} \left\{ \sum_{l=1}^{N} \langle l| \hat{O}^\dagger \hat{U}^\dagger(T, 0; \epsilon_{opt}) \hat{U}(t, 0; \epsilon_{opt})|l \rangle \right\} = 0. \tag{23}
\]

Eq. (23) is a necessary but not sufficient condition for the optimal field, as is also Eq. (10). Denoting as before by \( \tilde{\epsilon} \) a driving field generating the target unitary transformation up to a global phase, the left-hand-side of (23) gives,

\[
\text{Im} \left\{ \sum_{l=1}^{N} \langle l| \hat{O}^\dagger \hat{U}^\dagger(t, T; \tilde{\epsilon}) \hat{U}(t, T; \tilde{\epsilon}) \hat{O}|l \rangle \right\} = 0. \tag{24}
\]

(The property \( \text{Im}[\langle \Psi| \hat{\mu}|\Psi \rangle] = 0 \) for Hermitian operator \( \hat{\mu} \) was used). Contrary to Eq. (12), the phase \( \phi \) doesn’t appear in Eq. (24) due to the factor \( \langle l| \hat{U}^\dagger(T, 0, \tilde{\epsilon}) \hat{O}|l \rangle \) correcting each term in the sum. Using the same arguments leading to Eq. (13), it can be shown that the left-hand-side of Eq. (23) is null for \( \epsilon = 0 \) when the target unitary transformation is diagonal. The previous results imply that any field that generates the target unitary transformation up to a global phase fulfills the condition in Eq. (23) and in addition spurious solutions could be found, as in the first approach.

IV. CONCLUSIONS

In this study we have employed a modified formulation of OCT which uses the correction to the driving field \( \Delta \epsilon \) as central element. \( \Delta \epsilon = 0 \) is a necessary but not sufficient condition for obtaining the objective. The relations derived from this condition allow a better analysis of the control equations, in particular, the similarities and differences between the two approaches. Optimal solutions of the evolution equation approach will be also optimal solutions of the state to state approach. In this sense both approaches are equivalents. The
difference between them is a term in the state to state approach which modified the phases. This term can cause a phase ambiguity in the target unitary transformation. A careful choice of the initial set of states can solve this problem.

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