Local control theory for unitary transformations: Application to quantum computing without leakage

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We present a local optimal control strategy to produce desired unitary transformations. Unitary transformations are central to all quantum computational algorithms. Many realizations of quantum computation use a submanifold of states, comprising the quantum register, coupled by an external driving field to a collection of additional mediating excited states. Previous attempts to apply control theory to induce unitary transformations on the quantum register, while successful, produced pulses that drive the population out of the computational register at intermediate times. Leakage of population from the register is undesirable since often the states outside the register are prone to decay and decoherence, and populating them causes a decrease in the final fidelity. In this work we devise a local optimal control method for achieving target unitary transformations on a quantum register, while avoiding intermediate leakage out of the computational submanifold. The technique exploits a phase locking of the field to the system such as to eliminate the undesirable excitation. This method is then applied to produce an SU(6) Fourier transform on the vibrational levels of the ground electronic state of the Na$_2$ molecule. The emerging mechanism uses two photon resonances to create a transformation on the quantum register while blocking one photon resonances to excited states.

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In recent years there has been growing interest in the possibility of realizing quantum computers. Any such implementation must consist of a quantum register comprised of a selection of quantum states on which the computational operations can be performed. A physical realization of a quantum computer should therefore be able to produce these unitary transformations on the register by the use of external driving fields [1].

The general paradigm of quantum computing is to break up every computational operation into a sequence of simple unitary operations called quantum gates which can be considered the basic building blocks of quantum computation [2]. As the register size grows the number of quantum gates required to construct an arbitrary unitary operation increases rapidly, and therefore the total fidelity, which depends on the accumulation of errors at each step, decreases drastically [3]. It has been shown in [4, 5, 6] that Optimal Control theory (OCT) methods can be utilized in order to calculate a field that will directly induce an arbitrary target transformation. The OCT approach eliminates the need to decompose the unitary operator into fundamental operations; however the emerging fields are complicated and drive the population out of the computational submanifold at intermediate times. This is undesirable since in physical realizations the excited states are prone to decay and decoherence, and therefore their population at intermediate times causes a decrease in the final fidelity.

In this paper we use a variant of control theory, which we refer to as “local control”, to achieve a target unitary transformation on a quantum register with no intermediate leakage out of the quantum register. The technique exploits a phase locking of the field to the system such as to eliminate undesirable excitations. We demonstrate this approach by obtaining fields to produce an SU(6) FT on a quantum register consisting of a submanifold of vibrational levels on the ground electronic state of a diatomic molecule [12, 13] without populating the excited electronic vibrational states. The emerging mechanism uses two photon resonances to transform the quantum register while blocking one photon resonances to excited states. To some extent the method can be viewed as a systematic generalization of the methods of Monroe et al [14] and Sørensen and Mølmer [15] to an arbitrary number of qubits and arbitrary unitary transformations. The more complicated fields presented here can be realized using optical pulse shaping techniques [16, 17, 18].

The model Hamiltonian consists of a free part \( \hat{H}_0 \) and an interaction part \( \hat{V} = -\mu E(t) - \hat{\mu}^\dagger E^*(t) \) controlled by an external field \( E(t) \) through the dipole operator \( \hat{\mu} = \sum_{ij} \mu_{ij} |i\rangle \langle j| \), with \( \mu_{ij} \) the coupling strengths between the ground and excited states \( |i\rangle \) and \( |j\rangle \) respectively,

\[
\hat{H} = \hat{H}_0 - \mu E(t) - \hat{\mu}^\dagger E^*(t).
\] (1)

The system evolution can be described by a time dependent unitary transformation \( U(t) \), the dynamics of which is governed by the Schrödinger equation,

\[
\frac{\partial U(t)}{\partial t} = -\frac{i}{\hbar} \hat{H} U(t),
\] (2)

with the initial condition \( U(0) = I \). In order to eliminate the free Hamiltonian motion it is common practice to
switch to the interaction picture Hamiltonian

\[ \hat{H} \rightarrow \hat{\tilde{H}} = \exp \left( \frac{i}{\hbar} H_0 t \right) \hat{V} \exp \left( -\frac{i}{\hbar} H_0 t \right) \]

\[ = -\tilde{\mu}(t) E(t) - \tilde{\mu}^\dagger(t) E^*(t). \]  

(3)

with \( \tilde{\mu}(t) \equiv \exp \left( \frac{i}{\hbar} H_0 t \right) \tilde{\mu} \exp \left( -\frac{i}{\hbar} H_0 t \right) \).

The desired computation is represented by a certain unitary transformation \( O_r \), which is defined to operate solely on the restricted subspace constituting the quantum register and which must be obtained by the system at the final time \( T \). Denoting \( P_r \) to be a projection onto the restricted subspace we define \( U_r(t) = P_r U(t) P_r \) to be the portion of the evolution operator acting on the restricted computational subspace. The goal is therefore to obtain a control field \( E(t) \) which will maximize the overlap, \( J = |\text{Tr}(O_r^\dagger U_r(T))|^2 \), between the target \( O_r \) and \( U_r(t) \) at the final time, subject to the constraint that the computational manifold population \( C = \text{Tr}(U_r^\dagger(t) U_r(t)) \) remains fixed throughout. This constraint enforces the elimination of leakage from the computational manifold throughout the evolution.

We introduce, here, a local control method which continuously increases the objective \( J \) while simultaneously holding the constraint \( C \) fixed. At each time step, the algorithm constructs a field \( E(t) \) that fulfills the two conditions. The constraint \( dC/dt = 0 \), determines the direction of the field vector \( E(t) \) in the complex plane. The sign of the field, however, remains free and is chosen such as to make the time derivative of \( J \) positive, i.e. \( dJ/dt \geq 0 \), ensuring an increase in the objective at the next time step.

We now derive the equations determining the direction and magnitude of \( E(t) \) at each step. Note first that since \( U_r = P_r U P_r \) we have

\[ \hat{U}_r = P_r \frac{1}{i\hbar} \hat{H} U P_r. \]

The equation for the constraint is

\[ \dot{C} = \frac{d}{dt} \text{Tr}(U_r^\dagger U_r) \]

\[ = 2\text{Re} \left\{ \text{Tr}(U_r^\dagger U_r \frac{1}{i\hbar} \hat{H} U P_r) \right\} \]

\[ = -\frac{2}{\hbar} \text{Im} \{ \text{Tr}(U_r^\dagger U_r \tilde{\mu}(t) U P_r) E(t) \}
+ \text{Tr}(U_r^\dagger U_r \tilde{\mu}^\dagger(t) U P_r) E^*(t) \} = 0 \]  

(4)

Noticing that the trace operation is invariant under transposition of its argument and that the imaginary part changes sign under complex conjugation we can take the adjoint of the second term and write

\[ \dot{C} = -\frac{2}{\hbar} \text{Im} \{ \text{Tr}(U_r^\dagger P_r \tilde{\mu}(t) U P_r) E(t) \}
- \text{Tr}(P_r U^\dagger \tilde{\mu}(t) P_r U_r) E(t) \} \]

\[ = -2\text{Im} \{ g E(t) \} = 0 \]  

(5)

where \( g = \text{Tr}(U_r^\dagger P_r \tilde{\mu}(t) U P_r - P_r U^\dagger \tilde{\mu}(t) P_r U_r) \). One can now enforce fulfillment of the constraint, eq. [5], by choosing the electric field to be in the direction of \( g^* \) with (real) proportionality constant \( \alpha \) namely

\[ E(t) = \alpha \epsilon_g^*, \]  

(6)

with \( \epsilon_g^* \equiv g^*/|g| \) denoting the direction of \( g^* \) in the complex plane. We now use the freedom in choosing the sign of \( \alpha \) to assure monotonic increase in the objective.

\[ J = \frac{d}{dt} |\text{Tr}(O_r^\dagger U_r)|^2 \]

\[ = 2\text{Re} \left\{ \text{Tr}(O_r^\dagger U_r)^* \frac{d}{dt} \text{Tr}(O_r U_r) \right\} \]

\[ = 2\text{Re} \left\{ \eta^* \text{Tr}(O_r^\dagger P_r \frac{1}{i\hbar} \hat{H} U P_r) \right\} \]

\[ = \alpha 2\text{Re} \{ f \epsilon_g^* \} \geq 0, \]

(7)

where we define \( \eta \equiv \text{Tr}(O_r U_r) \) and \( f = -\frac{1}{\hbar} \text{Tr} \{ \eta^* O_r^\dagger P_r \tilde{\mu}(t) U P_r - \eta P_r U^\dagger \tilde{\mu}(t) P_r O_r \} \). Note that in advancing to the last line we have employed the same sequence of steps as in eq. [4] and [5]. In order to enforce an increase in \( J \), we choose

\[ \alpha = \text{Re} \{ f g^* \} \]

\[ \equiv (f \cdot g), \]

(8)

with \( (f \cdot g) \) denoting a scalar product in the complex plane, thus guaranteeing that \( dJ/dt \geq 0 \). The electric field is therefore chosen as

\[ E(t) = (f \cdot g) \epsilon_g^* \]  

(9)

It is important that \( E(t) \) depend on the magnitude of \( g^* \) and not only on its direction \( \epsilon_g^* \), since for a vanishing \( |g| \) the direction \( \epsilon_g^* \) becomes undefined and numerically unstable. We therefore wish that \( E \) be proportional to \( |g| \) such that a phase jump in \( g \) be accompanied by a vanishing of \( E \), thus avoiding abrupt phase jumps in the emerging field.
Note that there is still freedom in determining the magnitude of \( E(t) \), which can be utilized to control the order of magnitude of the field strength by multiplying by a positive envelope function, \( S(t) \). It is sometimes necessary for numerical reasons to limit the maximum allowed field such that \( |E(t)| < E_{\text{max}} \). This can be achieved by transforming \( \alpha \rightarrow E_{\text{max}} \tanh(\alpha/E_{\text{max}}) \) which preserves the sign of \( \alpha \) but saturates at constant value, \( E_{\text{max}} \).

Summing up, our algorithm requires calculating \( g \) and \( f \) at each time step and choosing a field according to

\[
E(t) = E_{\text{max}} \tanh \left( S(t)(f \cdot g)/E_{\text{max}} \right) \epsilon_g^*.
\]

In order to begin the control process it is necessary to seed a small fraction of population into the excited states at initial time. This can be done by exciting the system with a weak pulse tuned to the optical transition. Alternatively, one can begin with an initial condition slightly rotated from the identity. As the seeding is negligibly small, the emerging field will produce the target unitary transformation also when applied to the ‘pure’ initial condition \( U(0) = I \) as required.

We apply the local control technique described above to the implementation of an \( SU(N_r) \) Fourier transform on the ground potential surface of a two-electronic surface model of an \( \text{Na}_2 \) molecule. The first \( N_r \) vibronic states of the ground electronic surface, \( \chi^1 \Sigma^+_g \), comprise the quantum register. All ground states are coupled via the dipole coupling to the vibronic levels of the electronically excited surface, \( A^1 \Sigma^+_u \) (see figure 2). The final time for the implementation was taken to be 128 picoseconds. Figure 3 summarizes our results for producing an \( SU(6) \) transform,

\[
FT(6) = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
1 & w & w^2 & w^3 & w^4 & w^5 \\
1 & w^2 & w^4 & w^6 & w^8 & w^{10} \\
1 & w^3 & w^6 & w^9 & w^{12} & w^{15} \\
1 & w^4 & w^8 & w^{12} & w^{16} & w^{20} \\
1 & w^5 & w^{10} & w^{15} & w^{20} & w^{25}
\end{pmatrix}; \quad w \equiv \sqrt{1} = e^{2\pi i/6},
\]
on a submanifold of the two potential surfaces containing seven ground state vibrational levels and three excited state vibrational levels. The top plot shows the electric field obtained by the local control procedure. The middle plot shows the evolution of the absolute value of the unitary propagator elements under the derived field. The monotonic increase of the objective \( \sqrt{J} \) (solid) and constraint \( C \) (dashed) showing monotonic increase in the former while keeping the latter constant.

![FIG. 2: Schematic picture of \( \text{Na}_2 \) molecular model consisting of ground \( (\chi^1 \Sigma^+_g) \) and excited \( (A^1 \Sigma^+_u) \) electronic potential energy curves. A submanifold of the ground state levels constitutes the quantum register. The remaining levels serve as mediators which couple the register levels through interaction with the electric field. The goal is to produce a unitary transformation on the register levels with no intermediate population of the mediating states.](image)

![FIG. 3: Top: The control field obtained by the algorithm. Middle: Controlled evolution of the elements of the unitary propagator (absolute values). Bottom: Evolution of objective \( \sqrt{J} \) (solid) and constraint \( C \) (dashed) showing monotonic increase in the former while keeping the latter constant.](image)
We stress, however, that due to the smallness of the perturbation, once the field is obtained it can be applied to the desired ‘pure’ initial condition $U(0) = I$, with negligible deviations from the current results. As time progresses the elements rotate and shrink/expand to obtain the $SU(6)$ Fourier transform at the final time. It can be clearly seen that the elements at final time (c) divide the circle into six equal parts and thus are, up to an unimportant phase rotation, just powers of $w$, the sixth root of unity appearing in $FT(6)$.

Some understanding of the mechanism by which the leakage is avoided can be obtained by looking at the spectrum of the field $E(t)$ and its square $|E(t)|^2$ (top and bottom of figure 4 respectively). The spectrum $\tilde{E}(\omega)$ of the field intensity corresponds to one-photon processes. A glance at the plot of $\tilde{E}(\omega)$ (top of figure 5) reveals that there are ‘holes’ in this spectrum at precisely the points corresponding to transitions from the quantum register to the excited states, as indicated by the circles. These ‘holes’ are evidently responsible for the absence of excitations. As one-photon interactions are suppressed it must be two (and higher) photon processes which produce the evolution towards the desired target. The spectrum $|\tilde{E}|^2(\omega)$ of the field intensity corresponds to two-photon processes produced by absorption and immediate emission of a photon. The bottom plot of figure 5 shows that $|\tilde{E}|^2(\omega)$ displays peaks at the precise frequencies corresponding to energy differences between the register states, indicated in the figure by green circles. This implies that the field is in two-photon resonance with transitions corresponding to the register states but is detuned from one-photon resonance with excited state transitions.

The model system used above illustrates the general features of our local control method; however it suffers from the following drawbacks. First, the analysis described above was performed in the interaction picture where the $H_0$ motion is transformed away. In practice, however, this drift motion must be taken into account. Second, it is generally expected that the computational power scale exponentially with the physical resources such that for example $N_r$ physical bits carry $2^{N_r}$ entities of information. In the molecular system studied here, as in other studies of molecular quantum computation, this requirement is not satisfied since $N_r$ physical levels correspond to only $N_r$ information entities ($\log_2 N_r$ bits) namely the scaling is only linear. However, the control method we have proposed does not depend on the specific model studied; therefore it can be applied to alternative models which are both driftless and scalable.

In summary, we have shown that it is possible to systematically design fields to produce arbitrary unitary transformations while avoiding leakage from the quantum register.

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