Robust control of quantum systems in the presence of field fluctuations

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ABSTRACT

The impact of control field fluctuations on the optimal manipulation of quantum dynamics phenomena is investigated. The presence of significant field fluctuations is shown to break down the evolution into a sequence of partially coherent robust steps. Robustness occurs because the optimization process reduces sensitivity to noise-driven quantum system fluctuations. This process takes advantage of the observable expectation value being bilinear in the evolution operator and its adjoint. The consequences of this inherent robustness bodes well for the future success of closed loop quantum optimal control experiments.

Keywords: Quantum control, Laser fields, Laser noise, Optimal control

1. INTRODUCTION

Many optimal control calculations have been performed for manipulating quantum phenomena[1,2], and a number of successful closed loop optimal control experiments[3-14] have also been carried out where the optimal fields were directly identified in the laboratory using suitable learning control techniques[15-17]. An early point of speculation was that even modest field noise would effectively kill the successful achievement of quantum control in the strong field non-linear regime, where the quantum system could act to amplify the field noise. The intriguing recent experiments operating in this regime provide evidence that this speculation was incorrect. However, the detailed explanation for the enhanced robustness has remained unclear.

Learning control simulations indicate that closed loop experiments should naturally gravitate towards control fields that produce robustness with respect to the presence of field fluctuations[18-20]. The recent laboratory demonstrations of non-linear intense field controlled dissociation and rearrangement of molecules[4,7], as well as the manipulation of high harmonic generation[5], are consistent with this suggestion. Explicitly seeking robustness[19] as an additional control criterion can further enhance this stable behavior, and possibly even with little deterioration in the quality of the attained objective. Although it is possible under some special circumstances that field fluctuations may be helpful[21], the general expectation is that field noise will diminish the degree of attainable control. Control field noise may also influence the rate of convergence of the learning control experiments[17,20]. This paper will consider the relationship between (a) coherent quantum dynamics, (b) the presence of field fluctuations, (c) the nature of dynamical robustness, and (d) seeking robustness.

2. OPTIMAL CONTROL OF QUANTUM DYNAMICS

The quantum system has the Hamiltonian $H_0 = H_0 - \mu \cdot \varepsilon(t)$, where H_0 is the field-free Hamiltonian, μ is the electric dipole moment, and $\varepsilon(t)$ is the control field. The system initially is described by the density matrix $\rho(0)$ and the dynamics is given by

$$i\hbar \frac{\partial \rho}{\partial t} = \left[H, \rho\right]. \tag{1}$$

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In the present analysis, the system evolution occurs free of any environmental interactions. Solving this equation gives $\rho(t) = U(t,0)\rho(0)U^\dagger(t,0)$, where the time evolution operator $U(t,0)$ satisfies $i\hbar\frac{\partial}{\partial t}U = HU$, $U(0,0) = 1$. An objective operator O (taken as time-independent here) is specified such that the expectation value

$$\langle O(T)\rangle = \mathrm{tr}\left[\rho(0)U^\dagger(T,0)OU(T,0)\right] \tag{2}$$

at the target time T is the goal for controlled manipulation. The system is assumed to be controllable to an acceptable degree[22]. It is natural to pose the objective as achieving the best (i.e., the optimal) result for $\langle O(T)\rangle$. This view is fundamental to quantum optimal control theory[23], as well as for closed loop learning control in the laboratory[3-17,19,20]. Here optimization may refer to maximization, minimization, or some other specified criteria, which is summarized as

$$\underset{\varepsilon(t)}{\mathrm{Opt}}\langle O(T)\rangle \tag{3}$$

where the control field is varied until the objective is met, as best as possible. Any single laboratory experiment would operate with an electric field $\varepsilon(t) = \varepsilon_{opt}(t) + \delta\varepsilon(t)$ where $\delta\varepsilon(t)$ is a random disturbance around the nominal optimal field $\varepsilon_{opt}(t)$; in practice, a set of experiments would be performed to average over an ensemble of noise trajectories $\{\delta\varepsilon(t)\}$. The influence of the field fluctuations can depend on the overall magnitude of $\varepsilon_{opt}(t)$ and the degree of nonlinearity of the control process. Optimal control calculations[18-20] and experiments[3-14] indicate that there is significant robustness even in the presence of rather large amplitude field fluctuations. We assume that $\delta\varepsilon(t)$ is a random variable characterized by a distribution function $P(\delta\varepsilon(t))$, such that

$$\int D[\delta\varepsilon(t)]P(\delta\varepsilon(t)) = 1. \tag{4}$$

Equation (2) shows that the initial density operator $\rho(0)$ is transformed to the final objective expectation value $\langle O(T)\rangle$ under the simultaneous action of U(T,0) and $U^\dagger(T,0)$. This evolution occurs through a sequence of states $|\ell_i\rangle$, $i = 1, 2, \ldots, n$, where each quantum number ℓ_i may span many accessible values. These states will be identified in Section 3 as those associated with high quantum evolution phase sensitivity to control field fluctuations. Each of the states $|\ell_i\rangle$ denotes an intermediate "stopping-off" point along the way to the objective. We may rigorously decompose U(T(0)) as follows:

$$U(T,0) = \mathop{\sum\!\!\!\!\!\!\int}_{\ell'_i=1,\ldots n} U(T,t_n)|\ell'_n\rangle\langle\ell'_n|U(t_n,t_{n-1})|\ell'_{n-1}\rangle\langle\ell'_{n-1}|\ldots.$$

$$\ldots.|\ell'_2\rangle\langle\ell'_2|U(t_2,t_1)|\ell'_1\rangle\langle\ell'_1|U(t_1,0). \tag{5}$$

The symbol $\sum\!\!\!\!\!\!\int$ denotes a summation or integration over the intermediate state indices, as appropriate. On physical grounds, it is suggestive to think in terms of a sequence of evolving events under the influence of the electric field $\varepsilon(t)$, $0 \le t \le T$, broken into sub-intervals $\{\varepsilon_0(t), 0 \le t \le t_1\}$, $\{\varepsilon_1(t), t_1 \le t \le t_2\}, \ldots, \{\varepsilon_n(t), t_n \le t \le T\}$, such that the full field is a continuous concatenation of the individual pieces $\varepsilon(t) = [\varepsilon_0(t), \varepsilon_1(t), \ldots, \varepsilon_n(t)]$ taken in sequence.

An expression for $U^{\dagger}(T,0)$ analogous to U(T,0) in Eq. (5) may be written, and their combination utilized to represent the structure in Eq. (2):

$$
\begin{aligned}
\langle O(T)\rangle = \sum_{\ell_i=1,\ldots,n} \sum_{\ell'_i=1,\ldots n} \leftarrow \rho(0)\big|U^{\dagger}(t_1,0)\big|\ell_1\big\rangle\big\langle\ell_1\big|U^{\dagger}(t_2,t_1)\big|\ell_2\big\rangle\big\langle\ell_2\big|\ldots.. \\
\ldots.\big|\ell_{n-1}\big\rangle\big\langle\ell_{n-1}\big|U^{\dagger}(t_n,t_{n-1})\big|\ell_n\big\rangle\big\langle\ell_n\big|U^{\dagger}(T,t_n)\big|O\big|U(T,t_n)\big|\ell'_n\big\rangle \\
\times\big\langle\ell'_n\big|U(t_n,t_{n-1})\big|\ell'_{n-1}\big\rangle\big\langle\ell'_{n-1}\big|\ldots\ldots\ldots\big|\ell'_2\big\rangle\big\langle\ell'_2\big|U(t_2,t_1)\big|\ell'_1\big\rangle\big\langle\ell'_1\big|U(t_1,0)\big|\longrightarrow.
\end{aligned}
\tag{6}
$$

The arrows at the beginning and end of the expression imply that these operators are linked together to form a closed loop structure. Figure 1 depicts the sequence of steps from ρ(0) to $\langle O(T)\rangle$ without field noise, permitting coherent transfer of amplitude through each intermediate state. Each matrix element in Eq. (6) may be written in terms of its modulus and phase

$$
\big\langle\ell'_q\big|U(t_q,t_{q-1})\big|\ell'_{q-1}\big\rangle = \big|\big\langle\ell'_q\big|U(t_q,t_{q-1})\big|\ell'_{q-1}\big\rangle\big| \exp\big[i\phi(\ell'_q,\ell'_{q-1})\big] \ , \tag{7}
$$

such that Eq. (6) becomes:

$$
\begin{aligned}
\langle O(T)\rangle = \sum_{\ell_i=1,\ldots,n} \sum_{\ell'_i=1,\ldots n} \big\langle\ell'_1\big|U(t_1,0)\big|\rho(0)\big|U^{\dagger}(t_1,0)\big|\ell_1\big\rangle \\
\times \big|\big\langle\ell_2\big|U(t_2,t_1)\big|\ell_1\big\rangle\big|\big|\big\langle\ell'_2\big|U(t_2,t_1)\big|\ell'_1\big\rangle\big| \exp\big\{i\big[\phi(\ell'_2,\ell'_1)-\phi(\ell_2,\ell_1)\big]\big\} \\
\vdots \\
\times \big|\big\langle\ell_n\big|U(t_n,t_{n-1})\big|\ell_{n-1}\big\rangle\big|\big|\big\langle\ell'_n\big|U(t_n,t_{n-1})\big|\ell'_{n-1}\big\rangle\big| \exp\big\{i\big[\phi(\ell'_n,\ell'_{n-1})-\phi(\ell_n,\ell_{n-1})\big]\big\} \\
\times \big\langle\ell_n\big|U^{\dagger}(T,t_n)\big|O\big|U(T,t_n)\big|\ell'_n\big\rangle.
\end{aligned}
\tag{8}
$$

An arbitrary term in Eq. (8),

$$
S_{q,q-1} = \big|\big\langle\ell_q\big|U(t_q,t_{q-1})\big|\ell_{q-1}\big\rangle\big|\big|\big\langle\ell'_q\big|U(t_q,t_{q-1})\big|\ell'_{q-1}\big\rangle\big| \exp\big\{i\big[\phi(\ell'_q,\ell'_{q-1})-\phi(\ell_q,\ell_{q-1})\big]\big\} \tag{9}
$$

is a functional of the electric field $\varepsilon_{q-1}(t)$, $t_{q-1} \le t \le t_q$. In Eq. (8), it is understood that each phase $\phi(\ell_p, \ell_{p-1})$, $p = 2,\ldots,n$ will generally be a distinct functional of the electric field $\varepsilon_{p-1}(t)$.

In the laboratory learning control experiments, the final result is an ensemble average of Eq. (8) over the probability distribution function in Eq. (4)

$$
\langle O(T)\rangle_{\{\delta\varepsilon\}} \equiv \int D[\delta\varepsilon(t)]P(\delta\varepsilon(t))\,\langle O(T)\rangle. \tag{10}
$$

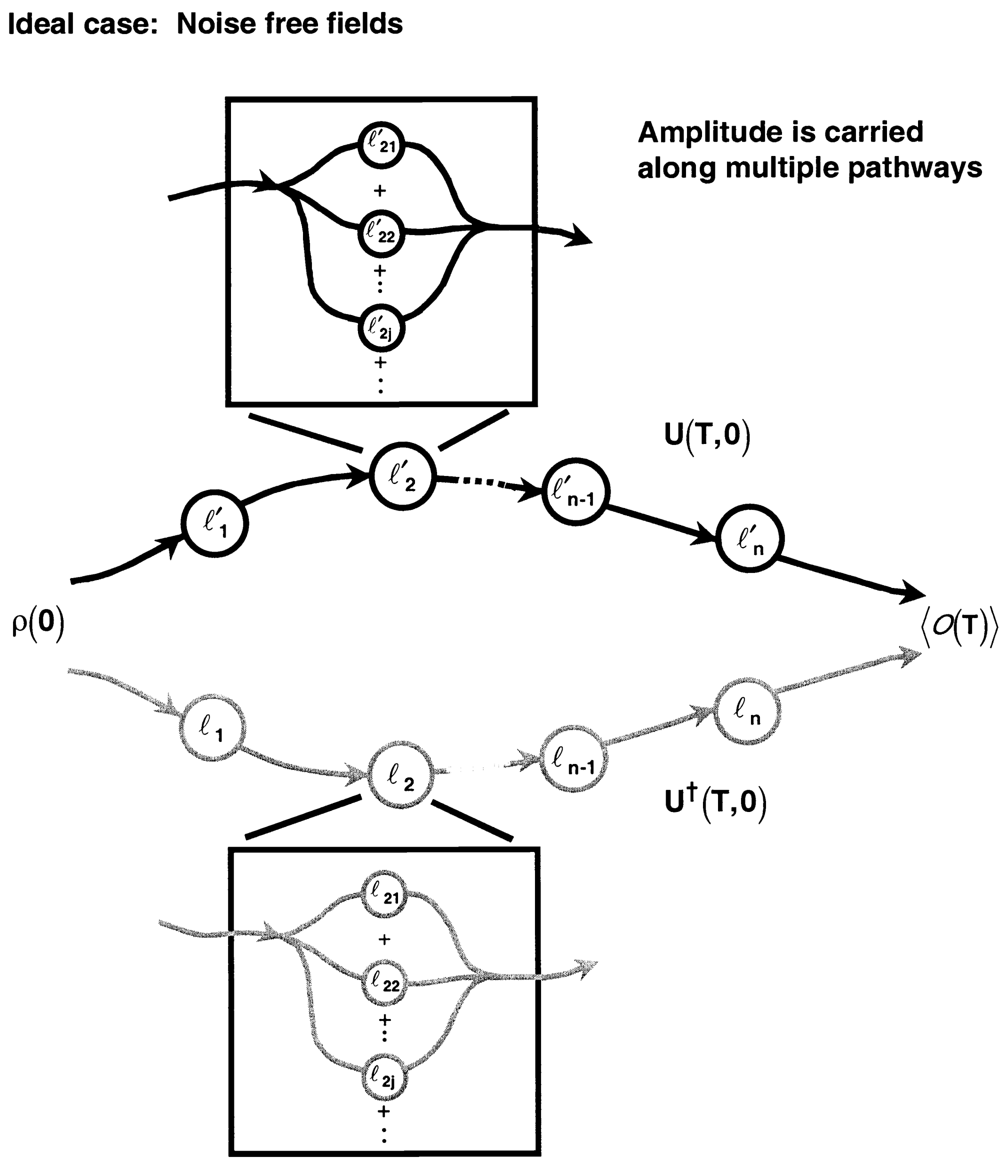

Figure 1. A schematic depicting the transformation from the initial density operator $\rho(0)$ to the final expectation value $\langle O(\mathrm{T})\rangle$ through a series of dynamical states $|\ell_1\rangle$ and $|\ell'_1\rangle$, i = 1,..., acting as stopping-off points on the excursion. In this case, the dynamics are noise-free with complete transfer of phase across each intermediate state depicted by the independent flow of amplitude for U and $\mathrm{U}^\dagger$. The many possible states are shown in the boxes.

The field fluctuations from one interval to the next are assumed to be statistically independent of each other, such that

$$P(\delta\varepsilon(t)) = \prod_{q=0}^{n} P_q\left(\delta\varepsilon_q(t)\right). \tag{11}$$

This factorized form implies that the noise fluctuations have a memory shorter than the time intervals $t_q - t_{q-1}$ for each of the physical evolution steps. The presence of correlated noise over extended time periods would change this assumption, and a careful analysis of laser pulse noise is necessary for a more elaborate analysis. Proceeding with the present assumption, combining Eqs. (8), (10), and (11) shows that each of the terms is a separate average over an ensemble of noise trajectories. A typical term in Eq. (9) becomes an average:

$$\left\langle S_{q,q-1}\right\rangle_{\{\delta\varepsilon_{q-1}\}} = \int D\left[\delta\varepsilon_{q-1}(t)\right] P_{q-1}\left(\delta\varepsilon_{q-1}(t)\right) S_{q,q-1}\left(\left[\delta\varepsilon_{q-1}(t)\right]\right). \tag{12}$$

The most sensitive functional dependence on the field fluctuations in Eq. (9) is assumed to arise in the phase factors, rather than the moduli. A stationary phase analysis can be performed sequentially on all of the terms in Eq. (8). This will lead to the form

$$\begin{aligned}\left\langle \mathcal{O}(T)\right\rangle_{\{\delta\varepsilon\}} \simeq \sum_{\ell_i, i=1,\ldots,n} & \left|\left\langle \ell_1 \middle| U(t_1,0)\middle|\rho(0)\middle|U^{\dagger}(t_1,0)\middle|\ell_1\right\rangle\right| \\ & \times\left|\left\langle \ell_1 \middle| U(t_1,t_2)\middle|\ell_2\right\rangle\right|^2 \cdots\cdots \left|\left\langle \ell_{n-1} \middle| U(t_{n-1},t_n)\middle|\ell_n\right\rangle\right|^2 \\ & \times\left\langle \ell_n \middle| U^{\dagger}(T,t_n)\middle|\mathcal{O}\middle|U(T,t_n)\middle|\ell_n\right\rangle .\end{aligned} \tag{13}$$

Comparison of the structure in Eq. (13) with that in Eq. (8) shows that the process of seeking optimally controlled system performance in the presence of field noise has broken the evolution $\rho(0) \rightarrow \left\langle \mathcal{O}(T)\right\rangle_{\{\delta\varepsilon\}}$ into a sequence of steps, as shown in Figure 2. Coherence is fully maintained within each step (e.g., $\left|\left\langle \ell_1 \middle| U(t_1,t_2)\middle|\ell_2\right\rangle\right|^2$), but is broken in going from one step to the next. An important point is that Eq. (13) represents an extreme limit where phase transmission across each stationary phase point is fully blocked. In practice, differing degrees of phase transmittal across at these points can occur.

When operating with intense fields, a tradeoff will likely exist. Control with intense fields has attractive features (e.g., the lifting of constraining resonant conditions), but significant field fluctuations can have a deleterious effect on the control process. The graduated influence of field noise evident in the analysis above should allow for a balance of good quality control while still assuring an acceptable level of robustness to field noise.

3. DISCUSSION

A basic premise is that the best control results will maximally utilize constructive and destructive (C/D) interferences to discriminate amongst the desired and undesired product channels[24]. Equation (13) strictly applies to the case of there at least being a single intermediate stop-off point, $n \geq 1$, on the path $\rho(0) \Rightarrow \langle \mathcal{O}\rangle$. In the laboratory, there will always be a finite amount of field noise, thereby likely corresponding to the presence of one or more intermediate stopping-off points on the control pathway, as shown in Figure 2. Each of these points breaks the C/D interference process into sub-pieces, likely resulting in less than full control. The search for optimality will attempt to drive up the degree of C/D interference manipulation, while assuring that the control results are as robust as possible to field noise. Partial transmission of phase information across the stop-off points can occur, which will be beneficial to C/D interference. The stable structure of Eq. (13) suggests that reasonable levels of field noise, even at high field intensities, may not result in a catastrophic loss of control. Perhaps the best evidence for this behavior is the success of the recent high field quantum control experiments involving molecular dissociation and rearrangement[7], as well as selective high harmonic generation[5].

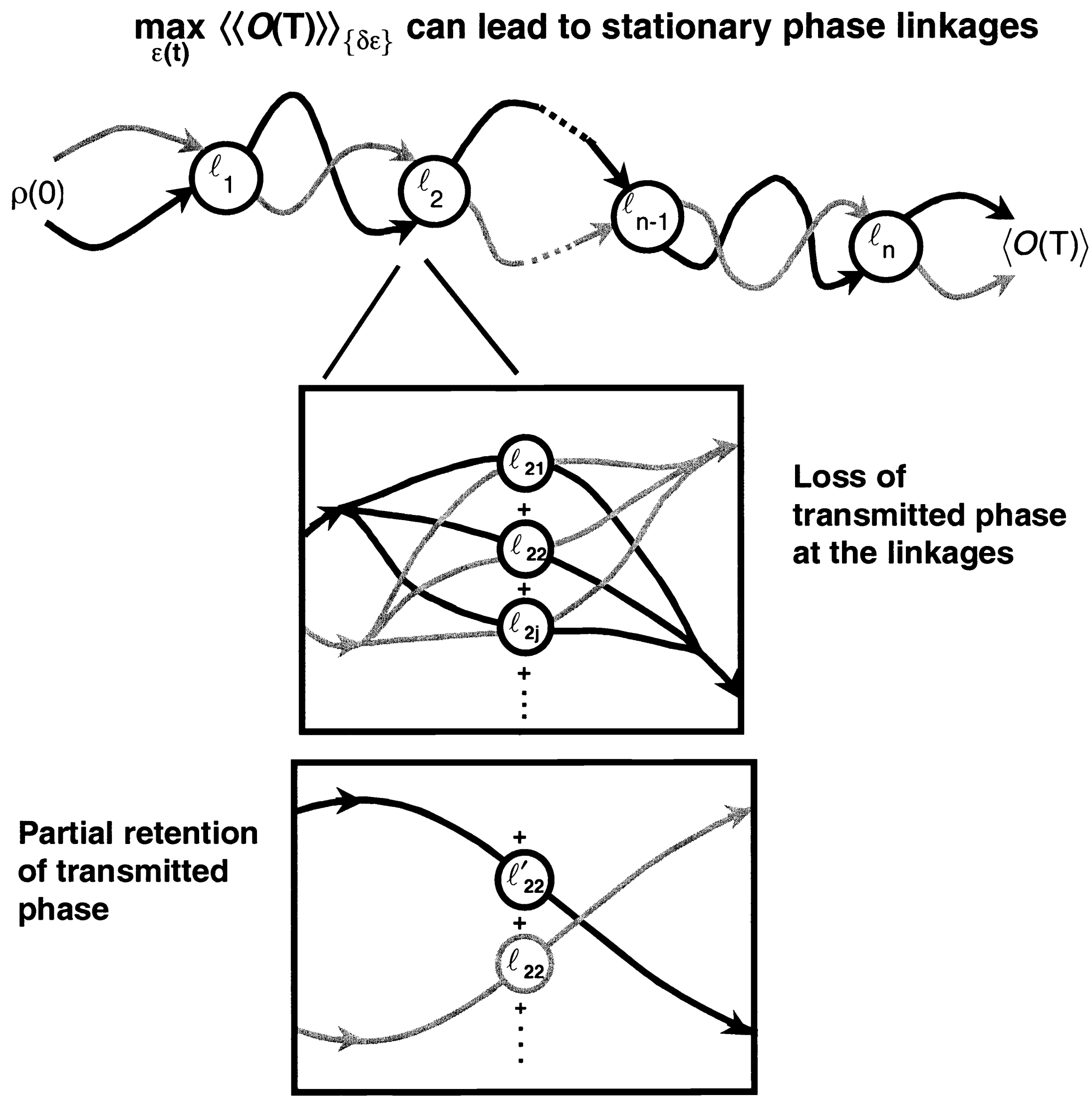

Figure 2. The structure arising along the path $\rho(0) \rightarrow \langle O(T) \rangle_{\{\delta\varepsilon\}}$ due to seeking optimal quantum system performance in the presence of control field noise. In spite of noise being present, the optimization process seeks to retain a maximum degree of control through manipulation of constructive/destructive interferences. The result is a reduction of the structure in Figure 1 down to a sequence of steps shown here and explicitly expressed in Eq. (13). Within each step (e.g., $\ell_1 \rightarrow \ell_2$), full quantum evolutionary coherence is retained while the process is broken in going from one step to the next (e.g., $\ell_1 \rightarrow \ell_2$ and then $\ell_2 \rightarrow \ell_3$). The interference retained within a step is depicted by the complex interleaving paths. The nature of the $|\ell_i\rangle$ states, their total number n, and their location along the excursion, is dictated by the ensemble of noise trajectories $\{\delta\varepsilon(t)\}$ associated with the control field. The bilinear nature of $\langle O(T) \rangle$, in terms of U and $U^\dagger$ is the origin of the inherent robustness in the evolution, expressed as a set of intermediate coherent steps towards the target $\langle O(T) \rangle$, rather than a total loss of control due to field noise. The resultant loss of phase transmitted, either total or partial, is indicated in the boxes shown the corresponding coupled or partially decoupled amplitudes.

One limiting class of experiments will be those carried out without any benefit of optimal field training to meet the objectives. The expectation is that this circumstance will utilize little, if any, beneficial C/D interferences, but perhaps exhibit a good degree of robustness to field noise. This regime should correspond to employing a maximum number of intermediate stop-off points in Eq. (13), producing a ladder of stepwise transitions to the final outcome.

Consider now the number of steps n on the way to the target in Eq. (13), as well as their location in time and quantum number space $\{t_q, \ell_q\}$. The sequence of points $\{t_q, \ell_q\}$ are those locations where there is *high* quantum evolution phase sensitivity to field fluctuations. In order to optimally achieve the control objective with good robustness, the quantum evolution phase sensitivity is diminished at $\{t_q, \ell_q\}$, by cancellation of the pairs of phases at the analogous points along the evolution of U(T,0) and $U^{\dagger}(T,0)$. Increasing noise levels should lead to more such intermediate phase sensitive points $\{t_q, \ell_q\}$, with the limit ultimately reducing the dynamics to a sequence of incoherently coupled steps. Such a chain of simple steps is still quantum mechanical, as governed by the system selection rules. The physical nature of the intermediate states $|\ell_q\rangle$, $q = 1, 2, \ldots, n$ is dictated by the optimal control process seeking the best system performance. These intermediate states might be members of the eigenstates of H_0 or superpositions of them to form virtual states. The guidance is strictly driven by seeking optimality.

4. CONCLUSION

This paper argued that a relationship exists between (a) the nature of quantum dynamics being bilinear in U and $U^{\dagger}$, (b) the presence of field fluctuations, (c) the attainment of optimality, and (d) the robustness of the control process. Although noise is expected to generally have a deleterious effect on achieving control, especially in the non-perturbative regime, the analysis showed that good control selectivity may still remain, with the power of optimality fighting to achieve the best results possible[25]. To push this analysis further, it would be very desirable to carefully assess the nature of shaped laser pulse noise.

In many applications, even a modest degree of stable control would be quite acceptable. A notable exception may arise in quantum information science[26], where the highest quality control is sought. Regardless of the application, seeking optimality should provide the best operational performance, including robustness. The analysis in this paper bodes well for the future success of control over quantum phenomena, including in the strong field regime.

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