Dynamical realizability of kinematical bounds on the optimization of observables for quantum systems

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Abstract

In previous work we derived kinematical bounds on the optimization of observables for mixed-state quantum systems and showed that they are dynamically realizable if the system is completely controllable. In this paper the problem of finding dynamically realizable bounds for systems that are not completely controllable is addressed. We derive such bounds for systems whose dynamics can be decomposed into subspace dynamics. We also study systems that are not decomposable yet fail to be completely controllable. For these systems, the question of dynamical realizability of the kinematical bounds depends on the accessibility of the target states for which the expectation value of the observable assumes its kinematical maximum.

1 Introduction

In [1] we derived upper and lower kinematical bounds for the expectation value (ensemble average) of arbitrary observables for mixed-state quantum systems. The question arises whether it is actually possible to steer the system in such a way that the observable assumes its kinematical upper or lower bound. This question of dynamical realizability of the kinematical bounds is of theoretical as well as practical interest. If the kinematical bounds are dynamically realizable then the values of the global extrema of the ensemble average of a given observable are known. Independent knowledge of the global extrema of the observable allows one to determine how close to the global maximum a given control steers the system, and thus to assess the effectiveness of the control in realizing the control objective. This can be a crucial step when one attempts to solve the global optimization problem of steering the system from its initial state to a target state for which the observable assumes its global maximum since most algorithms designed to find optimal controls [4, 5] are based on a set of differential equations that constitute necessary but not sufficient conditions for optimality. The control algorithms may thus produce controls that steer the system to a local maximum or even a minimum, for instance.

2 Mathematical Setup

We consider a quantum-mechanical system whose state space $\mathcal{H}$ is a separable Hilbert space. Any mixed state of the system can be represented by a density operator $\hat{\rho}(t)$ on $\mathcal{H}$ with eigenvalue decomposition

$$\hat{\rho}(t) = \sum_k w_k |\Psi_k(t)\rangle\langle\Psi_k(t)|, \tag{1}$$

where w_k are the eigenvalues and $|\Psi_k(t)\rangle$ the corresponding normalized eigenstates of $\hat{\rho}(t)$, which evolve in time according to the time-dependent Schrödinger equation. The eigenvalues satisfy

$$0 \le w_k \le 1 \quad \forall k, \qquad \sum_k w_k = 1. \tag{2}$$

Unless otherwise specified, we shall use the word "state" in the following to refer to a mixed quantum state represented by a density operator $\hat{\rho}$.

If the system is Hamiltonian, $\hat{\rho}(t)$ evolves according to

$$\hat{\rho}(t) = \hat{U}(t,t_0)\hat{\rho}_0\hat{U}(t,t_0)^\dagger, \tag{3}$$

where $\hat{U}(t,t_0)$ is the time-evolution operator of the system satisfying the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}\hat{U}(t,t_0) \tag{4}$$

with $\hat{U}(t_0,t_0) = \hat{1}$. $\hat{H}$ is the total Hamiltonian of the system. $\hat{\rho}(t)$ also satisfies the quantum Liouville equation

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = [\hat{H},\hat{\rho}(t)], \tag{5}$$

with initial condition $\hat{\rho}(t_0) = \hat{\rho}_0$.

Observables are represented by Hermitian operators $\hat{A}$ on $\mathcal{H}$ and we define their expectation value to be the *ensemble average*

$$\langle \hat{A}(t) \rangle = \mathrm{Tr}\left(\hat{A}\hat{\rho}(t)\right). \qquad (6)$$

3 Universal Kinematical Bounds on the Optimization of Observables

In [1] we proved the following results.

Theorem 1 *Let $\hat{A}$ be a Hermitian operator on $\mathcal{H}$ with eigenvalue decomposition*

$$\hat{A} = \sum_{i=1}^{m} a_i \hat{I}(a_i), \qquad (7)$$

and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$ be the eigenvalues a_i, counted with multiplicity and ordered in a non-increasing sequence. Then we have

$$\sum_{k=1}^{N} \lambda_{N-k+1} w_k \leq \mathrm{Tr}\left(\hat{A}\hat{\rho}(t)\right) \leq \sum_{k=1}^{N} \lambda_k w_k, \qquad (8)$$

provided that the weights w_k are also ordered in a non-increasing sequence, i.e., $w_1 \geq w_2 \geq \ldots \geq w_k \geq \ldots$.

Theorem 2 *$\langle A(t_F) \rangle$ assumes its upper bound if for $k = 1, \cdots, m$*

$$span_{j=1,\ldots,d(k)} |\Psi_{r(k,j)}(t_F)\rangle = E(a_k), \qquad (9)$$

and its lower bound if for $k = 1, \cdots, m$

$$span_{j=1,\cdots,d(k)} |\Psi_{r(k,j)}(t_F)\rangle = E(a_{N-k+1}), \qquad (10)$$

where $d(k) = \dim E(a_k)$, i.e., the dimension of the eigenspace belonging to the eigenvalue a_k and $r(k,j) = d(1) + \cdots + d(k-1) + j$.

Thus, to attain the kinematical maximum for an observable whose eigenvalues are distinct with multiplicity one, we need to find a unitary transformation that simultaneously maps the initial pure state with the largest probability w_1 onto the eigenspace corresponding to the largest eigenvalue of $\hat{A}$, the initial state with the second largest probability w_2 onto the eigenspace corresponding to the second largest eigenvalue of $\hat{A}$, and so forth. If $\hat{A}$ is a projector onto a subspace of dimension d, then realization of the kinematical upper bound requires finding a unitary transformation that maps the d initial states with the d largest probabilities onto the eigenspace corresponding to the eigenvalue one of $\hat{A}$.

4 Dynamical Realizability of the Universal Kinematical Bounds

To formulate the question of dynamical realizability precisely, let us define this expression as follows.

Definition 1 *A kinematical bound for an observable is* dynamically realizable *if there exists an admissible control-trajectory pair that steers the system from the initial state $\hat{\rho}(t_0)$ to a final state $\hat{\rho}(t_F)$, for which the expectation value of the target observable assumes its kinematical maximum or minimum.*

For a Hamiltonian quantum system, the only admissible trajectories are given by equation (3), where $\hat{\rho}_0$ is the initial state of the system and $\hat{U}(t, t_0)$ is the propagator satisfying (4). Since $\hat{H}$ is Hermitian, the propagator must be unitary.

The set of admissible controls depends on the constraints of the system considered. However, in general we can assume that an admissible control should be at least a bounded measurable function.

Equation (3) shows that the problem amounts to deciding whether every unitary operator $\hat{U}$ can be dynamically generated, i.e., $\hat{U} = \hat{U}(t_F, t_0)$. Since $U(N)$ is a group, it suffices to verify that every unitary operator is accessible from the identity. This motivates the following

Definition 2 *A non-dissipative quantum system is* completely *mixed-state* controllable *if every unitary operator in $U(N)$ is accessible from the identity operator $\hat{I}$ via a path that satisfies the dynamical law (4).*

If the system is completely controllable then every kinematically attainable target state can be reached dynamically from a given initial state. In this case, it is obvious that the kinematical bounds are always dynamically realizable, i.e., the kinematical upper and lower bounds correspond to the global maximum and minimum of $\langle \hat{A}(t_F) \rangle$, respectively, which can be attained if the system is driven with an optimal control $\mathbf{f}(t)$.

For control-linear systems, complete controllability can easily be verified numerically using the condition established by Ramakrishna et. al. [3].

Theorem 3 *An N-level quantum control system with Hamiltonian*

$$\hat{H} = \hat{H}_0 + \sum_{m=1}^{M} f_m(t) \hat{H}_m, \qquad (11)$$

where f_m are independent bounded measurable control functions, is completely controllable if and only if the

Lie algebra L_0 generated by the skew-Hermitian matrices $\{i\hat{H}_0, \ldots, i\hat{H}_M\}$ has dimension N^2 ($i = \sqrt{-1}$).

The question arises whether the universal kinematical bounds can dynamically realized for quantum systems that are not completely controllable, or whether improved bounds can be established in this case.

5 Dynamically Realizable Bounds for Decomposable Systems

One class of quantum systems that are obviously not completely controllable consists of decomposable systems, i.e., systems whose dynamics can be decomposed into independent subspace dynamics. For such systems the universal kinematical bounds can be improved.

Let us first consider a control-linear Hamiltonian system with a single control

$$\hat{H}(f(t)) = \hat{H}_0 + f(t)\hat{V}, \tag{12}$$

where $\hat{H}_0$ is the internal Hamiltonian of the unperturbed system and $\hat{V}$ defines the interaction with the control field $f(t)$.

In this case, the system is decomposable if there exists a basis $\mathcal{B}$ for the Hilbert space $\mathcal{H}$ such that $\hat{H}_0$ is diagonal and

$$\hat{V} = \hat{V}_1 \oplus \hat{V}_2 \doteq \left(\begin{array}{c|c} \hat{V}_1 & 0 \\ \hline 0 & \hat{V}_2 \end{array}\right). \tag{13}$$

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be orthogonal subspaces of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ and each $\hat{V}_\ell$ maps $\mathcal{H}_\ell$ to itself,

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2, \qquad \hat{V}_\ell : \mathcal{H}_\ell \to \mathcal{H}_\ell, \quad \ell = 1, 2. \tag{14}$$

It follows immediately that $\hat{H}(f(t))$ is block-diagonal,

$$\mathcal{H}(f(t)) = \hat{H}_1 \oplus \hat{H}_2 \doteq \left(\begin{array}{c|c} \hat{H}_1 & 0 \\ \hline 0 & \hat{H}_2 \end{array}\right) \tag{15}$$

and maps $\mathcal{H}_\ell$ to itself ($\ell = 1, 2$). Thus, the two subspaces $\mathcal{H}_1$ and $\mathcal{H}_2$ do not interact. Let $\mathcal{B}_\ell$ be the restriction of the basis $\mathcal{B}$ to the subspace $\mathcal{H}_\ell$; $\hat{P}_\ell$ be the projector onto the subspace $\mathcal{H}_\ell$ and N_ℓ denote the dimension of $\mathcal{H}_\ell$.

Given an observable $\hat{A}$ on $\mathcal{H}$, we define the restricted observables $\hat{A}_\ell = \hat{P}_\ell \hat{A}$ ($\ell = 1, 2$). Note that $\hat{A}_\ell$ is a Hermitian operator on the subspace $\mathcal{H}_\ell$, i.e.,

$$\hat{A}_\ell = \hat{P}_\ell \hat{A} \hat{P}_\ell : \mathcal{H}_\ell \to \mathcal{H}_\ell \quad \ell = 1, 2. \tag{16}$$

Let $\lambda_n^{(\ell)}$ denote the eigenvalues of $\hat{A}_\ell$, counted with multiplicity and ordered

$$\lambda_1^{(\ell)} \geq \lambda_2^{(\ell)} \geq \cdots \geq \lambda_{N_\ell}^{(\ell)}. \tag{17}$$

If $\hat{\rho}_\ell(t_0)$ is the density operator for subsystem ℓ, whose matrix representation with respect to the basis $\mathcal{B}_\ell$ is given by

$$\hat{\rho}_\ell(t_0) \doteq \mathrm{diag}(w_1^{(\ell)}, \ldots, w_{N_1}^{(\ell)}) \tag{18}$$

and $w_1^{(\ell)} \geq w_2^{(\ell)} \geq \cdots \geq w_{N_1}^{(\ell)}$ then we can apply Theorem 1 to obtain bounds for the expectation value of $\hat{A}_\ell$:

$$\sum_{n=1}^{N_\ell} w_{N_1-n+1}^{(\ell)} \lambda_n^{(\ell)} \leq \langle \hat{A}_\ell(t) \rangle \leq \sum_{n=1}^{N_\ell} w_n^{(\ell)} \lambda_n^{(\ell)}. \tag{19}$$

Notice that the total probability for each subspace is less or equal to one, and that the sum of the subspace probabilities must equal one, i.e.,

$$p_\ell = \sum_{n=1}^{N_\ell} w_n^{(\ell)} \leq 1, \quad p_1 + p_2 = 1. \tag{20}$$

If the probability for subspace ℓ is one then the initial ensemble is restricted to this subspace and since the subspaces do not interact, the ensemble will remain in this subspace forever, i.e., $p_\ell = 1$ for all times. In this case, $\langle \hat{A}(t) \rangle = \langle \hat{A}_\ell(t) \rangle$.

If both subspaces are initially occupied, i.e., both p_1 and p_2 are non-zero, then the density operator for the entire space $\mathcal{H}$ is the direct sum of the subspace density operators $\hat{\rho}_1(t_0)$ and $\hat{\rho}_2(t_0)$, i.e.,

$$\hat{\rho}(t_0) = \hat{\rho}_1(t_0) \oplus \hat{\rho}_2(t_0) \doteq \left(\begin{array}{c|c} \hat{\rho}_1(t_0) & 0 \\ \hline 0 & \hat{\rho}_2(t_0) \end{array}\right). \tag{21}$$

Since $\hat{H}$ maps each subspace to itself, we can conclude

$$\hat{\rho}(t) = \hat{\rho}_1(t) \oplus \hat{\rho}_2(t) \doteq \left(\begin{array}{c|c} \hat{\rho}_1(t) & 0 \\ \hline 0 & \hat{\rho}_2(t) \end{array}\right) \tag{22}$$

for $t > t_0$ and thus

$$\begin{aligned} \langle \hat{A}(t) \rangle &= \mathrm{Tr}\left(\hat{A}\hat{\rho}(t)\right) \\ &= \mathrm{Tr}\left(\begin{pmatrix} \hat{A}_1 & * \\ * & \hat{A}_2 \end{pmatrix}\begin{pmatrix} \hat{\rho}_1(t) & 0 \\ 0 & \hat{\rho}_2(t) \end{pmatrix}\right) \\ &= \mathrm{Tr}\begin{pmatrix} \hat{A}_1\hat{\rho}_1(t) & * \\ * & \hat{A}_2\hat{\rho}_2(t) \end{pmatrix} \\ &= \mathrm{Tr}\left(\hat{A}_1\hat{\rho}_1(t)\right) + \mathrm{Tr}\left(\hat{A}_2\hat{\rho}_2(t)\right) \end{aligned}$$

Since $\hat{\rho}_\ell(t)$ and $\hat{A}_\ell$ ($\ell = 1, 2$) are operators on $\hat{H}_\ell$, we can apply (19). Thus we have

Theorem 4 *Consider a decomposable quantum system with Hamiltonian $\hat{H} = \hat{H}_0 + f(t)\hat{V}$ where $\hat{H}_0$ is diagonal and $\hat{V}$ is of the form (13), which is initially in a state $\hat{\rho}_0$ as in (21). Then the expectation value of an arbitrary* *observable $\hat{A}$ is bounded by*

$$\langle \hat{A}(t)\rangle \geq \sum_{n=1}^{N_1} w_n^{(1)}\lambda_{N_1-n+1}^{(1)} + \sum_{n=1}^{N_2} w_n^{(2)}\lambda_{N_2-n+1}^{(2)} \quad (23)$$

$$\langle \hat{A}(t)\rangle \leq \sum_{n=1}^{N_1} w_n^{(1)}\lambda_n^{(1)} + \sum_{n=1}^{N_2} w_n^{(2)}\lambda_n^{(2)}, \quad (24)$$

where $\lambda_n^{(\ell)}$ are the eigenvalues of the subspace observable $\hat{A}_\ell$ ($\ell = 1,2$) counted with multiplicity and ordered in a non-increasing sequence.

The upper bound is attained at $t = t_F$ if for $k_\ell = 1,\cdots,m_\ell$ ($\ell = 1,2$)

$$span_{j=1,\ldots,d(k_\ell)} |\Psi^{(\ell)}_{r(k_\ell,j)}(t_F)\rangle = E(a^{(\ell)}_{k_\ell}), \quad (25)$$

and the lower bound is realized if for $k_\ell = 1,\cdots,m_\ell$ ($\ell = 1,2$)

$$span_{j=1,\cdots,d(k_\ell)} |\Psi^{(\ell)}_{r(k_\ell,j)}(t_F)\rangle = E(a^{(\ell)}_{N_1-k_\ell+1}), \quad (26)$$

where $d(k_\ell) = \dim E(a^{(\ell)}_{k_\ell})$ and $r(k_\ell, j) = d(1) + \cdots + d(k_\ell - 1) + j$,

This theorem provides improved bounds for decomposable systems and it is easy to see how it can be generalized to systems consisting of more than two non-interacting subsystems or control-linear systems with multiple controls. The improved bounds are dynamically realizable if all the subsystems are simultaneously completely controllable.

6 Applications of Bounds for Decomposable Systems

As a particular example, we consider the problem of energy maximization for a decoupled four-level system initially in thermal equilibrium, i.e.,

$$\hat{\rho}_0 = \sum_{n=1}^{4} w_n |n\rangle\langle n| \doteq \begin{bmatrix} w_1 & 0 & 0 & 0 \\ 0 & w_2 & 0 & 0 \\ 0 & 0 & w_3 & 0 \\ 0 & 0 & 0 & w_4 \end{bmatrix} \quad (27)$$

with weights $w_1 = 0.3850$, $w_2 = 0.2758$, $w_3 = 0.1976$ and $w_4 = 0.1416$ (Boltzmann distribution) whose internal Hamiltonian is given by

$$\hat{H}_0 = \sum_{n=1}^{4} E_n |n\rangle\langle n| \doteq \begin{bmatrix} 0.494762 & 0 & 0 & 0 \\ 0 & 1.45286 & 0 & 0 \\ 0 & 0 & 2.36906 & 0 \\ 0 & 0 & 0 & 3.24336 \end{bmatrix} \quad (28)$$

The target observable is the energy of the system,

$$\hat{A} = \hat{H}_0. \quad (29)$$

and the aim is to maximize the expectation value of $\hat{A}$ at the target time $t_F = 200$ fs, starting at $t_0 = 0$, subject to the constraints that the evolution of the system satisfy the quantum Liouville equation and that the pulse fluence be as small as possible. We study two cases of interactions.

Case A:

$$\hat{H}_1 = f(t)\sum_{n=1}^{3} d_n(|n\rangle\langle n+1| + |n+1\rangle\langle n|) \doteq f(t)\begin{bmatrix} 0 & 1.0 & 0 & 0 \\ 1.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.73205 \\ 0 & 0 & 1.73205 & 0 \end{bmatrix} \quad (30)$$

Case B:

$$\hat{H}_1 = f(t)\,(|1\rangle\langle 4| + |4\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2|) \doteq f(t)\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad (31)$$

where $f(t)$ is the external control field, which is to be determined. Both of these systems are decomposable and hence not completely controllable.

In case A, the expectation value of the observable is bounded by

$$1.5186 \leq \langle \hat{A}(t)\rangle \leq 1.6722. \quad (32)$$

according to Theorem 4. These bounds are dynamically attainable since each of the subsystems is completely controllable. Hence the relative yield is

$$\text{yield} = \frac{\langle \hat{A}(t_F)\rangle}{1.6722}. \quad (33)$$

In case B, the expectation value of the observable is bounded by

$$1.518570 \leq \langle \hat{A}(t)\rangle \leq 2.259226, \quad (34)$$

according to Theorem 4. Notice that these bounds are exactly the same as the kinematical bounds for the Morse oscillator model. Although the whole system is not completely controllable, the bounds are also dynamically realizable since both subsystems are controllable. Hence, the relative yield is

$$\text{yield} = \frac{\langle \hat{A}(t_F)\rangle}{2.259226}. \quad (35)$$

Figs 1–3 show the results of a control computation for case A, Figs 4–6 show the results of a control computation for case B. In both cases, the final yield is close to

100%, showing that our control algorithm did indeed produce a control that steers the system to a target state for which the expectation value of the internal energy (target observable) is close to its kinematical maximum. Furthermore, observe the simultaneous inversion of populations one/two and three/four in Fig. 2, as well as the simultaneous inversion of populations one/four and two/three in Fig. 5, exactly as predicted by Theorem 4.

7 Non-decomposable Systems Failing to be Completely Controllable

The question arises whether there are systems that are not completely controllable but still coupled in a way that the dynamics can not easily be decomposed into independent subspace dynamics. Unfortunately, the answer is yes. In such a case it is usually not easy to determine whether the kinematical bounds are dynamically realizable. In general, all that can be said is that dynamical realizability of the kinematical bounds for a particular observable depends on whether at least one of the target states for which the kinematical bound is attained is dynamically accessible from the initial state. Clearly, this depends on the choice of the observable, i.e., for some observables the kinematical bounds may still be dynamically attainable while for others they are not.

Example 1 *We performed computations for a four-level harmonic oscillator with*

$$\hat{H}_0 = \begin{bmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 1.5 & 0 & 0 \\ 0 & 0 & 2.5 & 0 \\ 0 & 0 & 0 & 3.5 \end{bmatrix}, \tag{36}$$

with the non-standard interaction term

$$\hat{H}_1 = f(t) \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{37}$$

This system differs from the standard harmonic oscillator in that all the transition dipole moments d_n are equal to one instead of $d_n = \sqrt{n}$. While the standard harmonic oscillator is always completely controllable [6] this system is not *completely controllable [7] although it is clearly* not *decomposable.*

Our preliminary computations maximizing (1) the energy of the system, i.e., $\hat{A} = \hat{H}_0$, and (2) the transition dipole moment $\hat{A} = \hat{V}$, assuming

$$\hat{\rho}_0 = \begin{bmatrix} 0.4 & 0 & 0 & 0 \\ 0 & 0.3 & 0 & 0 \\ 0 & 0 & 0.2 & 0 \\ 0 & 0 & 0 & 0.1 \end{bmatrix}, \tag{38}$$

indicate that it still seems to be possible to control the system rather effectively. The final yield after 20 iterations in the first case was 97.75 %. In the second case, the final yield after 20 iterations was 95.69%. [The figures have been omitted due to space constraints.]

This example shows that further investigation of systems that are not completely controllable is necessary.

8 Conclusion

We have presented universal kinematical bounds on the optimization of observables for non-dissipative quantum systems as well as general criteria for the dynamical realizability of these bounds. In particular, we showed that the kinematical bounds are always dynamically realizable if the system is completely controllable.

Improved bounds were derived for decomposable systems and it was demonstrated using several examples how these bounds can be used to assess the effectiveness of a numerically obtained "optimal" control in realizing the control objective.

In the last section we briefly examined the problems posed by systems that are neither completely controllable nor decomposable. We presented an example of a system of this type, for which we were nevertheless able to closely approximate the kinematical bounds dynamically for two different observables. The last example shows that complete controllability is not required for dynamical realizability of kinematical bounds and suggests further study of "partially" controllable, non-decomposable systems.

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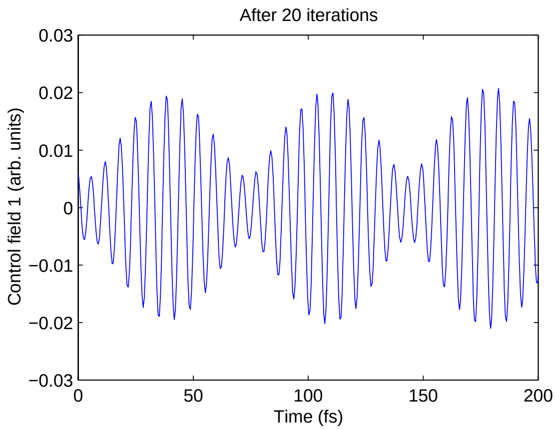

Figure 1: Energy maximization for a decoupled four-level system (Case A) initially in thermal equilibrium: optimal control field

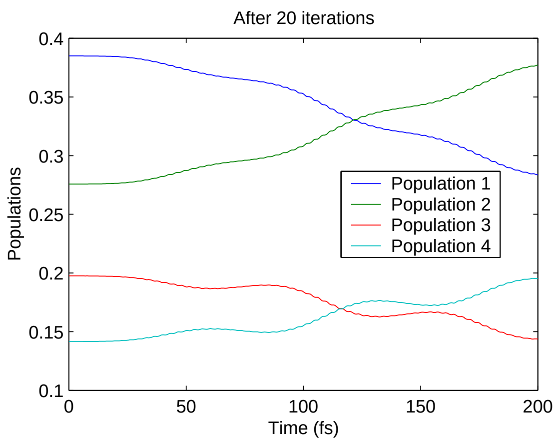

Figure 2: Energy maximization for a decoupled four-level system (Case A) initially in thermal equilibrium: evolution of the energy level populations

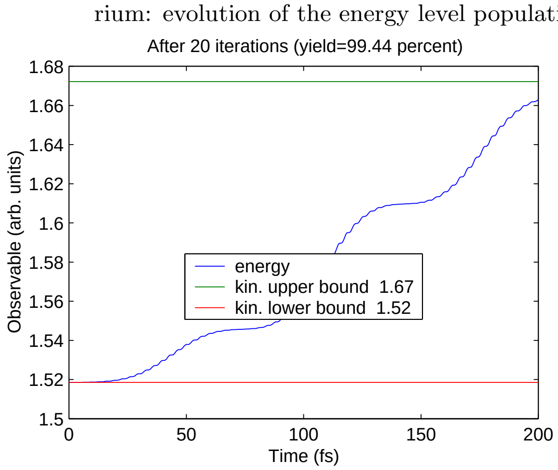

Figure 3: Energy maximization for a decoupled four-level system (Case A) initially in thermal equilibrium: evolution of the observable

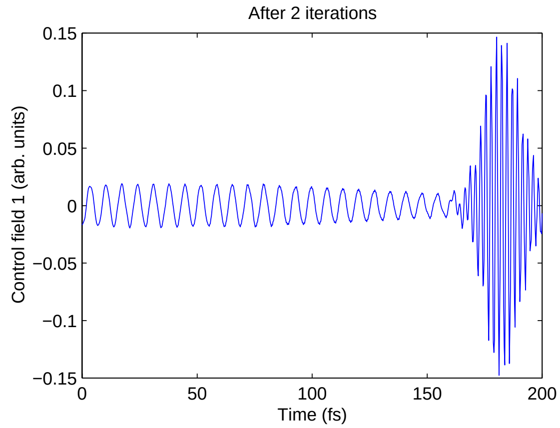

Figure 4: Energy maximization for a decoupled four-level system (case B) initially in thermal equilibrium: optimal control field

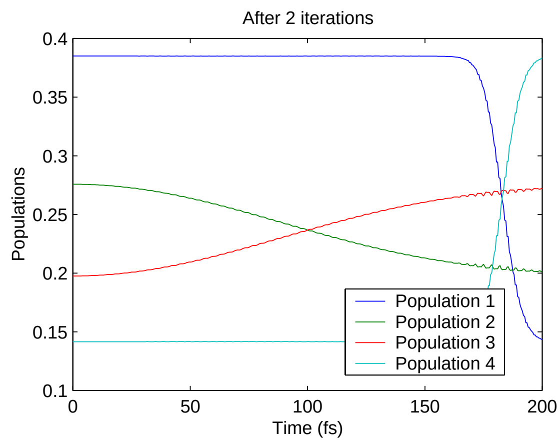

Figure 5: Energy maximization for a decoupled four-level system (case B) initially in thermal equilibrium: evolution of the energy level populations

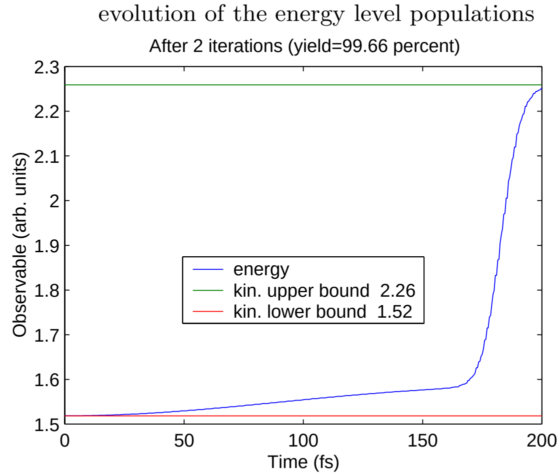

Figure 6: Energy maximization for a decoupled four-level system (case B) initially in thermal equilibrium: evolution of the observable