Projector Space Optimization in Quantum Control

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PROJECTOR SPACE OPTIMIZATION IN QUANTUM CONTROL *

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Abstract. We investigate in this work the numerical resolution of a quantum control problem; the specificity of the approach is that, instead of searching directly for the optimal laser intensity that drives the system toward its target, we consider here as main variable the evolution semigroup i.e. the set of propagators indexed with time. The precise form of the generator of the semigroup (e.g. dipolar) is then enforced as a constraint. We present both an algorithm and associated numerical results.

INTRODUCTION

Following successful quantum control experiments in the late 90s [1–4, 6, 7, 20] that build on the introduction of the evolutionary paradigm [5] a large number of works [8, 11–13, 17, 18, 21, 23] investigated numerically the control of quantum phenomena with laser fields.

The mean that allows to control the system is thus the laser field, more precisely its intensity. Traditionally, the numerical simulations considered some description of the interaction of the laser and the system, of which the most used is the *dipole approximation*, and performed optimizations considering the laser intensity as main variable.

We propose in this work a different view of the problem: we place ourselves in the evolution semigroup of unitary propagators and ask that the resulting Hamiltonian be consistent with the chosen approximation type.

The balance of the paper is as follows: we introduce the main notations and the technical choices that determine our problem in Section 1. Our specific optimization algorithm is presented in Sections 2 and 3 followed in Section 4 by numerical results.

1. PROBLEM SETTING

We consider a quantum system evolving under the Schrödinger equation (we use atomic units, i.e $\hbar = 1$):

$$\begin{aligned} i\frac{d}{dt}\psi(x,t) &= H(t)\psi(x,t), \\ \psi(t=0) &= \psi_{init} \end{aligned} \tag{1}$$

where $\psi(x,t)$ is the wavefunction, ψ_{init} is the initial data and $H(t)$ the Hamiltonian of the system. We assume that the system is described as finite dimensional, so that H is a $N \times N$ complex Hermitian matrix with entries in $\mathbb{C}$ and $\psi(x,t) \in \mathbb{C}^{\mathbb{N}}$. The initial data ψ_{init} verifies $\|\psi_{init}\| = 1$.

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This finite dimensional configuration represents an approximation of an infinite dimensional system. The same formulation of the system given by (1) can be expressed using the time evolution operator $U(t)$ $U(N)$, called the propagator:

$$\begin{aligned} i\frac{d}{dt}U(t) &= H(t)U(t) \\ U(t=0) &= I \end{aligned} \tag{2}$$

with the property $\psi(x,t) = U(t)\psi(x,0)$. We recall that $U(N)$ is the space of unitary matrices

$$U(N) = \{A \in \mathbb{C}^{N\times N}; AA^* = A^*A = Id\} \tag{3}$$

In the following we suppose that our system it is submitted to an external interaction taken here as an electric field. In the dipole approximation [9, 16, 19] the Hamiltonian $H(t)$ has the following form:

$$H(t) = H_0 + \varepsilon(t)\mu, \tag{4}$$

where H_0 is the internal Hamiltonian of the system $\varepsilon(t) \in \mathbb{R}$ is the intensity of the laser field and $\mu \in \mathbb{R}^{N\times N}$ the (coupling) dipole moment operator.

Both H_0 and μ are known, self adjoint operators. The control is here $\varepsilon(t)$ which can be chosen to influence the evolution of the system.

Our goal is to design an algorithm that finds an (optimal) laser field $\varepsilon(t)$ such that, under the control $\varepsilon(t)$, the system evolves from the initial state $U(t=0) = I$ to the final state $U(t=T) = U_T$.

We work in a space $\mathcal{H}_N$, of the hermitian matrices with the scalar product defined by:

$$\forall A, B \in \mathcal{H}_N \ < A, B >= real(tr(AB^*)), \tag{5}$$

where B^* is the transposed-conjugate of the matrix. This scalar product induces a norm on the space of Hermitian matrices:

$$\forall A \in \mathcal{H}_N \ \|A\| = \sqrt{< A, A >}. \tag{6}$$

Instead of searching for the intensity ε [12,21,22] we take here a different view and search for a path $U(t)$ in propagator space such that the corresponding Hamiltonian will be of type (4). This leads us to minimize the following functional

$$\int_0^T \|H - \Pi_{H_0+Span(\mu)}(H)\|^2 dt, \tag{7}$$

with the constraints:

- $H(t) = i\dot{U}(t)U^*(t)$ for every t in $[0,T]$
- $U^*(t)U(t) = U(t)U^*(t) = I$ for every t in $[0,T]$.

Since $\|H - \Pi_{H_0+Span(\mu)}(H)\| = \min_{\xi\in\mathbb{R}} \|H - H_0 - \xi\mu\| = \|H - H_0 - \Pi_{Span(\mu)}(H - H_0)\|$ our minimization problem can be written as :

$$\begin{cases} \min\limits_{U} \int_0^T \|H(t) - (H_0 + \Pi_{Span(\mu)}(H(t) - H_0))\|^2 dt \\ H(t) = i\dot{U}(t)U^*(t) \text{ for every t in } [0,T], \\ U^*(t)U(t) = U(t)U^*(t) = I \text{ for every t in } [0,T], \\ U(t=0) = I, U(t=T) = U_T. \end{cases} \tag{8}$$

Note that when $H(t) = H_0 + \varepsilon(t)\mu$, since $\Pi_{Span(\mu)}(H - H_0)) = \varepsilon(t)\mu$, we can define our laser field as

$$\epsilon(t) = \frac{< (H(t) - H_0), \mu >}{< \mu, \mu >}.$$

Once a path $\widetilde{U}(t)$ in propagator space has been given, to improve it we will search $U(t)$ of the form $U(t) = \widetilde{U}(t)\exp(iA(t))$, with $A(t) \in \mathcal{H}_N$. Since $U(t)U^*(t) = \widetilde{U}(t)e^{iA(t)}e^{-iA(t)}\widetilde{U}^*(t) = I$ for every $t \in [0,T]$, and replacing $H(t) = iU(t)U^*(t)$ we obtain a cost functional depending on $A(t)$ with no constraints:

$$J(U) = J^c_{\widetilde{U}}(A) = \int_0^T \|i\dot{U}(t)U^*(t) - (H_0 + \Pi_{Span(\mu)}(i\dot{U}(t)U^*(t) - H_0))\|^2 dt \tag{9}$$

$$U(t=0) = I, U(t=T) = U_T. \tag{10}$$

We discretize the interval $[0,T]$ with points $t_j = jT/N$; this allows to write an approximation for $\dot{U}(t)$ (e.g. by finite differences) . For a given integer N, we define the discretization parameter $\Delta T = T/N$, and U_j, A_j, H_j, ε_j represent approximations for $U(j\Delta T)$,$A(j\Delta T)$ $H(j\Delta T)$, $\varepsilon(j\Delta T)$. In the following we denote $\varepsilon = (\varepsilon_j)_{0\le j\le N}$, $U = (U_j)_{0\le j\le N}$, $A = (A_j)_{0\le j\le N}$, $H = (H_j)_{0\le j\le N}$. We consider the time discretized version of the cost function

defined in (9):

$$J_{\widetilde{U}}(A) = \Delta T \sum_{j=0}^{N} \|i\widehat{\dot{\widetilde{U}_j}e^{iA_j}}\widehat{\widetilde{U}_j e^{iA_j}}^* - (H_0 + \Pi_{Span(\mu)}(i\widehat{\dot{\widetilde{U}_j}e^{iA_j}}\widehat{\widetilde{U}_j e^{iA_j}}^* - H_0))\|^2 dt \tag{11}$$

$$A_j \in \mathcal{H}_N$$

$$U_0 = I, U_N = U_T.$$

2. ITERATION ALGORITHM

In order to minimize $J_U(A)$ with respect to A we use a gradient type method. At step $k-1$, for a given U^{k-1} we minimize $J_{U^{k-1}}(A)$ by taking $U^k = U^{k-1}e^{iA^k}$; we can easily verify that the property $U^k(U^k)^* = I$ holds at every step k.

To compute $\dot{U}^k$ we propose a centered finite differences formula:

$$\begin{aligned} H_j^k &= i\dot{U}_j^k(U_j^k)^* = i\frac{U_{j+1}^k - U_{j-1}^k}{2\Delta T}\frac{(U_{j+1}^k)^* + (U_{j-1}^k)^*}{2} \\ &= i\frac{U_{j+1}^k(U_{j+1}^k)^* + U_{j+1}^k(U_{j-1}^k)^* - U_{j-1}^k(U_{j+1}^k)^* - U_{j-1}^k(U_{j-1}^k)^*}{4\Delta T} \\ &= i\frac{U_{j+1}^k(U_{j-1}^k)^* - U_{j-1}^k(U_{j+1}^k)^*}{4\Delta T} \\ &= i\frac{U_{j+1}^{k-1}e^{iA_{j+1}^k}e^{-iA_{j-1}^k}(U_{j-1}^{k-1})^* - U_{j-1}^{k-1}e^{iA_{j-1}^k}e^{-iA_{j+1}^k}(U_{j+1}^{k-1})^*}{4\Delta T} \end{aligned} \tag{12}$$

Now we consider an iteration algorithm for solving the minimization problem (8). The iteration procedure is specified as follows:

Step $k \ge 2$

$$\begin{aligned} A_j^k &= -\rho\frac{\partial J_{U^{k-1}}(A)}{\partial A_j} \; for\; every\; j = 1,..,N-1 \\ U_j^k &= U_j^{k-1}e^{iA_j^k} \; for\; every\; j = 1,..,N-1 \end{aligned}$$

where ρ is a positive constant. Note that the new value of the functional $J(U^k)$ is:

$$J(U^k) = J_{U^{k-1}}(A) \quad = \quad \Delta T \sum_{j=0}^{N} \|i\dot{U}_j^k (U_j^k)^* - (H_0 + \Pi_{Span(\mu)}(i\dot{U}_j^k (U_j^k)^* - H_0))\|^2 dt$$

The boundary condition in each step are:

$$U_0^k = I, A_0^k = 0, U_N^k = U_T,$$

The corresponding control field at each iteration step can be written as:

$$\epsilon_j^k \quad = \quad \frac{< (H_j^k - H_0), \mu >}{< \mu, \mu >} \; for \; every \; j = 0, .., N.$$

In the following for simplicity reasons we note $\Pi_{Span(\mu)} = \Pi$ and $P = I - \Pi$ (I is the identity operator).

3. GRADIENT COMPUTATION

We explain in this section how to compute the variation $\frac{\partial J_{U^{k-1}}(A)}{\partial A_j}$.

Theorem 3.1. *The gradient of $J_{U^k}(A)$ is given by:*

$$\nabla J_{U^k}(A) = \Big(- 2(U_{j-1}^{k-1})^*(P(H_{j-1}^k)(0) - P(H_0))U_j^{k-1} - 2(U_j^{k-1})^*(P(H_{j-1}^k)(0) - P(H_0))U_{j-2}^{k-1} + \quad (13)$$

$$2(U_j^{k-1})^*(P(H_{j+1}^k)(0) - P(H_0))U_{j+2}^{k-1} + 2(U_{j+2}^{k-1})^*(P(H_{j+1}^k)(0) - P(H_0))U_j^{k-1}\Big)_{j=1,..,N-1} \quad (14)$$

Proof. In order to have an explicit formula for the gradient of $J_{U^k}(A)$ we will compute the partial derivatives of $J_{U^k}(A)$ with respect to A_j for every $j = 2, ..., N$ around the point $A = (0, 0, ..., 0)$.

$$\begin{aligned}
\frac{\partial J_{U^k}(A)}{\partial A_j}(A=0) \quad &= \quad \Delta T \frac{\partial}{\partial A_j}\Big(\sum_{j=0}^{N} \|H_j^k - \Pi H_j^k + \Pi H_0 - H_0\|^2\Big)\Big|_{A=0} \\
&= \quad \Delta T \frac{\partial}{\partial A_j}\Big(\sum_{j=0}^{N} < H_j^k - \Pi H_j^k + \Pi H_0 - H_0, H_j^k - \Pi H_j^k + \Pi H_0 - H_0 > \Big)\Big|_{A=0} \\
&= \quad \Delta T \Big\{ \frac{\partial}{\partial A_j} < P(H_{j-1}^k)(A_j) - P(H_0), P(H_{j-1}^k)(A_j) - P(H_0) > + \\
&\quad + \frac{\partial}{\partial A_j} < P(H_{j+1}^k)(A_j) - P(H_0), P(H_{j+1}^k)(A_j) - P(H_0) > \Big\}\Big|_{A=0}.
\end{aligned}$$

Continuing the computation we obtain

$$\begin{aligned}
&\frac{\partial}{\partial A_j} < P(H_{j-1}^k)(A_j) - P(H_0), P(H_{j-1}^k)(A_j) - P(H_0) >= \\
&\frac{\partial}{\partial A_j}(< P(H_{j-1}^k)(A_j), P(H_{j-1}^k)(A_j) > + \\
&+2 < P(H_{j-1}^k)(A_j), -P(H_0) > + < P(H_0), P(H_0) >)
\end{aligned}$$

which at the first order gives:

$$
\begin{aligned}
&< P(H_{j-1}^k)(A_j+\delta A_j), P(H_{j-1}^k)(A_j+\delta A_j) > \\
&+2 < P(H_{j-1}^k)(A_j+\delta A_j), -P(H_0) > + < P(H_0), P(H_0) >= \\
&=< P(H_{j-1}^k)(A_j), P(H_{j-1}^k)(A_j) > +2 < P(H_{j-1}^k)(A_j), P(H_{j-1}^k)\frac{\partial}{\partial A_j}H_{j-1}^k(\delta A_j) > \\
&+2 < P(H_{j-1}^k)(A_j), -P(H_0) > +2 < P(H_{j-1}^k)\frac{\partial}{\partial A_j}H_{j-1}^k(\delta A_j), -P(H_0) > + \\
&< P(H_0), P(H_0) > +O(\delta A_j)^2.
\end{aligned}
$$

We proceed now by identification to obtain:

$$
\begin{aligned}
&\frac{\partial}{\partial A_j} < P(H_{j-1}^k)(A_j) - P(H_0), P(H_{j-1}^k)(A_j) - P(H_0) >= \\
&= 2 < P(H_{j-1}^k)(A_j), P(H_{j-1}^k)\frac{\partial H_{j-1}^k}{\partial A_j}(\delta A_j) > \\
&+2 < P(H_{j-1}^k)\frac{\partial H_{j-1}^k}{\partial A_j}(\delta A_j), -P(H_0) > \\
&= 2 < P(H_{j-1}^k)(A_j) - P(H_0), P(H_{j-1}^k)\frac{\partial H_{j-1}^k}{\partial A_j}(\delta A_j) > \\
&= 2 < P^*(P(H_{j-1}^k)(A_j) - P(H_0)), \frac{\partial H_{j-1}^k}{\partial A_j}(\delta A_j) > \\
&= 2 < P(H_{j-1}^k)(A_j) - P(H_0), \frac{\partial H_{j-1}^k}{\partial A_j}(\delta A_j) > .
\end{aligned}
\tag{15}
$$

Using the same method we can also prove:

$$
\begin{aligned}
&\frac{\partial}{\partial A_j} < P(H_{j+1}^k)(A_j) - P(H_0), P(H_{j+1}^k)(A_j) - T(H_0) >= \\
&= 2 < P(H_{j+1}^k)(A_j) - P(H_0), \frac{\partial H_{j+1}^k}{\partial A_j}(\delta A_j) > .
\end{aligned}
\tag{16}
$$

In order to compute $\frac{\partial H_{j-1}^k}{\partial A_j}$ and $\frac{\partial H_{j+1}^k}{\partial A_j}$ we will use relation (12), and a first order approximation to obtain:

$$
\begin{aligned}
H^k_{j-1}(A_j+\delta A_j)\big|_{A=0} &= \Big(i\frac{U^{k-1}_j e^{iA_j+i\delta A_j}e^{-iA_{j-2}}(U^{k-1}_{j-2})^*}{4\Delta T} - \\
&\quad -i\frac{U^{k-1}_{j-2}e^{iA_{j-2}}e^{-iA_j-i\delta A_j}(U^{k-1}_j)^*}{4\Delta T}\Big)\big|_{A=0} \\
&= \Big(i\frac{U^{k-1}_j(I+iA_j+i\delta A_j)(I-iA_{j-2})(U^{k-1}_{j-2})^*}{4\Delta T} - \\
&\quad i\frac{U^{k-1}_{j-2}(I+iA_{j-2})(I-iA_j-i\delta A_j)(U^{k-1}_j)^*}{4\Delta T}\Big)\big|_{A=0} \\
&= i\frac{U^{k-1}_j(U^{k-1}_{j-2})^* - iU^{k-1}_{j-2}(U^{k-1}_j)^*}{4\Delta T} + \\
&\quad i\frac{U^{k-1}_j i\delta A_j(U^{k-1}_{j-2})^* - iU^{k-1}_{j-2}(-i\delta A_j)(U^{k-1}_j)^*}{4\Delta T} + O(\delta A_j)^2.
\end{aligned}
$$

Again by identification we determine that:

$$
\frac{\partial H^k_{j-1}(A_j)}{\partial A_j}(\delta A_j)\big|_{A=0} = i\frac{U^{k-1}_j i\delta A_j(U^{k-1}_{j-2})^* - iU^{k-1}_{j-2}(-i\delta A_j)(U^{k-1}_j)^*}{4\Delta T}. \tag{17}
$$

Same arguments can be invoked to prove :

$$
\frac{\partial H_{j+1}(A_j)}{\partial A_j}(\delta A_j)\big|_{A=0} = i\frac{U^{k-1}_{j+2} i\delta A_j(U^{k-1}_j)^* - iU^{k-1}_j(-i\delta A_j)(U^{k-1}_{j+2})^*}{4\Delta T}. \tag{18}
$$

Substituting (17), (18) into (15) and respectively (16) we obtain:

$$
\begin{aligned}
\frac{\partial J_{U^k}}{\partial A_j}(\delta A_j)(A=0) &= \Delta T\Big\{2 < P(H^k_{j-1}) - P(H_0), \frac{-U^{k-1}_j\delta A_j(U^{k-1}_{j-2})^* - U^{k-1}_{j-2}(\delta A_j)(U^{k-1}_j)^*}{4\Delta T} > \\
&\quad +2 < P(H^k_{j+1}) - P(H_0), \frac{+U^{k-1}_{j+2}\delta A_j(U^{k-1}_j)^* + U^{k-1}_j(\delta A_j)(U^{k-1}_{j+2})^*}{4\Delta T} > \Big\} \\
&= -0.5 real(tr((P(H^k_{j-1}) - P(H_0))U^{k-1}_j(\delta A_j)(U^{k-1}_{j-2})^*) \\
&\quad -(P(H^k_{j-1}) - P(H_0))U^{k-1}_{j-2}(\delta A_j)(U^{k-1}_j)^*)) \\
&\quad +0.5 real(tr((P(H^k_{j+1}) - P(H_0))U^{k-1}_{j+2}(\delta A_j)(U^{k-1}_j)^*) \\
&\quad +(P(H^k_{j+1}) - P(H_0))U^{k-1}_j(\delta A_j)(U^{k-1}_{j+2})^*)).
\end{aligned}
$$

Using the property of the scalar product $real(tr(AB^*)) = real(tr(AB))$ and the properties of the trace, by identification we obtain the relation (13) which concludes the proof.

□

The previous theorem allows to define the set C of the critical points of $J_U(A)$

$$
\begin{aligned}
C = \Big\{ & A = (A0, A_1, ..., A_N), A_j \in \mathcal{H}_N, \forall j = 0, ..N \Big| -2(U^{k-1}_{j-1})^*(P(H_{j-1})(0) - P(H_0)U^{k-1}_j \\
& -2(U^{k-1}_j)^*(P(H_{j-1})(0) - P(H_0)U^{k-1}_{j-2} + 2(U^{k-1}_j)^*(P(H_{j+1})(0) - P(H_0)U^{k-1}_{j+2} \\
& +2(U^{k-1}_{j+2})^*(P(H_{j+1})(0) - P(H_0)U^{k-1}_j = 0,\ j = 1, ..., N-1\Big\}.
\end{aligned} \tag{19}
$$

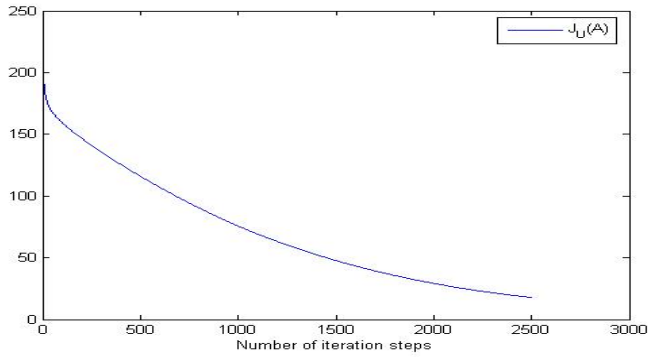

FIGURE 1. Convergence of the functional J towards the minimum value vs the number of iterations.

4. NUMERICAL SIMULATIONS

In order to demonstrate the efficiency of the algorithm, we choose a five-dimensional test system [14, 15] having internal Hamiltonian H_0 and dipole moment operator μ:

$$H_0 = \begin{pmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.2 & 0 & 0 & 0 \\ 0 & 0 & 1.3 & 0 & 0 \\ 0 & 0 & 0 & 2.0 & 0 \\ 0 & 0 & 0 & 0 & 2.15 \end{pmatrix}, \ \mu = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{pmatrix}$$

Numerical simulations have been performed for a final time $T = 200$, which represents approximately 32 times the natural period, at which the system without control oscillates. The system evolves between the initial state $U_0 = I_5$ and the final state $U_T = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$. The functional $J(U)$ is positive and as we can see in $Fig.1$ the algorithm obtains linear convergence towards the minimum point, zero. As soon as the minimum point is reached we also obtain the optimal laser field, which representation is given by $Fig.3$.

After that we solve the equation (2) [10, 15] with $H(t) = H_0 + \varepsilon\mu$, where ε is the laser field given by the optimization algorithm, starting from the initial point U_0. In $Fig.4$ we represent $|U(1,1)|^2$ and $|U(5,1)|^2$ as functions of time, and we observe that the final state U_T is reached.

The algorithm provides satisfying results for a discretization time step $\Delta T < 10^{-1}$. If we choose the value of $\Delta T = 10^{-1}$ we accelerate the convergence of the functional towards the minimum point, but instead the laser field thus obtained doesn't allow the evolution of our system between the two chosen states.

If we take a small value for ΔT the error decreases and we can reach the final state U_T , but we need a larger number of iterations. The numerical simulations presented in $Fig.1$, $Fig.2$ $Fig.3$ and $Fig.4$ have been performed for $\Delta T = 0.04$, and $\rho = 0.01$.

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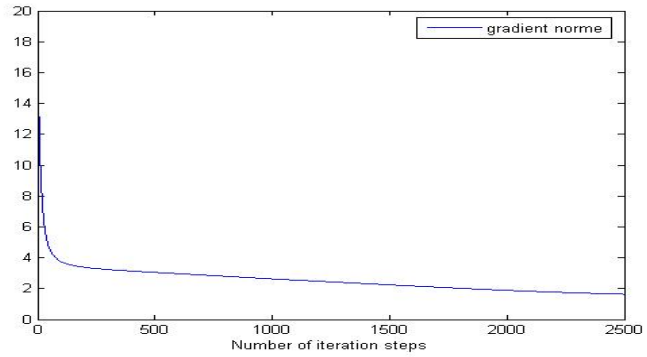

FIGURE 2. The value of the gradient norme $\|\nabla J\|$ vs the number of iterations.

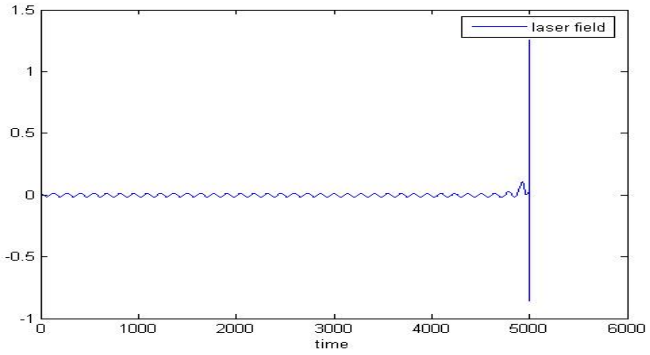

FIGURE 3. Optimized laser field as a function of time.

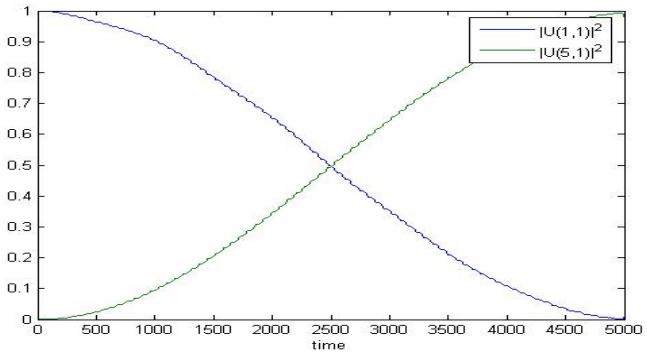

FIGURE 4. The values of $|U(1,1)|^2$ and $|U(5,1)|^2$ as functions of time.

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