Advanced computational methodologies for solving quantum control problems

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Application fields of quantum control methodologies

1. Quantum control: state transitions, laser induced chemistry, magnetic and optical trapping.
2. Quantum computing: qubits, data operations.
3. Quantum transport, superfluids of atoms, vortices.
4. Construction of barriers, channels, etc. for few atoms.
5. Amplification of material waves: laser of atoms.
6. Semiconductor nanostructures.
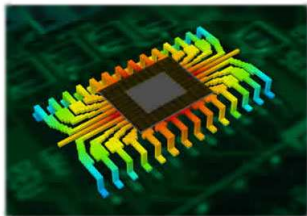
New challenges from quantum control problems

The possibility to manipulate states of atoms and molecules by means of laser pulses or magnetic fields opens new technological perspectives.

The solution of quantum control problems poses new challenges involving optimal control theory, numerical analysis, and scientific computing.

Quantum control models define an important class of nonlinear control mechanisms.

Quantum mechanical models

▶ One-particle Schrödinger equation, $\psi = \psi(x, t)$ or $\psi = \psi(t)$

$$i \frac{\partial}{\partial t} \psi = (H_0 + V_0 + V_{control}) \psi$$

▶ BEC Condensate Gross-Pitaevskii equation, $\psi = \psi(x, t)$

$$i \frac{\partial}{\partial t} \psi = \left(-\frac{1}{2} \nabla^2 + V_0 + V_{control} + g |\psi|^2 \right) \psi$$

▶ Time-dependent Kohn-Sham equation, $\psi_i = \psi_i(x, t)$

$$i \frac{\partial}{\partial t} \psi_i = \left(-\frac{1}{2} \nabla^2 + V_{ext} + V_{Hartree}(\rho) + V_{exc}(\rho) + V_{control} \right) \psi_i$$

where ψ_i, $i = 1, \ldots, N$ are the K-S orbitals; $\rho = \sum_{i=1}^{N} |\psi_i|^2$ is the one-electron density.

▶ Multi-particle (n) Schrödinger equation, $\psi = \psi(x_1, x_2, \ldots, x_n, t)$

$$i \frac{\partial}{\partial t} \psi = \left(-\frac{1}{2} \sum_{i=1}^{n} \nabla_i^2 + \sum_{i=1}^{n} V_i + \sum_{i,j=1}^{n} U_{ij} + V_{control} \right) \psi$$

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Quantum mechanics structure and objectives

Dynamically stable systems exist with confining potentials V_0

$$\left\{ -\nabla^2 + V_0(x) - E_j \right\} \phi_j(x) = 0, \quad j = 1, 2, \ldots,$$

where $\phi_j \in \mathcal{H}$ represent the eigenstates and E_j represent the energy. Here, $\mathcal{H}$ is a complex Hilbert space.

Control may be required to drive state transitions $\phi_i \longrightarrow \phi_j$.

The expectation value of a physical observable A when the system is in a state ψ is given by $(\psi, A\psi)$.

Control may be required to maximize observable expectation.

An Hermitian operator O may represent a transformation regardless of initial and final states (e.g., quantum gates).

Control may be required to obtain best performance of O.

Quantum control mechanisms

Laser pulses, electric fields, and magnetic fields represent physically meaningful control mechanisms. They are represented by potentials that sum up to the stationary one

$$V(x, t) = V_0(x) + V_{control}(x, t)$$

The dipole approximation of the electric control field modeling a laser pulse results in the form

$$V_{control}(x, t) = u(t) x$$

where $u : (0, T) \to \mathbb{R}$ is the modulating control amplitude.

A magnetic potential for manipulating a BEC is given by

$$V_{control}(x, u(t)) = -\frac{u(t)^2 d^2}{8c} x^2 + \frac{1}{c} x^4$$

where u is a parameter control function.

Mathematical issues of quantum control problems

- ▶ **Finite- and infinite-dimensional quantum systems**
  Finite-level systems are characterized by $H_0, V \in \mathbb{C}^{n \times n}$, while
  H_0 is unbounded in ∞-dim systems and $V : \Omega \times (0, T) \to \mathbb{R}$.

- ▶ **Existence and uniqueness of quantum optimal control**
  Existence of optimal solutions can usually be proven.
  Uniqueness usually does not occur: for dipole control, if $u(t)$
  is a minimizer, then so is $-u(t)$.

- ▶ **Exact and approximate controllability**
  A finite-level system is controllable iff $Lie\{i\,H_0, i\,V\} = su(n)$,
  the Lie algebra of zero-trace skew-Hermitian $n \times n$ matrices;
  see, e.g., Dirr & Helmke. For infinite-dimensional systems, see
  Beauchard & Coron, Chambrion, Mason, Sigalotti & Boscain,
  and Turinici.

- ▶ **Accurate and fast solution schemes for optimal control**
 Gradient schemes, monotonic schemes, Newton schemes, and
  multigrid schemes.

Optimal control of finite-level quantum systems

Optimal control of a finite-level quantum system

Quantum systems with a finite number of states model artificial atoms (semiconductor quantum dots) and quantum devices (quantum gates).

Consider a Λ-type three-level system with two stable states ψ_1 and ψ_2 (conservative), and one unstable state ψ_3 (dissipative).
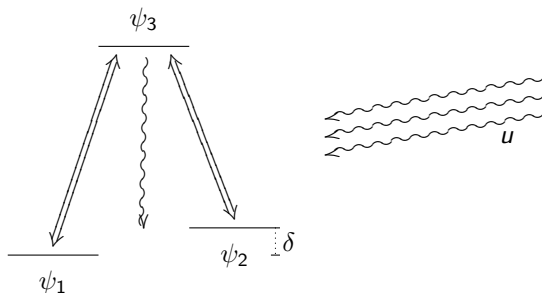
Finite-level quantum models

Governed by Schrödinger-type equations for a n-component wave function $\psi : [0, T] \to \mathbb{C}^n$ as follows

$$i\dot{\psi}(t) = H(u(t))\,\psi(t), \qquad \psi(0) = \psi_0,$$

for $t \in [0, T]$ and $T > 0$ is a given terminal time.

The function $u : [0, T] \to \mathbb{C}^m$ represents the external control field. Alternatively $u = (u_1, \ldots, u_{2m})$ and $u_i : [0, T] \to \mathbb{R}$

The linear Hamiltonian $H(u) = H_0 + V(u)$, consists of

A free Hamiltonian $H_0 \in \mathbb{C}^{n \times n}$ describing the unperturbed (uncontrolled) system;

A control Hamiltonian $V(u) \in \mathbb{C}^{n \times n}$ modeling the coupling of the quantum state to the control field u.

The objective of the quantum control

Control is applied to reach a target state at $t = T$.
One needs to avoid population of dissipative states during the control process, while having limited laser resources.
These modeling requirements may result in the following

$$
\begin{aligned}
J(\psi, u) \;=\; & \frac{1}{2} \left| \psi(T) - \psi_d \right|_{\mathbb{C}^n}^2 + \frac{\gamma}{2} \left\| u \right\|_{L^2(0,T;\mathbb{C})}^2 + \frac{\mu}{2} \left\| \dot{u} \right\|_{L^2(0,T;\mathbb{C})}^2 \\
& + \frac{1}{2} \sum_{j \in J} \alpha_j \left\| \psi_j \right\|_{L^2(0,T;\mathbb{C})}^2
\end{aligned}
$$

where ψ_d is the desired terminal state; $\gamma > 0$ and μ, $\alpha_i \geq 0$ are weighting factors; ψ_j denotes the j-th (dissipative) component of ψ.

First-order necessary optimality conditions

For the quantum optimal control problem

$$\min J(\psi, u), \text{ subject to } i\dot{\psi}(t) = H(u(t))\,\psi(t), \quad \psi(0) = \psi_0$$

Theorem
Suppose that $x = (\psi, u) \in X$ is a local solution to the optimal control problem. Then there exist (unique) Lagrange multipliers $p \in H^1(0, T; \mathbb{C}^n)$ ($\mu > 0$) satisfying

$$i\dot{\psi} = H(u(\cdot))\psi$$
$$i\dot{p} = H(u(\cdot))^* p - \alpha_j(\psi)_j$$
$$-\mu\ddot{u} + \gamma u = \Re e(p \cdot (V_r'(u)\psi)^*) + i\,\Re e(p \cdot (V_i'(u)\psi)^*)$$

where

$$\psi(0) = \psi_0, \qquad i p(T) = \psi(T) - \psi_d, \qquad u(T) = u(0) = 0.$$

Second-order optimality conditions

Consider the following optimal control problem

$$\begin{cases} \min_u J(\psi, u) & := & \frac{1}{2}|\psi(T) - \psi_d|^2 + \frac{\gamma}{2}\|u\|^2 \\ c(\psi, u) & := & i\dot\psi - a\,\psi - u\,\psi = 0 \end{cases}$$

The solution of the SE for a given u provides $\psi = \psi(u)$. We obtain the reduced objective $\hat{J}(u) = J(\psi(u), u)$. The reduced Hessian

$$(\nabla^2 \hat{J} \delta u, \delta u) = (W\delta u)(W\delta u)^* + 2\Re e(p\,\delta u, W\delta u) + \gamma(\delta u, \delta u).$$

where $W = W(\psi(u), u) = c_\psi(\psi(u), u)^{-1} c_u(\psi(u), u)$.

Because of unitary of evolution, we have $|p(t)| = |p(T)| = |\psi(T) - \psi_d|$.

Therefore, we have that $|\Re e(p\,\delta u, W\delta u)| \leq C(|u|)\,|\psi(T) - \psi_d|\,\|\delta u\|^2$.

For sufficiently small values of the tracking error $|\psi(T) - \psi_d|$ positiveness of the reduced Hessian is obtained.

Control of a Λ-type three-level model

Free Hamiltonian

$$H_0 = \frac{1}{2} \begin{pmatrix} -\delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & -i\Gamma_o \end{pmatrix}$$

where the term $-i\Gamma_o$ accounts for environment losses (spontaneous photon emissions, scattering of gamma rays from crystals).
The coupling to the external field is given by

$$V(u) = -\frac{1}{2} \begin{pmatrix} 0 & 0 & \mu_1 \, u \\ 0 & 0 & \mu_2 \, u \\ \mu_1 \, u^* & \mu_2 \, u^* & 0 \end{pmatrix}$$

where μ_1 and μ_2 describe the coupling strengths of states ψ_1 and ψ_2 to the inter-connecting state ψ_3 (e.g., optical dipole matrix elements).
Initial and final states are given by

$$\psi_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \text{ and } \psi_d = \begin{pmatrix} 0 \\ e^{-i\delta T} \\ 0 \end{pmatrix}$$

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Importance of optimization parameters

Smaller values of γ result in smaller $|\psi(T) - \psi_d|_{\mathbb{C}^3}$.

As μ increases, $|\psi(T) - \psi_d|_{\mathbb{C}^3}$ increases: additional smoothness of the control function (slightly) reduces the capability of tracking.

Larger μ makes the problem behaving better, resulting in a smaller number of iterations.

By taking $\alpha = \alpha_3 > 0$, dissipation is reduced and therefore better tracking is achieved.

γ	μ	α	$|\psi(T) - \psi_d|_{\mathbb{C}^3}$	J	CPU
10^{-7}	10^{-7}	0.05	$8.6 \cdot 10^{-4}$	$2.37 \cdot 10^{-3}$	19.6
10^{-7}	10^{-9}	0.05	$3.7 \cdot 10^{-4}$	$5.46 \cdot 10^{-4}$	55.6
10^{-7}	0	0.05	$6.9 \cdot 10^{-5}$	$1.41 \cdot 10^{-4}$	424.8
10^{-7}	0	0	$1.2 \cdot 10^{-3}$	$2.33 \cdot 10^{-6}$	763.1
10^{-4}	10^{-4}	0.05	$3.3 \cdot 10^{-2}$	$6.52 \cdot 10^{-2}$	47.3
10^{-4}	10^{-6}	0.05	$4.4 \cdot 10^{-3}$	$9.03 \cdot 10^{-3}$	42.3
10^{-4}	0	0.05	$2.7 \cdot 10^{-3}$	$5.68 \cdot 10^{-3}$	17.2
10^{-4}	0	0	$8.3 \cdot 10^{-3}$	$3.34 \cdot 10^{-4}$	5.5

Optimal solutions

With $\delta = 10$, $\Gamma_0 = 0.01$, $\mu_1 = \mu_2 = 1$, and $\gamma = 10^{-4}$, $\alpha_3 = 0.01$. We have $\mu = 0$ (top) and $\mu = 10^{-6}$ (bottom). Control (left) and state evolution (right).
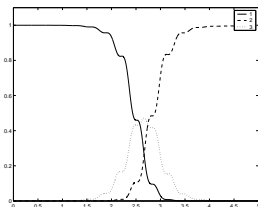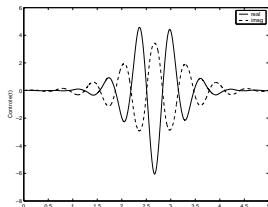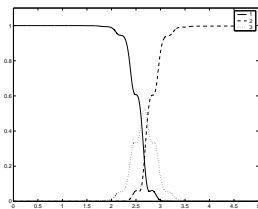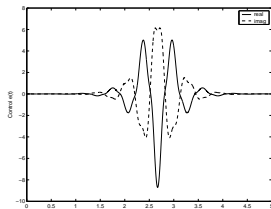
Performance of NCG, Cascadic-NCG, and CNMS schemes

The NCG scheme provides better performance while refining the computational mesh. There is a lack of robustness of the CNMS scheme for small $\gamma = 10^{-3}$ and severe convergence criteria $\|\nabla \hat{J}\| < tol_{abs}$.

	$N = 2048$		$N = 4096$	
tol_{abs}	CPU(NCG)	CPU(CNMS)	CPU(NCG)	CPU(CNMS)
10^{-4}	1.17	1.28	2.32	1.39
10^{-5}	4.32	12.63	9.26	15.92
10^{-6}	5.01	48.00	17.21	*no conv*

Dramatic improvement with the Cascadic-NCG version

	$\gamma = 10^{-4}$		$\gamma = 10^{-6}$	
N	CPU(NCG)	CPU(C-NCG)	CPU(NCG)	CPU(C-NCG)
4096	40.54	6.26	254.70	58.10
8192	112.57	12.71	319.46	134.00
16384	312.17	27.42	626.84	279.46

Computational effort to solve for $tol_{abs} = 10^{-6}$; $\gamma_0 = 0.01$, $\alpha_3 = 0.05$; in C-NCG coarsest level $N = 1024$.

Optimal control of infinite-dimensional quantum systems

Bose Einstein condensates model

Consider a bosonic gas (e.g. Rubidium) trapped in a magnetic field. By lowering the confining potential, atoms with higher energy escape and the remaining atoms condensate to a lower temperature.

The mean-field dynamics of the condensate is described by the Gross-Pitaevskii equation (GPE)

$$i \frac{\partial}{\partial t} \psi(x, t) = \left(-\frac{1}{2} \nabla^2 + V(x, u(t)) + g |\psi(x, t)|^2 \right) \psi(x, t)$$

We consider $V(x, u(t))$ is a potential produced by a magnetic microtrap. The control function $u(t)$ parameterizes the variation of the confining potential with time.

Magnetic trap with optical plug
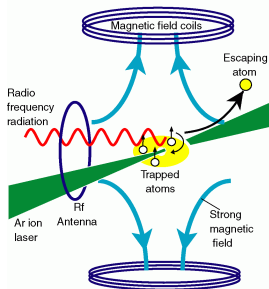
Control of matter at small scales

Trapping and coherent manipulation of cold neutral atoms in microtraps near surfaces of atomic chips is the focus of the present research towards control of matter at small scales.

This achievement has boosted developments in the atomic interferometry, the construction of quantum gates, the microscopic magnetic field imaging, quantum data encoding, etc..

At the base of all these developments is the ability to manipulate Bose-Einstein condensates (BEC) subject to a control potential.

We consider the problem to split and transport a BEC being confined in a single well $V(x, 0)$ at $t = 0$ to a double well $V(x, 1)$ at time $t = T$. We have

$$V(x, u(t)) = -\frac{u(t)^2 \, d^2}{8c} \, x^2 + \frac{1}{c} \, x^4$$

where $c = 40$ and d is the width of the double well potential.

Optimal control formulation and optimality system

Consider a BEC at the initial state ψ_0 and a target state ψ_d.

$$J(\psi, u) = \frac{1}{2}\left(1 - \left|\langle\psi_d|\psi(T)\rangle\right|^2\right) + \frac{\gamma}{2}\int_0^T (\dot{u}(t))^2 \, dt$$

Optimal control problem: Minimize the cost function $J(\psi, u)$ subject to the condition that ψ fulfills the Gross-Pitaevskii equation.

The optimal solution is characterized by the optimality system

$$i\frac{\partial}{\partial t}\psi = \left(-\frac{1}{2}\nabla^2 + V_u + g|\psi|^2\right)\psi$$

$$i\frac{\partial}{\partial t}p = \left(-\frac{1}{2}\nabla^2 + V_u + 2g|\psi|^2\right)p + g\,\psi^2\,p^*$$

$$\gamma\ddot{u} = -\Re e\langle\psi|\frac{\partial V_u}{\partial u}|p\rangle\,,$$

where $\langle u, v\rangle = \int_\Omega u(x)^* v(x)\, dx$. We have the initial and terminal conditions

$$\psi(0) = \psi_0 \quad \text{and} \quad ip(T) = -\langle\psi_d|\psi(T)\rangle\,\psi_d$$

$$u(0) = 0\,, \quad u(T) = 1\,.$$

The choice of the control space and the gradient

For a given potential $V(x, u(t))$, we have a unique $\psi(u) = \psi(x, t)$. In terms of u we have the reduced objective $\hat{J}(u) = J(\psi(u), u)$.
The Taylor series of $\hat{J}(u)$ in a Hilbert space X is

$$\hat{J}(u + \epsilon\varphi) = \hat{J}(u) + \epsilon \left(\nabla\hat{J}(u), \varphi\right)_X + \frac{\epsilon^2}{2} \left([\nabla^2\hat{J}(u)]\varphi, \varphi\right)_X + O(\epsilon^3)$$

For $X = L^2(0, T; \mathbb{R})$, the reduced gradient is given

$$\nabla\hat{J}_{L^2}(u) = -\gamma\,\ddot{u} - \Re e\langle\psi|\frac{\partial V_u}{\partial u}|p\rangle,$$

In the case $X = H^1(0, T; \mathbb{R})$ formulation, we have that

$$-\frac{d^2}{dt^2}[\nabla\hat{J}_{H^1}(u)] = -\gamma\ddot{u} - \Re e\langle\psi, \frac{\partial V_u}{\partial u}p\rangle,$$

with $[\nabla\hat{J}(u)](0) = 0$ and $[\nabla\hat{J}(u)](T) = 0$.
The H^1 gradient $\nabla\hat{J}_{H^1}(u)$ has the same regularity as u, while the L^2 gradient does not.
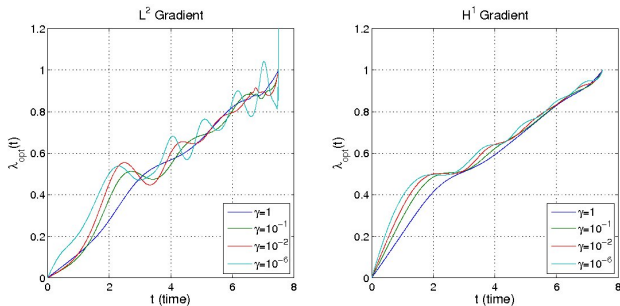
Optimal controls obtained on different X spaces

Figure: Dependence of the optimal control function on the regularization parameter γ for the L^2 and H^1 spaces. More oscillating controls are obtained with smaller γ. $M = 3200$ time steps with $g = 10$ and $T = 7.5$.

A nonlinear conjugate gradient on X space

Step 1. Given $k = 1$, u_1, $d_1 = -g_1$, if $\|g_1\|_X < tol$ then stop.

Step 2. Compute $\tau_k > 0$ satisfying the Armij-Wolfe conditions

$$\hat{J}(u_k + \tau_k d_k) \leq \hat{J}(u_k) + \delta\,\tau_k\,(g_k, d_k)_X$$
$$(g(u_k + \tau_k d_k), d_k)_X > \sigma\,(g_k, d_k)_X, \qquad 0 < \delta < \sigma < 1/2$$

Step 3. Let $u_{k+1} = u_k + \tau_k\,d_k$.

Step 4. Compute $g_{k+1} = \nabla\hat{J}_X(u_{k+1})$.
If $\|g_{k+1}\|_X < tol_{abs}$ or $\|g_{k+1}\|_X < tol_{rel}\|g_1\|_X$ or $k = k_{\max}$ then stop.

Step 5. Compute β_k by (Hager-Zhang)

$$\beta_k = \frac{(\sigma_k, g_{k+1})_X}{(d_k, y_k)_X}, \qquad \sigma_k = y_k - 2d_k\frac{(y_k, y_k)_X}{(y_k, d_k)_X}, \quad y_k = g_{k+1} - g_k$$

Step 6. Let $d_{k+1} = -g_{k+1} + \beta_k\,d_k$.

Step 7. Set $k = k + 1$, goto Step 2.

BFGS on X space

With BFGS the search direction is given by $p_k = -H_k \nabla \hat{J}(u_k)$.
By the Sherman-Morrison-Woodbury formula, we have

$$H_{k+1} = H_k + \frac{s_k^\top y_k + y_k^\top H_k y_k}{(s_k^\top y_k)^2}(s_k s_k^\top) - \frac{H_k y_k s_k^\top + s_k y_k^\top H_k}{s_k^\top y_k}$$

where $s_k = \tau_k p_k$. Supposing X is either $L^2(0, T; \mathbb{R})$ or $H^1(0, T; \mathbb{R})$, the function space analog of the outer product is a dyadic operator $x \otimes y : X \to X$. The action of this operator on a third element $v \in X$ can be expressed in terms of the inner product $(x \otimes y) v = (y, z)_X v$. One obtains the descent directions
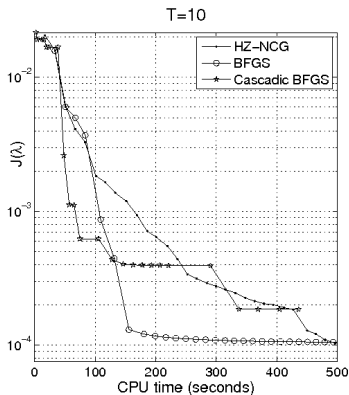
$$p_k = -H_0 g_k - \sum_{j=0}^{k-1} c_j [d_j (s_j, g_k)_X s_j - (z_j, g_k)_X s_j - (s_j, g_k)_X z_j]$$

where $c_j = (s_j, y_j)_X^{-1}$, $d_j = 1 + c_j (y_j, z_j)$, and for $z_k = H_k y_k$, we have.

$$z_k = H_0 y_k + \sum_{j=0}^{k-1} c_j \{ [d_j (s_j, y_k)_X - (z_j, y_k)_X] s_j - (s_j, y_k)_X z_j \}.$$

Results with HZ-NCG and BFGS on H^1 space

mesh	$\hat{J}$	$\|\nabla \hat{J}\|$	iterations	CPU time (sec)
400	1.6605×10^{-2}	1.4288×10^{-1}	15	3.8407×10^{1}
800	5.5963×10^{-4}	4.5284×10^{-2}	62	2.8107×10^{2}
1600	2.9634×10^{-4}	1.0733×10^{-2}	30	3.6334×10^{2}
3200	1.0562×10^{-4}	3.6378×10^{-3}	37	9.6153×10^{2}

MultiGrid OPTimization framework

The MGOPT solution to the optimization problem $\min_u \hat{J}(u)$ requires to define a hierarchy of minimization problems

$$\min_{u_k} \hat{J}_k(u_k) \qquad k = 1, 2, \ldots, L$$

where $u_k \in X_k$ and $\hat{J}_k(\cdot)$ is the reduced objective.

Among spaces X_k, restriction operators $I_k^{k-1} : X_k \to X_{k-1}$ and prolongation operators $I_{k-1}^k : X_{k-1} \to X_k$ are defined.
Require that $(I_k^{k-1}u, v)_{k-1} = (u, I_{k-1}^k v)_k$ for all $u \in X_k$ and $v \in X_{k-1}$.

We also choose an optimization scheme as 'smoother' (NCG, BFGS, ...)

$$u_k^\ell = O_k\left(u_k^{\ell-1}\right)$$

That provides sufficient reduction

$$\hat{J}_k(O_k(u_k^\ell)) < \hat{J}_k(u_k^\ell) - \eta \|\nabla \hat{J}_k(u_k^\ell)\|^2$$

for some $\eta \in (0, 1)$.

MGOPT Algorithm

Initialize u_k^0. If $k = 1$, solve $\min_{u_k} \hat{J}_k(u_k) - (f_k, u_k)_k$ and return. Else if $k > 1$,

1. *Pre-optimization*: $u_k^\ell = O_k(u_k^{\ell-1}, f_k)$, $\ell = 1, 2, \ldots, \gamma_1$

2. *Coarse grid problem*
   Restrict the solution: $u_{k-1}^{\gamma_1} = I_k^{k-1} u_k^{\gamma_1}$
   Fine-to-coarse correction: $\quad \tau_{k-1} = \nabla \hat{J}_{k-1}(u_{k-1}^{\gamma_1}) - I_k^{k-1} \nabla \hat{J}_k(u_k^{\gamma_1})$
   $$f_{k-1} = I_k^{k-1} f_k + \tau_{k-1}$$
   Apply MGOPT to the coarse grid problem:

   $$\min_{u_{k-1}} \hat{J}_{k-1}(u_{k-1}) - (f_{k-1}, u_{k-1})_{k-1}$$

3. *Coarse grid correction*
   Prolongate the error: $\quad d = I_{k-1}^k(u_{k-1} - u_{k-1}^{\gamma_1})$
   Perform a line search in the direction d to obtain a step length α_k.
   Coarse grid correction: $u_k^{\gamma_1+1} = u_k^{\gamma_1} + \alpha_k d$

4. *Post-optimization*: $u_k^\ell = O_k(u_k^{\ell-1}, f_k)$, $\ell = \gamma_1 + 2, \ldots, \gamma_1 + \gamma_2 + 1$

Computational performance of CNCG and MGOPT

	CNCG		MGOPT	
γ	$\frac{1}{2}\big(1 - \big|\langle\psi_d, \psi(T)\rangle\big|^2\big)$	CPU	$\frac{1}{2}\big(1 - \big|\langle\psi_d, \psi(T)\rangle\big|^2\big)$	CPU
10^{-2}	$2.23 \cdot 10^{-2}$	17	$9.69 \cdot 10^{-4}$	116
10^{-4}	$4.54 \cdot 10^{-4}$	202	$6.01 \cdot 10^{-4}$	82
10^{-6}	$1.38 \cdot 10^{-2}$	14	$8.78 \cdot 10^{-4}$	78

Table: Computational performance of the CNCG and MGOPT schemes; $T = 7.5$ and $g = 10$.

	CNCG		MGOPT	
g	$\frac{1}{2}\big(1 - \big|\langle\psi_d, \psi(T)\rangle\big|^2\big)$	CPU	$\frac{1}{2}\big(1 - \big|\langle\psi_d, \psi(T)\rangle\big|^2\big)$	CPU
25	$3.89 \cdot 10^{-4}$	53	$7.08 \cdot 10^{-4}$	149
50	$2.35 \cdot 10^{-3}$	80	$9.84 \cdot 10^{-3}$	76
75	$5.54 \cdot 10^{-3}$	90	$1.85 \cdot 10^{-3}$	163
100	$4.94 \cdot 10^{-1}$	50	$5.44 \cdot 10^{-3}$	257

Table: Computational performance of the CNCG and MGOPT schemes for different values of g; $T = 7.5$, $\gamma = 10^{-4}$, mesh 128×1250.

Time evolution for linear and optimized u control

The linear $u(t) = t/T$ is the standard choice for the optimal control (left).
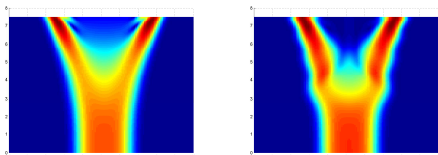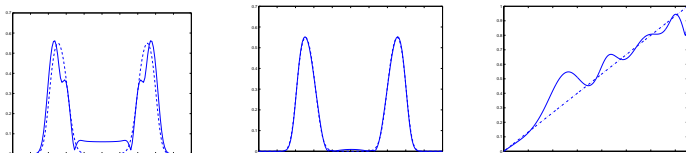

Tracking and control profile

Figure: The function $|\psi(x,t)|$ on the space-time domain (top) for the linear (left) and optimized (right) control. The corresponding profiles at $t = T$ (bottom, continuous line) compared to the desired state (dashed line). The tracking error $\frac{1}{2}\left(1 - \left|\langle\psi_d, \psi(T)\rangle\right|^2\right)$ results $6.26\,10^{-2}$ (lin) and $1.22\,10^{-3}$ (opt). MGOPT, Mesh 128×1250; $\gamma = 10^{-4}$.

Dipole quantum control

Electronic states of a charged particle in a well potential

The control of quantum electronic states has a host of applications such as control of photochemical processes and semiconductor lasers.

Consider a confining potential $V_0(x)$ with a 'well' envelope. The eigenproblem

$$\left\{ -\partial_x^2 + V_0(x) - E_j \right\} \phi_j(x) = 0, \quad j = 1, 2, \ldots,$$

defines eigenfunctions representing the eigenstates with energy E_j.

A representative potential with applications in semiconductor nanostructures is the infinite barrier well potential where $V_0(x) = 0$ for $x \in (0, \ell)$ and $V_0(0) = +\infty$ and $V_0(\ell) = +\infty$.
The infinite barrier condition is equivalent to homogeneous Dirichlet boundary conditions for the wavefunction and thus we have
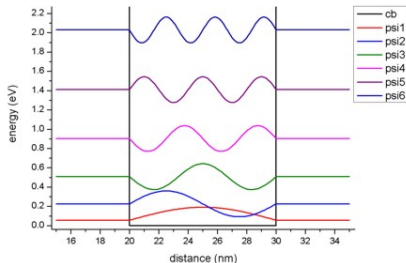
$$E_j = \frac{j^2 \pi^2}{\ell^2} \qquad \text{and} \qquad \phi_j(x) = \sin(j\pi x/\ell).$$

Electric dipole transitions and a GaAs quantum well
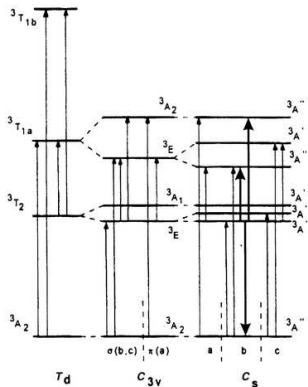
Six lowest wavefunctions in a 10 nm GaAs quantum well ("infinite barriers")

Transitions $\phi_j \longrightarrow \phi_k$

Electric dipole control

Consider a control field modeling a laser pulse. Using the dipole approximation results in the following

$$V(x, t) = V_0(x) + u(t)\, x$$

where $u : (0, T) \to \mathbb{R}$ is the modulating control amplitude.
The quantum state of a charged particle subject to this potential is governed by the time-dependent Schrödinger equation ($c(\psi, u) = 0$)

$$i\frac{\partial}{\partial t}\psi(x, t) = \left\{ -\frac{\partial}{\partial x^2} + V(x, t) \right\} \psi(x, t), \qquad (x, t) \in Q = \Omega \times (0, T),$$

Objective of the control

$$J(\psi, u) := \frac{1}{2} \left(1 - \|P\psi(\cdot, T)\|_{\mathcal{H}}^2 \right) + \frac{\gamma}{2} \|u\|_{\mathcal{U}}^2$$

where the projector $P\psi = (\psi_d, \psi)_{\mathcal{H}}\, \psi_d$.
We denote $\mathcal{H} = L^2(\Omega; \mathbb{C})$, $\mathcal{U} = H_0^1(0, T; \mathbb{R})$ and $\|u\|_{\mathcal{U}}^2 = \|u\|^2 + \alpha \|\dot{u}\|^2$

Dipole control optimality system

Introduce the Lagrangian

$$L(\psi, u, p) = J(\psi, u) + \Re e \int_0^T \int_\Omega p^*(x, t) c(\psi, u)(x, t) \, dxdt$$

where p is the Lagrange multiplier. The following first-order optimality system characterizes the optimal solution

$$\left\{ i\partial_t + \partial_x^2 - V_0(x) - u(t)\, x \right\} \psi(x, t) = 0$$

$$\left\{ i\partial_t + \partial_x^2 - V_0(x) - u(t)\, x \right\} p(x, t) = 0$$

$$-\gamma\, u + \gamma\alpha\, \ddot{u} + \Re e \int_\Omega p^*(x, t)\, x\, \psi(x, t)\, dx = 0$$

with homogeneous Dirichlet boundary conditions, and initial and terminal conditions given by

$$\psi(x, 0) = \psi_0(x)$$

$$p(x, T) = i\, (\psi_d(\cdot), \psi(\cdot, T))_{\mathcal{H}}\, \psi_d(x)$$

$$u(0) = 0, \quad u(T) = 0$$

Discretization: modified Crank-Nicholson scheme

Our MCN scheme results in the following

$$\psi_k - \psi_{k-1} = -\frac{i\delta t}{4}[H(t_k) + H(t_{k-1})][\psi_k + \psi_{k-1}].$$

Spatial discretization $\mathbf{H}_k$ of the Hamiltonian $H(t_k)$ is by linear FEM. We have that $\mathbf{H}_k = \mathbf{H}_k^\top$, which is important for preserving unitarity of the time-stepping method. Let $\mathbf{A}_k = \frac{\delta t}{4}[\mathbf{H}_k + \mathbf{H}_{k-1}]$.

$$\mathbf{B}_k = \begin{pmatrix} \mathbf{I} & \mathbf{A}_k \\ -\mathbf{A}_k & \mathbf{I} \end{pmatrix}.$$

This gives the following representation of the equality constraint

$$\mathbf{c}_k(\mathbf{y}, \mathbf{u}) = \mathbf{B}_k \mathbf{y}_k - \mathbf{B}_k^\top \mathbf{y}_{k-1}, \quad \mathbf{y}_k = \begin{pmatrix} \Re e[\psi_k] \\ \Im m[\psi_k] \end{pmatrix},$$

where $\mathbf{y}$ is a compact notation for the set of state vectors at each time step $\mathbf{y}_1, \ldots, \mathbf{y}_{N_t}$ and similarly for $\mathbf{u}$.

Discrete optimality system

Let **S** corresponds to multiplication by i. We have that

$$\mathbf{S} = \left(\begin{array}{cc} \mathbf{0} & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{array} \right), \quad (\psi_d, \psi)_{\mathcal{H}} \text{ corresponds to } \left(\begin{array}{c} \mathbf{y_d}^\top \\ \mathbf{y_d}^\top \mathbf{S} \end{array} \right) \mathbf{y}$$

In this representation, we can rewrite the objective in the form

$$J(\mathbf{y}, \mathbf{u}) = \frac{1}{2} \left[1 - \mathbf{y}_{N_t}^\top \left(\begin{array}{cc} \mathbf{y_d} & -\mathbf{Sy_d} \end{array} \right) \left(\begin{array}{c} \mathbf{y_d}^\top \\ \mathbf{y_d}^\top \mathbf{S} \end{array} \right) \mathbf{y}_{N_t} \right] + \frac{\gamma}{2} \mathbf{u}^\top \mathbf{K} \mathbf{u}$$

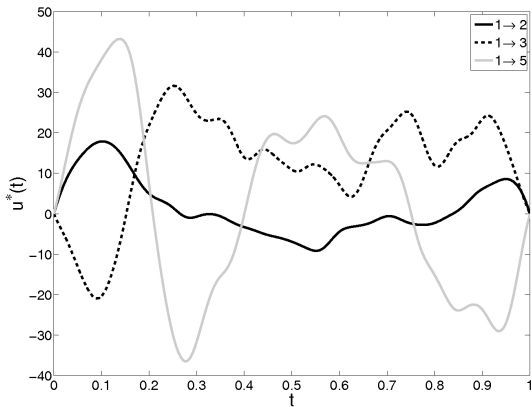The matrix **K** is the discretization of $I - \alpha \partial_t^2$. We have the Lagrangian

$$\mathbf{L}(\mathbf{y}, \mathbf{u}, \mathbf{p}) = J(\mathbf{y}, \mathbf{u}) + \sum_{k=1}^{N_t} \mathbf{p}_k^\top \mathbf{c}_k(\mathbf{y}, \mathbf{u})$$

Differentiating this Lagrangian with respect to its arguments and setting the derivatives to zero gives the discrete optimality system

$$\mathbf{B}_k \mathbf{y}_k = \mathbf{B}_k^\top \mathbf{y}_{k-1}$$
$$\mathbf{B}_k^\top \mathbf{p}_k = \mathbf{B}_{k+1} \mathbf{p}_{k+1}$$
$$\gamma \mathbf{K} \mathbf{u} = \mathbf{f}$$

Results with globalized Newton method: optimal controls

Optimal controls for transitions from the first state to the second, the third, and the fifth states.

Results with globalized Newton method: minimization

Iteration	$J_{SD} - J^*$	$J_{NCG} - J^*$	$J_{KN} - J^*$
1	2.4969×10^{-1}	2.4969×10^{-1}	2.4969×10^{-1}
2	1.3070×10^{-2}	1.3070×10^{-2}	1.5346×10^{-2}
3	6.4184×10^{-3}	6.4184×10^{-3}	5.1099×10^{-3}
4	5.5337×10^{-3}	5.3438×10^{-3}	2.2381×10^{-4}
5	4.8170×10^{-3}	3.1011×10^{-3}	1.8383×10^{-4}
6	4.2081×10^{-3}	2.3384×10^{-3}	1.6253×10^{-5}
7	3.6768×10^{-3}	1.2475×10^{-3}	2.7534×10^{-6}
8	3.2177×10^{-3}	9.1869×10^{-5}	3.3921×10^{-7}
9	2.8141×10^{-3}	5.9258×10^{-5}	4.7022×10^{-9}

Table: Convergence of the steepest descent scheme, the nonlinear CG scheme, and the Krylov-Newton scheme to reach the optimal cost $J^* = J(u^*)$.

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Some references

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3. A. B. and G. von Winckel, *Multigrid methods and sparse-grid collocation techniques for parabolic optimal control problems with random coefficients*, SIAM J. Sci. Comp., 31 (2009), 2172-2192.

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6. A. B., J. Salomon, and S. Volkwein, *Formulation and numerical solution of finite-level quantum optimal control problems*, J. Comput. Appl. Math., 216 (2008), 170–197.

7. A. B., G. Stadler, and U. Hohenester, *Optimal quantum control in nanostructures: Theory and application to a generic three-level system*, Phys. Rev. A 66, (2002) 053811.

Joint works with

Greg von Winckel (University of Graz), quantum modeling, Newton and quasi-Newton methods, sparse grids, uncertainty.

Stefan Volkwein (University of Konstanz), theory of quantum control problems.

Ulrich Hohenester (University of Graz), theoretical physics, quantum optics, nanophysics.

Julien Salomon (University of Dauphine, Paris), monotonic schemes.

Georg Stadler (University of Texas, Austin), theory of quantum control problems.

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Work in progress

1. Solution of quantum control problems under uncertainty

2. Robust control strategies

3. Quantum control problems on lattices

4. Multi-particle control problems

5. Design of nano devices

Thanks for your attention