Quantum models and optimal control problems

by

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Application of quantum control

1. Quantum control: state transitions, laser induced chemistry, magnetic and optical trapping.
2. Quantum computing: qubits, data operations.
3. Quantum transport, BEC, superfluids of atoms, vortices.
4. NMR and magnetic resonance imaging.
5. Quantum optics.
6. Semiconductor nanostructures.

Quantum mechanical frameworks

There are nine formulations of nonrelativistic quantum mechanics (QM): the wavefunction, matrix, path integral, phase space, density matrix, second quantization, variational, pilot wave, and Hamilton–Jacobi formulations.

A covariant formulation leads to a relativistic quantum mechanics (RQM).

Most of quantum optimal control problems have been formulated in the context of nonrelativistic quantum mechanics in the wavefunction and density matrix formulations.

The research field of quantum optimal control problems is wide open.

Wavefunction models

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

$$i\,\partial_t\,\psi = (H_0 + V_{control})\,\psi$$

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

$$i\,\partial_t\,\psi = \left(-\frac{1}{2}\Delta + V_0 + V_{control} + g\,|\psi|^2\right)\psi$$

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

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

Other QM models

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

$$i\,\partial_t\,\psi_i = \left(-\frac{1}{2}\Delta + V_{ext} + V_{Hartree}(\rho) + V_{exc}(\rho) + V_{control}\right)\psi_i$$

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

- The Wigner equation, $f = f(x,p,t)$

$$\partial_t\, f + p\cdot\nabla_x f = \Theta_{V_0+V_{control}}[f]$$

- The Liouville-von Neumann equation, $\rho = \rho_{ij}(t)$

$$\partial_t\,\rho = -\frac{1}{i\hbar}[\rho, H_0 + V_{control}].$$

- The stochastic Schrödinger equation, etc.

Control mechanisms

Many finite-dimensional controlled quantum systems can be written in a real representation as follows

$$\dot{X} = \left[A + \sum_{n=1}^{N_C} B_n \, u_n \right] X$$

where X represents a quantum state, A and B_n are skew-symmetric matrices, and $u_n : [0, T] \to \mathbb{R}$ are control functions. This structure appears frequently in, e.g., optimal control of spins.

In the case of infinite-dimensional controlled quantum systems, the original formulation in complex Hilbert spaces is preferred.

$$i \, \partial_t \, \Psi = \left\{ \left[\frac{1}{2} |p|^2 + \vec{A}(x,t) \cdot p + V(x,t) \right] \otimes I_2 + \vec{B}(t) \cdot \vec{I} \right\} \Psi .$$

In this Pauli equation for the spinor Ψ, the magnetic field $\vec{B}(t)$ and/or a potential $V(t,x) = V_0(x) + x \circ u(t)$ may play the role of control functions.

Control's physical objectives

Dynamically stable systems exist with confining potentials V_0.

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

where the ϕ_j represent the eigenstates and the E_j represent the energy.

Control may be required to quickly steer state transitions: $\phi_i \longrightarrow \phi_j$.

Control may be required to break bound states: dissociation of molecules.

Control may be required to maximize/minimize observable expected values $(\psi, O\psi)$, where O represents a physical observable.

If the Hermitian operator O represents a transformation (regardless of initial and final states) like a quantum gate, control may be required to obtain best performance of O.

Model purpose and cost of control

The purpose of the control is formulated by means of a cost functional to be optimised. This functional usually has a composite structure:

$$J(X, u) = J_1(X) + J_2(u).$$

The first term could represent a quantum expected value of an observable; e.g., $\langle \psi, O\, \psi \rangle$, to be maximized along the time evolution (thus involving a time integration) or at final time. On the other hand, it may correspond to a requirement on the state configuration.

The second term represents the cost of the control to be minimized in the given control space denoted with $\mathcal{U}$.

Moreover, we can pose additional restrictions for the admissible controls and require:

$$u \in U_{ad} \subseteq \mathcal{U}$$

A quantum control problem

A class quantum optimal control problem

$$\begin{aligned} \min \quad J(X,u) &:= J_1(X) + J_2(u) \\ \partial_t X &= \left[\mathcal{A} + u\,\mathcal{B}\right] X \\ X(\cdot,0) &= X_0, \qquad \mathcal{T}X = 0 \\ u &\in U_{ad} \end{aligned}$$

Analytical issues: Well-posedness (existence of solutions), Fréchet differentiability of the optimal control components, optimality conditions.

Assuming a unique solution of the governing model for a given control, we have the control-to-state map: $u \mapsto X(u)$. Thus the optimal control can be equivalently written as follows

$$\min_{u \in U_{ad}} \hat{J}(u) := J(X(u), u),$$

where $\hat{J}$ is the reduced cost functional.

The optimality system

In order to derive the first-order necessary optimality conditions, one can use the Lagrange multipliers method based on the Lagrange function:

$$L(\psi, u, \lambda) = J(\psi, u) + \mathrm{Re}\, \langle \partial_t X - \left[\mathcal{A} + u\,\mathcal{B}\right] X, Z \rangle,$$

where Z is the Lagrange multiplier and $\langle \cdot, \cdot \rangle$ a complex scalar product.

Let u be an optimal control, and $X = X(u)$. The Lagrange multiplier Z is the function satisfying the optimality system

$$\begin{aligned} D_X L(X, u, Z)(\delta X) &= 0 \\ D_Z L(X, u, Z)(\delta Z) &= 0 \\ D_u L(X, u, Z)(\delta u) &\geq 0, \qquad u + \delta u \in U_{ad}. \end{aligned}$$

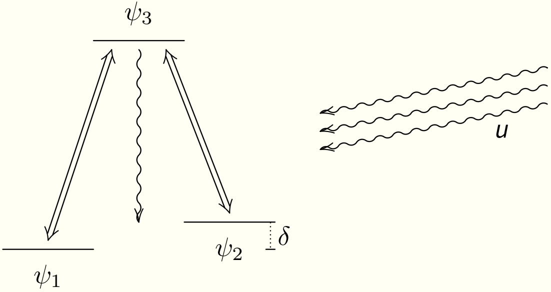
This system is equivalent to the optimality condition:

$$\left(\nabla \hat{J}(u), v - u\right) \geq 0 \qquad v \in U_{ad}.$$

A finite-level quantum system

Quantum systems with a finite number of states may 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):



Model of the Λ system

A Schrödinger-type equation for a n-component wave function $\psi : [0, T] \to \mathbb{C}^n$ has the form

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

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

The function $u : [0, T] \to \mathbb{C}$ represents the external control field. We write $u = u_r + i\,u_i$.

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

a free Hamiltonian $H_0 \in \mathbb{C}^{n\times n}$ describing the uncontrolled system;

a control potential $V(u) \in \mathbb{C}^{n\times n}$ modelling the coupling of the quantum state with the control field u.

Control's objective and costs

The purpose is to reach a target state at $t = T$, while limiting population of dissipative states during the control process, and using minimal laser resources.

These requirements can be modelled as follows

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

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

We have a quantum optimal control problem:

$$
\min J(\psi, u), \quad \text{s.t.} \quad i\,\dot{\psi}(t) = H(u(t))\,\psi(t), \quad \psi(0) = \psi_0,\ u \in \mathcal{U}
$$

$\mathcal{U} = H^1(0, T; \mathbb{C})$, where H^1 costs promote slow varying controls.

Optimality system

$$
\begin{aligned}
i\,\dot\psi &= H(u)\,\psi, \qquad \psi(0) = \psi_0,\\
i\,\dot p &= H(u)^*\,p - \alpha_j\,(\psi)_j, \qquad i\,p(T) = \psi(T) - \psi_T\\
-\gamma\,\ddot u + \beta\,u &= \mathrm{Re}(p\cdot(\partial_{u_r}V(u)\,\psi)^*) + i\,\mathrm{Re}(p\cdot(\partial_{u_i}V(u)\,\psi)^*)\\
u(T) &= 0, \qquad u(0) = 0.
\end{aligned}
$$

With free hamiltonian and control potential given by

$$
H_0 = \frac{1}{2}\begin{pmatrix} -\delta & 0 & 0\\ 0 & \delta & 0\\ 0 & 0 & -i\Gamma_o \end{pmatrix}, \qquad V(u) = -\frac{1}{2}\begin{pmatrix} 0 & 0 & \mu_1\,u\\ 0 & 0 & \mu_2\,u\\ \mu_1\,u^* & \mu_2\,u^* & 0 \end{pmatrix}
$$

where the term $-i\,\Gamma_o$ accounts for environment losses, e.g., spontaneous photon emissions, scattering of gamma rays from crystals.
The 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 target states: $\psi_0 = (1,0,0)$ and $\psi_T = (0,1,0)$.

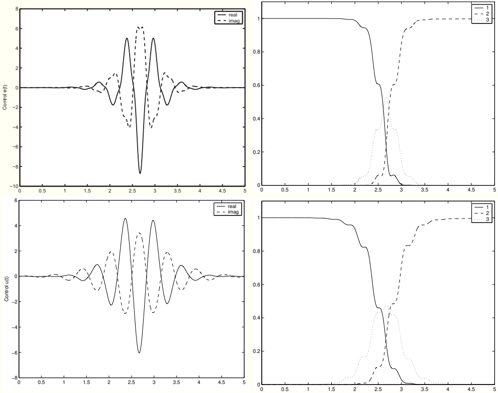
Choice of optimization weights

Smaller values of β and γ result in smaller $|\psi(T) - \psi_d|_{\mathbb{C}^3}$.
As γ increases: additional smoothness of the control function (slightly) reduces the capability of targeting, but problem better conditioned.
By taking $\alpha = \alpha_3 > 0$: dissipation is reduced and we have better targeting.

β	γ	α	$\lvert\psi(T) - \psi_T\rvert_{\mathbb{C}3}$	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 $\beta = 10^{-4}, \alpha_3 = 0.01$. We have $\gamma = 0$ (top) and $\gamma = 10^{-6}$ (bottom).



Control (left) and state evolution (right).

The choice of L^1 control costs

Consider a spin optimal control problem where the governing model is derived from the Pauli equation:

$$\min \quad J(X,u) := \frac{1}{2}\|X(T) - X_T\|_2^2 + \frac{\nu}{2}\sum_{n=1}^{N_C}\|u_n\|_{L^2}^2 + \beta\sum_{n=1}^{N_C}\|u_n\|_{L^1}$$

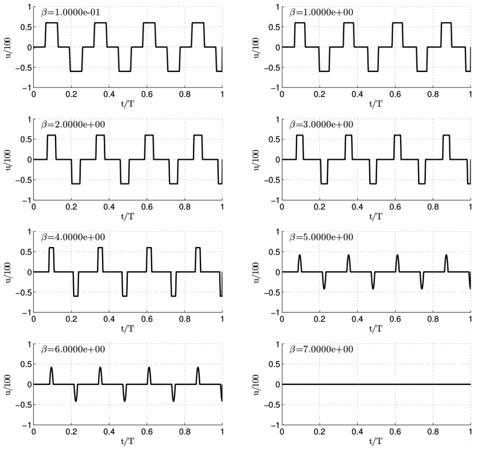
$$\text{s.t.} \quad \dot{X} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] X \;,\; X(0) = X_0.$$

The L^1 cost promotes sparsity and pulsed-shaped controls are obtained:

- easy implementation in laboratory pulse shapers;
- explanation of NMR pulses;
- mathematical challenging.

Control of 2 uncoupled spin-$\frac{1}{2}$

$X_0 = \uparrow\uparrow \qquad X_T = \rightarrow\rightarrow$



An open quantum spin system

The Liouville - von Neumann master equation is augmented with an additional 'dissipator' term $D(\rho)$ as follows

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho] + i\hbar\, D(\rho)$$

where the dissipation is given in the following Lindblad form

$$D(\rho) = C\rho C^\dagger - \frac{1}{2}\left\{C^\dagger C, \rho\right\}$$

where $\{A,B\} = AB + BA$, and C represents a quantum observable that is also a 'dissipation' channel.

To model continuous quantum measurements (diffusive case) of an open quantum system a stochastic term is added:

$$d\rho = \left(-i\,\frac{1}{\hbar}[H,\rho] + D(\rho)\right)\,dt + \left(\rho C^\dagger + C\rho - Tr(\rho(C + C^\dagger))\,\rho\right)dW_t$$

A stochastic Bloch model

This stochastic master equation (Belavkin equation) corresponds to the following stochastic Schrödinger equation

$$d\psi = -\left(iH + \frac{1}{2}[C^\dagger C - 2q_t C + q_t^2 I]\right)\psi\, dt + (C - q_t I)\ \psi\, dW$$

where $q_t = \frac{1}{2}\langle\psi, (C + C^\dagger)\psi\rangle$.

In particular, we consider the stochastic Schrödinger equation corresponding to the damped Bloch model of a two-level spin quantum system (qubit):

$$d\psi = -\left(iH + \frac{g}{2}\sigma^\dagger\sigma - g\langle\sigma^\dagger\rangle\sigma\right)\psi dt + \sqrt{g}\,\sigma\,\psi\, dW$$

A stochastic Bloch model

The stochastic Bloch model with polar coordinates on the Bloch sphere:

$$\begin{cases} d\varphi(t) = & B_\varphi(\varphi,\theta)\,dt + \sigma_{11}(\varphi,\theta)dW_1 + \sigma_{12}(\varphi,\theta)dW_2 \\ d\theta(t) = & B_\theta(\varphi,\theta)\,dt + \sigma_{21}(\varphi,\theta)dW_1 + \sigma_{22}(\varphi,\theta)dW_2, \end{cases}$$

$$\begin{aligned} B_\varphi(\varphi,\theta) &= A_\varphi(\varphi(t),\theta(t)) \\ \sigma_{11}(\varphi,\theta) &= -\sqrt{\tfrac{g}{2}}\frac{1+\cos(\theta(t))}{\sin(\theta(t))}\sin(\varphi(t)) \\ \sigma_{12}(\varphi,\theta) &= \sqrt{\tfrac{g}{2}}\frac{1+\cos(\theta(t))}{\sin(\theta(t))}\cos(\varphi(t)) \\ B_\theta(\varphi,\theta) &= A_\theta(\varphi(t),\theta(t)) + g\frac{1+\cos(\theta(t))}{\sin(\theta(t))}\left(1-(1+\cos(\theta(t))\cos(\theta(t))/4\right) \\ \sigma_{21}(\varphi,\theta) &= \sqrt{\tfrac{g}{2}}(1+\cos(\theta(t)))\cos(\varphi(t)), \qquad \sigma_{22}(\varphi,\theta) = \sqrt{\tfrac{g}{2}}(1+\cos(\theta(t)))\sin(\varphi(t)), \end{aligned}$$

The Fokker-Planck equation

The evolution of the probability density function (PDF) associated to the stochastic Bloch system is modelled by a FP equation on the sphere.

$$
\begin{aligned}
\partial_t f \quad &= \quad -\partial_\phi (A_\phi[\phi,\theta]\, f) \\
&- \quad \partial_\theta \left[\left(A_\theta[\phi,\theta] + g \frac{1+\cos(\theta)}{\sin(\theta)} \left(1 - \frac{(1+\cos(\theta))\cos(\theta)}{4} \right) \right) f \right] \\
&+ \quad \frac{g}{4} \partial_\phi^2 \left(\frac{1+\cos(\theta)}{1-\cos(\theta)}\, f \right) + \frac{g}{4} \partial_\theta^2 \left((1+\cos(\theta))^2\, f \right)
\end{aligned}
$$

with $f(\phi,\theta,t) \geq 0$ (positivity) and $\int_0^{2\pi} \int_0^{\pi} f(\phi,\theta,t) d\phi d\theta = 1$ (conservativeness). We also have $f(\phi,\theta,t) = 0$ for $\theta = 0$. These conditions are satisfied by the initial PDF $f_0 = f(\phi,\theta)$.

The formulation of control objectives with the PDF and the Fokker-Planck equation provides a consistent framework for the optimal control of stochastic models.

FP optimal control

The control mechanism in the Bloch system is the action of magnetic fields (u, v) as follows:

$$\begin{aligned} A_\varphi(\varphi, \theta, u, v) &= \omega + a\cot(\theta)\,(u\,\sin(\varphi) + v\,\cos(\varphi)) \\ A_\theta(\varphi, \theta, u, v) &= -a\,(u\,\cos(\varphi) - v\,\sin(\varphi)) \end{aligned}$$

We consider the following cost functional:

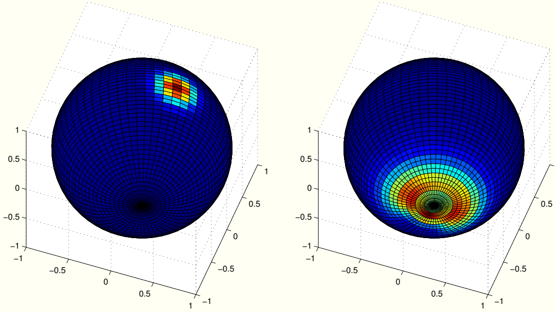
$$J(f, u, v) := \frac{1}{2}\|f(\cdot, T) - f_d(\cdot)\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|(u, v)\|^2_{L^2(0,T)}$$

where f_d represents the desired target PDF, e.g., a Gaussian.

A feedback control strategy can be constructed based on the model predictive control strategy where optimal control problems are solved in a sequence of time windows.

From the equator to the south pole

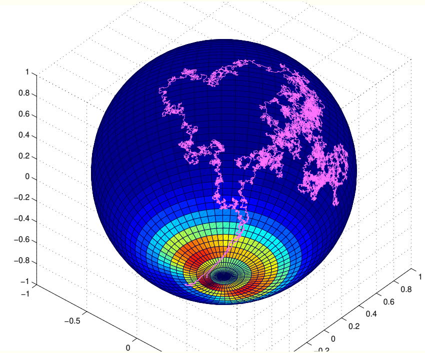
The initial PDF is a narrow normalized 2D Gaussian placed at the equator $(\theta, \phi) = (\pi/2, \pi)$ with variance $\sigma = \pi/20$. The target PDF is a Gaussian on the south pole with variance $\sigma = \pi/8$.



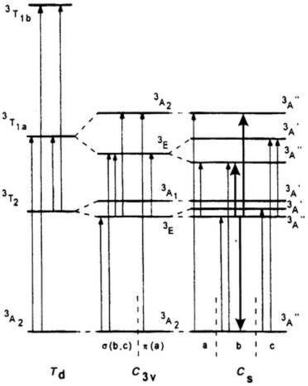
We set $g = 1, \omega = 0.01, a = 7g/\sqrt{2}$, and consider a time horizon of $T = 4$ and $N = 10$ time windows.

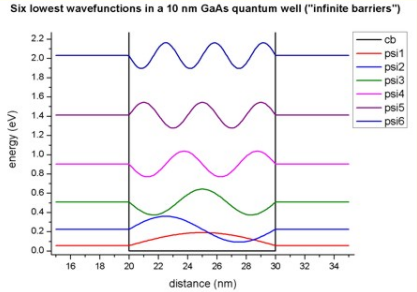
Controlled stochastic trajectories

We plot two stochastic trajectories on the sphere, corresponding to the an optimal control that drives the spin orientation from the equator to the south pole.
For this purpose, we plug the optimal controls in the stochastic model for the θ, φ and compute the trajectories using the Euler-Maruyama scheme.



Transitions in a quantum well





Transitions $\phi_j \longrightarrow \phi_k$

$$E_j = \frac{j^2\pi^2}{\ell^2}\,, \qquad \phi_j(x) = \sin(j\pi x/\ell).$$

Electric dipole control

Consider a control field modelling a laser pulse by dipole approximation:

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

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

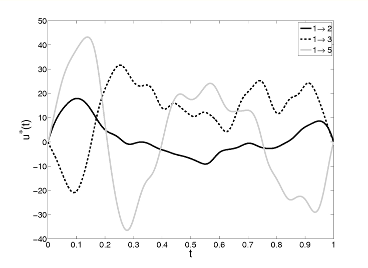
$$i\,\partial_t \psi(x,t) = \left\{ -\frac{\partial}{\partial x^2} + V(x,t) \right\} \psi(x,t), \qquad \psi(x,0) = \psi_0(x).$$

Objective of the control

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

where $\mathcal{U} = H_0^1(0,T;\mathbb{R})$ and $\|u\|_{\mathcal{U}}^2 = \|u\|^2 + \alpha\,\|\dot{u}\|^2$. The target is one of the eigenstates: $\psi_d = \phi_j$.

Results with a Newton method



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

Optimal control for the transition from the 1-st to the 4-th eigenstate:

Results with different methods

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}

Minimisation by the steepest descent scheme, the nonlinear CG scheme, and the Krylov-Newton scheme.

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):

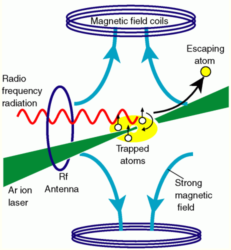
$$i\,\partial_t \psi(x,t) = \left(-\frac{1}{2}\nabla^2 + V(x,t)\right) + g\,|\psi(x,t)|^2\right)\psi(x,t)$$

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

A control mechanism for BEC

In our case $V(x,t)$ is a control potential produced by a magnetic microtrap. Its purpose is to split and transport a BEC.

Magnetic trap with optical plug



Assume that a BEC is confined in a single well $V(x,0)$ at $t=0$ and in a double well $V(x,T)$ at time $t=T$. We have

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

where $c=40$ and d is the width of the double well potential, u is a modulating function.

A BEC optimality system

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

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

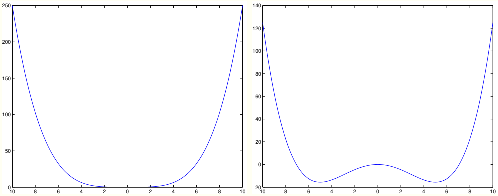
$$i\,\partial_t\psi = \left(-\frac{1}{2}\nabla^2 + V_u + g|\psi|^2\right)\psi, \qquad \psi(0) = \psi_0$$

$$i\,\partial_t p = \left(-\frac{1}{2}\nabla^2 + V_u + 2g|\psi|^2\right)p + g\,\psi^2\,p^*, \quad i\,p(T) = -\langle\psi_d|\psi(T)\rangle\,\psi_d$$

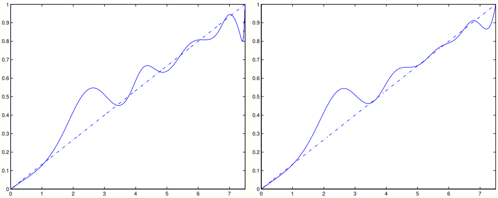
$$\gamma\ddot{u} = -\mathrm{Re}\langle\psi|\frac{\partial V_u}{\partial u}|p\rangle, \qquad u(0) = 0\,, \quad u(T) = 1$$

The initial state ψ_0 and the target state ψ_d are the ground-states wavefunctions of the GPE with single- ($u = 0$) and double-well ($u = 1$) potential, respectively.

Optimal controls & potentials

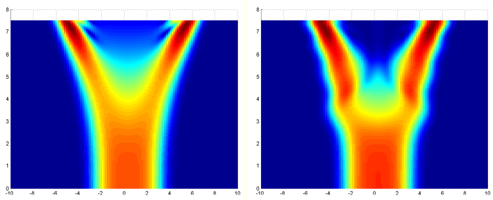


The potential V for $u = 0$ (left) and $u = 1$.

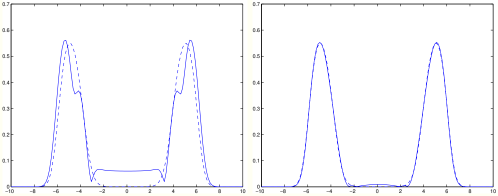


The optimal u and its linear approximation. Result for $\gamma = 10^{-4}$ (left) and for $\gamma = 10^{-2}$.

BEC manipulation



The function $|\psi(x, t)|$ on the space-time domain for the linear (left) and optimized (right) control.



The corresponding profiles at $t = T$ (continuous line) compared to the desired state (dashed line).

The TDDFT approach

The Schrödinger equation of a multi-electron system results in prohibitive computational power requirements. To bypass this high-dimensional problem, a time-dependent density functional theory (TDDFT) has been proposed.

The foundation of TDDFT on the Runge-Gross (RG) theorem:
there is a unique mapping between the time-dependent external potential of a system and its time-dependent electronic density. This implies that the wavefunction depending upon $3N$ space variables, is equivalent to the density, which depends upon only 3 space variables, and that many properties of a system can thus be determined from knowledge of the density alone.

The TDDFT Model

We have a nonlinear coupled system of N single particle SE where the interaction is modelled with a Kohn-Sham potential v_{KS}. A control function u enters in an external potential $v_{ext} = v_{ext}^0 + v_{ext}'(u)$.

$$i\frac{\partial}{\partial t}\psi_j(x,t) = \left(-\frac{1}{2}\Delta + v_{ext}(x,t;u) + v_{KS}(x,\rho(x,t))\right)\psi_j(x,t) \quad j = 1\ldots,N,$$

$$\rho(x,t) = \sum_{i=1}^{N}|\psi_i(x,t)|^2, \quad v_{KS}(x,\rho(x,t)) = \int_\Omega \frac{\rho(y,t)}{|x-y|}dy + v_x(\rho(x,t)) + v_c(\rho(x,t)),$$

where ψ_j represents the wave function of the jth particle.

$$\psi_j \in W = \left\{\psi \in L^2(0,T;H^1(\mathbb{R}^n)), \int_{\mathbb{R}^n}|\psi(x,t)|^2dx = 1,\ \forall t \in [0,T]\right\}.$$

We assume the adiabatic local density approximation, where the potentials v_x, v_c at (x,t) only depend on $\rho(x,t)$.

A TDDFT optimal control problem

$$\min_{\psi \in W^N,\, u \in L^2(0,T)} J(\psi, u) \text{ s.t. } \psi \text{ solves the TDDFT Model,}$$

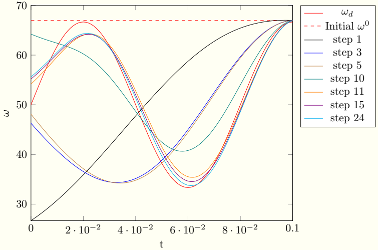
where the cost functional models different objectives:
$J := J_\beta + J_\gamma + J_\eta + J_\nu$

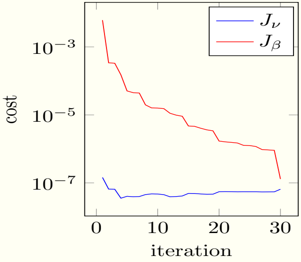
$$\begin{aligned} J(\psi, u) &= \frac{\beta}{2} \int_0^T \int_\Omega (\rho(x,t) - \rho_d(x,t))^2 dxdt \\ &+ \frac{\gamma}{2} \int_\Omega \left(\rho(x,T) - \rho_T(x)\right)^2 dx \\ &+ \frac{\eta}{2} \int_\Omega \chi_A \, \rho(x,T) dx + \frac{\nu}{2} \int_0^T u(t)^2 dt, \end{aligned}$$

with $\nu > 0$, $\beta, \gamma \geq 0$, and $\chi_A > 0$ is a characteristic function with support in A.

Numerical experiment I

Consider a two-dimensional quantum dot modelled by a harmonic potential, $v^0_{ext}(x,t) = \omega_0\, x^2$, and the control represents oscillator strength, $v'_{ext}(x,t;u) = u(t)\, x^2$, $(\beta,\gamma,\eta,\nu) = (1,0,0,1e-8)$.

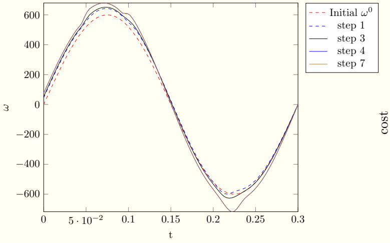


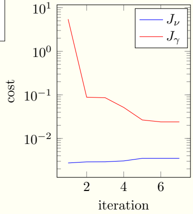


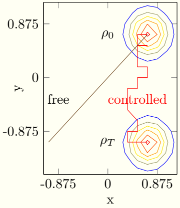
In this experiment, the desired density evolution is obtained with $u = \omega_0 + (\omega_0/3)\, sin(5\pi t/2)$, $\omega_0 = 50$.

Numerical experiment II

Consider a two-dimensional quantum dot modeled by a harmonic potential, $v^0_{ext}(x,t) = \omega_0\, x^2$, and a dipole control, $v'_{ext}(x,t;u) = u(t)\, x$, $(\beta,\gamma,\eta,\nu) = (0,1,0,1e-7)$.



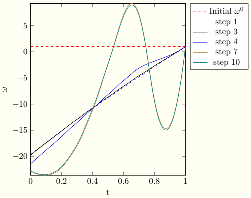


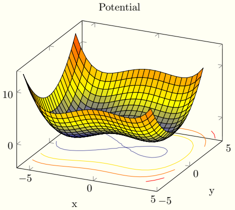


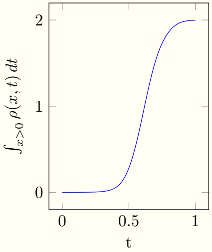
In this experiment, the target density ρ_T is a coerent state of the harmonic oscillator.

Numerical experiment III

Consider a two-dimensional quantum dot modelled by the following 4th-order asymmetric double-well,
$v^0_{ext}(x,t) = x^4/64 + x^3/32 - x^2/4 + y^2/2$, and dipole control. We have $(\beta,\gamma,\eta,\nu) = (0,0,1,1e-6)$.







Ensemble optimal control problems

In a statistical framework, a phase-space density-based optimal control formulation appears to be appropriate.

A Wigner ensemble optimal control problem:

$$\min J(f,u) := \Phi(f) + \Gamma(f) + \kappa(u),$$
$$\text{s.t.} \qquad \partial f + p \cdot \nabla_x f - \Theta_{V_0 + V_{control}(u)}[f] = 0, \qquad f_{|t=0} = f_0,$$

where

$$\Theta_U[f](x,p,t) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \delta U(x,\eta,t) f(x,p',t) e^{-i(p-p')\cdot\eta} \, \mathrm{d}p' \, \mathrm{d}\eta$$

The ensemble cost functional:

$$J(f,u) = \int_0^T \int_{\mathbb{R}^{2n}} \phi(x,p,t)\, f(x,p,t)\, dx\, dp\, dt - \int_{\mathbb{R}^{2n}} \gamma(x,p)\, f(x,p,T)\, dx\, dp$$
$$+ \frac{1}{2} \int_0^T \left(\gamma \, |u(t)|^2 + \nu \, |\dot{u}(t)|^2 \right) dt$$

Open topics

Some open topics in the field of quantum optimal control problems:

- Other QM formulations
- Control in a relativistic setting
- Control in a quantum statistical framework
- Open quantum systems and feedback control
- Time-dependent quantum field theory
- High-dimensional problems
- Formulation of inverse problems/hamiltonian identification
- Functional and numerical analysis issues
- Laboratory implementation

Thank you for your attention!

The book and the software

Software published in Computer Physics Communications
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Codes available at the International Computer Program Library on Mendeley Data:
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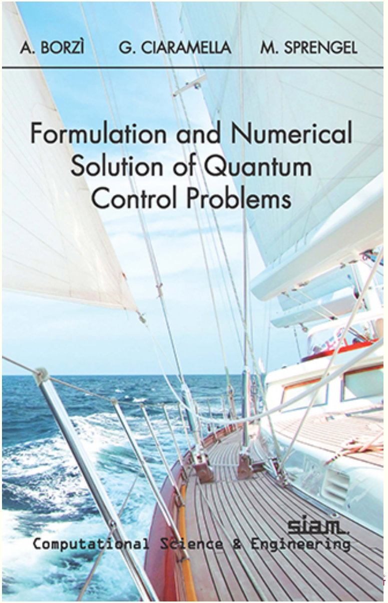

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