Introduction to Quantum Dynamics and Control

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UC Berkeley

Lecture: Numerical Methods of Optimal Control

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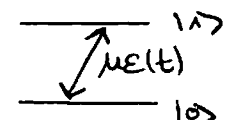
1. Problem Description

Set $\{\Psi_k^{in}(t=0)\}$ should be mapped to set $\{\Psi_k^{tgt}(T)\}$
with time evolution operator $\hat{U}(T,0;\varepsilon(t))$ ← control

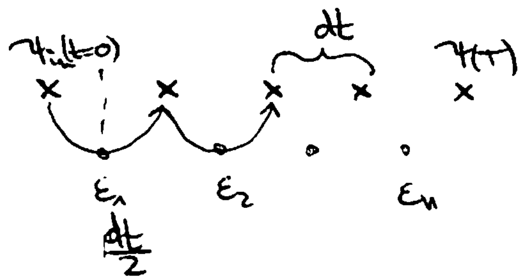
$\hat{U}$: operator that maps state according to equation of motion, propagated from 0 to T

TDSE: $i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \hat{H}(\varepsilon(t))|\Psi\rangle$; e.g. $\hat{H} = \begin{pmatrix} V_0 & \mu\varepsilon(t) \\ \mu\varepsilon(t) & V_1 \end{pmatrix}$



What is the control that brings the system from its initial state to its target state?

2. Discretization



control is piecewise constant, switches at points of time grid

$$\hat{U}(T,0;\varepsilon(t)) = \prod_{i=n} \underbrace{e^{\frac{i}{\hbar}\hat{H}(\varepsilon_i)dt}}_{\hat{U}_i} = \hat{U}_n \ldots \hat{U}_2 \hat{U}_1 |\Psi_{in}\rangle$$

Propagation: Runge-Kutta or Chebychev if more precision is required.

3. Optimization Functionals

OCT: minimize a functional of the control ε
includes measure of success, possibley penalties (cost functional) for the control and/or the system evolution

iterative procedure: start with guess $\varepsilon^{(0)}(t)$, find improvement $\varepsilon^{(1)}(t) = \varepsilon^{(0)}(t) + \Delta\varepsilon(t)$, repeat

Measure of success : Fidelities

e.g. for gate optimization [Palao, Kosloff, PRA 68, 062308 (2003)]
Map all basis states according to unitary transformation $\hat{O}$

$|0\rangle \overset{!}{\rightarrow} \hat{O}|0\rangle$, $|1\rangle \overset{!}{\rightarrow} \hat{O}|1\rangle$ (single qubit)

$$\frac{1}{N}\sum_{k=1}^{N} \langle \varphi_k^{in} | \hat{O}^+ \hat{U} | \varphi_k^{in} \rangle \longrightarrow \begin{cases} \frac{1}{N}\left|\sum \langle \ldots \rangle\right| & \text{gate fidelity} \\ \frac{1}{N^2}\left|\sum \langle \ldots \rangle\right|^2 & F_{sm} \\ \frac{1}{N}\,\mathrm{Re}\sum \langle \ldots \rangle & F_{re} \text{ (global phase sensitivity)} \end{cases}$$

Fidelity is functional of states at final time T

Add intermediate-time constraints for full optimization functional:

$$J = \underbrace{J_T[\{\varphi_k(T)\}]}_{1-F} + \int_0^T J_t[\{\varphi_k(t)\}, \varepsilon(t), t]\, dt \overset{!}{\longrightarrow} 0$$

4. Krotov-Method

[Reich et al. JCP 136, 104103 (2012) — arxiv: 1008.5126v1]
[Sklarz, Tannor. PRA 66, 053619 (2002)]

Specify $J_t = \underbrace{g_a[\varepsilon(t), t]}_{} + g_b[\{\varphi_k(t), t\}]$

usual choice: $\frac{\lambda_a}{S(t)}(\varepsilon(t) - \varepsilon_{ref}(t))^2$; with $\varepsilon_{ref} = \varepsilon^{(0)}$: $\boxed{g_a = \frac{\lambda_a}{S(t)}\Delta\varepsilon^2}$

Optimization Equations

Minimize J by choosing control ε, but such that dynamics of states follows eq. of motion
Idea of Krotov: auxillary functional with additional arb. potential Φ, use freedom in Φ to construct improved field

$$J = J_T(\{\varphi_k(T)\}) + \int_0^T g_a(\varepsilon(t))\,dt + \int_0^T g_b(\{\varphi_k(t)\})\,dt$$

$$\downarrow$$

$$L = G(\{\varphi_k(T)\}) - \Phi(\{|\varphi_k(0)\rangle, 0) - \int_0^T R(\{\varphi_k(t)\}, \varepsilon(t), t\; dt$$

with

$$G = J_T[\{\varphi_k(T)\}] + \Phi(\{\varphi_k(T)\}, T)$$

$$R = -\left(g_a[\varepsilon(t), t] + g_b[\{\varphi_k(t)\}, t]\right) + \frac{\partial \Phi}{\partial t} + \sum_{k=1}^{N}\Big[\nabla_{|\varphi_k\rangle}\Phi \cdot \underset{\substack{\uparrow \\ \text{eq. of motion: } \dot{\varphi}_k}}{f_k}[\varphi_k, \varepsilon, t] + \nabla_{\langle\varphi_k|}\Phi\, f_k^+[\varphi_k, \varepsilon, t]\Big]$$

$$\boxed{\text{For any potential } \Phi : \quad L \equiv J}$$

Expand Φ into states:

$$\Phi[\{\varphi_k\}, t] = \sum_k \left[\langle \chi_k(t)|\varphi_k(t)\rangle + \langle\varphi_k(t)|\chi_k(t)\rangle\right] + \underset{\text{(second order)}}{\cdots}$$

① Maximize L with respect to the states (by choosing coefficients $|\chi\rangle$ appropriately) $\rightarrow$ any change in control will then improve L

$\Rightarrow$ eq. of motion for χ:

$$\boxed{\begin{aligned} \frac{d}{dt}|\chi(t)\rangle &= -\frac{i}{\hbar}\hat{H}^+[\varepsilon^{(0)}(t)]|\chi^{(0)}(t)\rangle + \nabla_{\langle\varphi_k|} g_b \\ |\chi_k^{(0)}(T)\rangle &= -\nabla_{\langle\varphi_k|} J_T \end{aligned}}$$

② Minimize L with respect to the field ($\rightarrow R$-functional)

$$\left.\frac{\partial G}{\partial \varepsilon}\right|_{\varepsilon^{(1)}, \varphi^{(1)}} = 2\,\mathrm{Im}\left[\sum_{k=1}^{N}\langle\chi_k^{(0)}(t)|\left(\frac{\partial H}{\partial \varepsilon}\right)_{\varepsilon^{(1)}, \varphi^{(1)}}|\varphi_k^{(1)}(t)\rangle\right.$$

$$\boxed{\Rightarrow \Delta\varepsilon = \frac{S(t)}{\lambda_a}\,\mathrm{Im}\left[\sum_{k=1}^{N}\langle\chi_k^{(0)}(t)|\frac{\partial H}{\partial \varepsilon}|\varphi_k^{(1)}(t)\rangle\right.} + \text{higher order}$$

Comments:

- expanding Φ up to second order in states [Reich] may be required
  first order: $J_T'', g_b'' \geq 0$ eq. of motion linear in states, control
- system Hamiltonian enters as $\frac{\partial \hat{H}}{\partial \varepsilon}$, usually $\frac{\partial \hat{H}}{\partial \varepsilon} = \hat{\mu}$
  but other equations of motion might be used.
- Final-time functional / fidelity enters through boundary condition for $|\chi\rangle$

$$F_{re} = \frac{1}{N} \mathrm{Re} \sum_{k=1}^{N} \langle \varphi^{tgt} | \varphi_k(T) \rangle = \frac{1}{N} \sum_{k=1}^{N} \frac{1}{2} \left(\langle \varphi_k^{tgt} | \varphi_k(T) \rangle + \langle \varphi_k(T) | \varphi_k^{tgt} \rangle \right)$$

$$\Rightarrow |\chi_k(T)\rangle = \frac{1}{N} \cdot \frac{1}{2} |\varphi_k^{tgt}\rangle$$

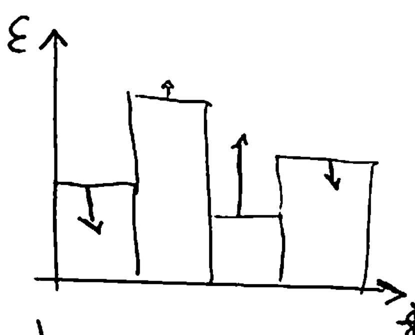
$$F_{sm} \Rightarrow |\chi_k(T)\rangle = \frac{1}{N^2} \left(\sum_{k'} \langle \varphi_{k'}^{tgt} | \varphi_k \rangle \right) |\varphi_k^{tgt}\rangle$$

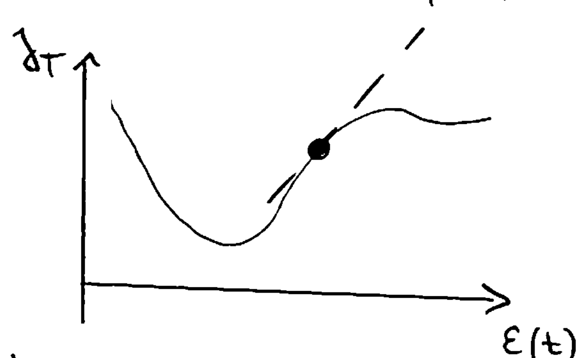
$\Rightarrow$ Slides

$\Rightarrow$ example of application: [Goerz et al. J. P.B. At. Mol. Opt. Phys. 44, 154011]; www.physik.uni-kassel.de/en/koch.html

5. Gradient Ascent

Alternative algorithm to Krotov [Khaneja et al. J. Mag. Res. 172, 296 (2005)]





change pulse in direction of gradient:

$$\varepsilon^{(1)}(t) = \varepsilon^{(0)}(t) - \alpha \frac{\partial J_T}{\partial \varepsilon(t)}$$

second order ($\hat{=}$ Newton) is necessary to reach convergence

LBFGSB is an algorithm that approximates Hessian from first derivatives (black - box - algorithm)

Calculation of gradient - $\frac{\partial J_T}{\partial \varepsilon(t)}$

Assume $J_T \sim \langle \varphi_k^{tgt} | \hat{U}(T,0) | \varphi_k^{in} \rangle$; $U(T,0) = \prod_{i=n}^{1} \hat{U}_i$

$$\frac{\partial \hat{U}}{\partial \varepsilon_i} = \prod_{j=n}^{i+1} \hat{U}_j \left(\frac{\partial \hat{U}_i}{\partial \varepsilon(t_i)} \right) \prod_{j=i-1}^{1} \hat{U}_j \qquad U_i = e^{-i \hat{H}(\varepsilon_i) dt} \longrightarrow \text{series expansion}$$

$$\boxed{\frac{\partial \hat{U}_i}{\partial \varepsilon_i} = \sum_{n=1}^{N} \frac{(-i dt)^n}{n!} \sum_{k=0}^{n-1} \hat{H}^k \left(\frac{\partial H(\varepsilon_i)}{\partial \varepsilon_i} \right) \hat{H}^{n-k-1}}$$

truncate after sufficient N

Note:

- krotov is sequential ($\varepsilon^{(1)}$ enters update), gradient method is not
- Convergence is not strictly guaranteed
- different derivatives need to be calculated: $\frac{\partial J_T}{\partial \varepsilon}$ vs. $\frac{\partial J_T}{\partial \langle \varphi_k |}$