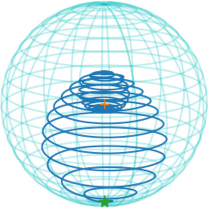
Second International Youth Workshop
''Mathematical Methods in the Problems of Quantum Technologies''
(November 26, 2018, Moscow)

On Some Methods for Constructing Optimal Controls for Quantum Systems

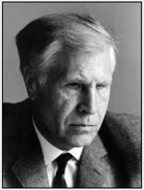


Oleg V. Morzhin
Steklov Mathematical Institute of Russian Academy of Sciences

1. Optimal Control Problems for Quantum Systems

Optimal Control Theory

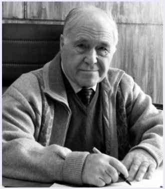
- The optimal control theory (since the mid-20th century) is a mathematical branch devoted to optimization of controls in dynamical systems defined by ordinary differential equations, partial differential equations, etc.
- There are different directions for applications of this theory: aviation, robotics, etc.
- Founders: for example,



L.S. Pontryagin

R.E. Bellman

A.G. Butkovsky



V.F. Krotov

For example: Pontryagin L.S., Boltyanskii V.G., Gamkrelidze R.V., Mishchenko E.F. *The mathematical theory of optimal processes* / Transl. from Russian. New York, London, John Wiley & Sons, Inc., 1962.

(Optimal) Control of Quantum Systems

Some books & reviews

- Butkovskiy A.G., Samoilenko Y.I. *Control of quantum-mechanical processes and systems*. Moscow: Nauka, 1984. (English edition was published in 1990.)
- D'Alessandro D. *Introduction to quantum control and dynamics.* Boca Raton, CRC Press, 2007.
- Brif C., Chakrabarti R., Rabitz H. Control of quantum phenomena: past, present and future, *New J. Phys.* Vol. 12, Issue 7, 075008 (2010).
- Bonnard B., Sugny D. *Optimal control with applications in space and quantum dynamics*. Springfield, American Institute of Math. Sciences, 2012.
- Koch C.P. Controlling open quantum systems: Tools, achievements, and limitations, *J. Phys.: Condens. Matter*. Vol. 28. Issue 21, 213001 (2016).
- Borzì A., Ciaramella G., Sprengel M. *Formulation and numerical solution of quantum control problems*. Philadelphia, SIAM, 2017.

Optimal Control of Quantum Systems

Quantum Systems

- individual molecules, atoms, etc;
- **closed** (w.r.t. environment) and **open** quantum systems;
- modeling with help of quantum mechanical equations: **Schrödinger, Gross–Pitaevskii, Liouville–von Neumann** for closed systems, and, for example, **Lindblad equation** for open systems.

Optimal Quantum Control — actively developed since the late 1970s

- quantum systems are modeled as **controlled** by external actions: **coherent** (e.g., shaped laser field) or **incoherent** (for example, temperature of the environment);
- control functions should be **optimizated** according to minimizing of some **cost functional** ($\mathcal{J}(u) \to \min$) and possible **constraints** for control functions (values, spectrum) and quantum states;
- final time T can be non-fixed and to be minimized ($\mathcal{J}(u,T) = T \to \min$).

Optimal Control of Quantum Systems

Quantum Systems

- individual molecules, atoms, etc;
- **closed** (w.r.t. environment) and **open** quantum systems;
- modeling with help of quantum mechanical equations: **Schrödinger, Gross–Pitaevskii, Liouville–von Neumann** for closed systems, and, for example, **Lindblad equation** for open systems.

Optimal Quantum Control — actively developed since the late 1970s

- quantum systems are modeled as **controlled** by external actions: **coherent** (e.g., shaped laser field) or **incoherent** (for example, temperature of the environment);
- control functions should be **optimizated** according to minimizing of some **cost functional** ($\mathcal{J}(u) \to \min$) and possible **constraints** for control functions (values, spectrum) and quantum states;
- final time T can be non-fixed and to be minimized ($\mathcal{J}(u,T) = T \to \min$).

Control Optimization in Schrödinger Equation

Schrödinger equation with controlled Hamiltonian

$$\frac{d\psi(t)}{dt} = -\frac{i}{\hbar}\mathbf{H}[u(t)]\psi(t), \quad \psi(0) = \psi_0, \quad \psi(t) \in \mathcal{H}, \tag{1}$$

$$\mathbf{H} = \mathbf{H}_0(t) + \sum_{l=1}^{m} \mathbf{H}_l u_l(t), \tag{2}$$

where $\mathcal{H}$ – some Hilbert space (for example, $\mathcal{H} = L^2(\mathbb{R}^d; \mathbb{C}^M)$, $\mathcal{H} = \mathbb{C}^n$).

Cost criterion

$$J = J_T(\psi(T)) + \lambda_u \int_0^T \|u(t)\|^2 dt \to \min, \quad \lambda_u \geq 0, \tag{3}$$

$$J_T = 1 - |\langle \psi(T), \psi_{\text{target}} \rangle|^2 \ \text{ with some given target state } \ \psi_{\text{target}}, \tag{4}$$

$$J_T = -\langle \psi(T), O\psi(T) \rangle \quad (O = O^\dagger). \tag{5}$$

Control Optimization in Schrödinger Equation

Schrödinger equation with controlled Hamiltonian

$$\frac{d\psi(t)}{dt} = -\frac{i}{\hbar}\mathbf{H}[u(t)]\psi(t), \quad \psi(0) = \psi_0, \quad \psi(t) \in \mathcal{H}, \tag{1}$$

$$\mathbf{H} = \mathbf{H}_0(t) + \sum_{l=1}^{m} \mathbf{H}_l u_l(t), \tag{2}$$

where $\mathcal{H}$ – some Hilbert space (for example, $\mathcal{H} = L^2(\mathbb{R}^d; \mathbb{C}^M)$, $\mathcal{H} = \mathbb{C}^n$).

Cost criterion

$$J = J_T(\psi(T)) + \lambda_u \int_0^T \|u(t)\|^2 dt \to \min, \quad \lambda_u \geq 0, \tag{3}$$

$$J_T = 1 - |\langle \psi(T), \psi_{\mathrm{target}} \rangle|^2 \ \text{ with some given target state } \ \psi_{\mathrm{target}}, \tag{4}$$

$$J_T = -\langle \psi(T), O\psi(T) \rangle \quad (O = O^\dagger). \tag{5}$$

Optimal Control Problem for Unitary Transformations

Closed Quantum System & Cost

$$\frac{dU(t)}{dt} = -\frac{i}{\hbar}\mathbf{H}[u(t)]U(t), \quad U(0) = I_N, \tag{6}$$

where $U(t)$ is the unitary operator.
Cost functional: for example,

$$J = -\frac{1}{N^2}\left|\mathrm{Tr}\{W^\dagger U(T)\}\right|^2 \to \min, \tag{7}$$

where the unitary matrix W means some quantum gate.

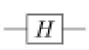
For instance,

- Palao J.P., Kosloff R. Quantum computing by an optimal control algorithm for unitary transformations, *Phys. Rev. Lett.* Vol. 89, No. 18, 188301 (2002).
- Palao J.P., Kosloff R. Optimal control theory for unitary transformations, *Phys. Rev. A.* Vol. 68. Issue 6, 062308 (2003).

Examples of Quantum Gates

Quantum gates, the building blocks of quantum circuits are represented by unitary matrices.

1-Qubit Quantum Gates ($N = 2$): Hadamard gate

$$W^H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$ Circuit representation: 

(8)

2-Qubit Quantum Gate ($N = 2^2$): controlled-NOT transform and quantum Fourier transform

$$W^{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad W^{QFT} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}. \qquad (9)$$

Nielsen M.A., Chuang I.L. Quantum computation and quantum information solutions: 10th Anniversary Edition. Cambridge Univ. Press, 2011.

Control Optimization in Gross-Pitaevskii Equation

Gross-Pitaevskii equation with controlled potential V

$$\frac{d\psi(t)}{dt} = -\frac{i}{\hbar}\Big(K + V(t, u(t)) + \kappa\,|\psi(t)|^2\Big)\psi(t), \quad \psi(0) = \psi_0, \tag{10}$$

where $\psi(t) \in L^2(\mathbb{R}^d; \mathbb{C})$, $K = -\dfrac{\hbar^2}{2m}\nabla^2$. Potential V can be different, for example, with polynomial dependence on u:

$$V = p_2\,(x - u(t))^2 + p_4\,(x - u(t))^4 + p_6\,(x - u(t))^6\,, \tag{11}$$

Objective criterion

$$\mathcal{J} = 1 - \big|\,\langle \psi_{\mathrm{target}}, \psi(T)\rangle\,\big|^2 \to \min \tag{12}$$

S. van Frank, M. Bonneau, J. Schmiedmayer, et al. Optimal control of complex atomic quantum systems, *Scientific Reports*. No. 6, 34187 (2016).

Control Optimization in Lindblad equation

Markovian Master Equation

$$\frac{d}{dt}\rho = \mathcal{L}(\rho) = -\frac{i}{\hbar}\Big[\mathbf{H}[u(t)], \rho\Big] + \mathcal{L}_D(\rho), \quad \rho(0) = \rho_0, \tag{13}$$

$$\mathcal{L}_D(\rho) = \sum_k \gamma_k \Big(A_k \rho A_k^\dagger - \frac{1}{2}\Big\{ A_k^\dagger A_k, \rho \Big\}\Big), \tag{14}$$

where $\rho(t)$ is the density operator ($\rho \geq 0$, $\mathrm{Tr}\rho = 1$); A_k are the Lindblad operators for modeling various dissipative channels.

Cost criterion

For example, maximization of the Hilbert–Schmidt product under the given target state $\rho_{\rm target}$:

$$J = \mathrm{Tr}\left\{\rho(T)\rho_{\rm target}\right\} \to \max \tag{15}$$

Koch C.P. Controlling open quantum systems: Tools, achievements, and limitations, *J. Phys.: Condens. Matter.* Vol. 28, 213001 (2016).

Minimal Time Control in Open Two-Level System

Optimizating both coherent and incoherent controls

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}\left[\widehat{\mathbf{H}}_0 + \widehat{\mathbf{V}}v, \rho\right] + \gamma D(\rho, n), \quad \rho(0) = \rho_0, \tag{16}$$

$$\begin{aligned} D(\rho, n) &= n\Big(\sigma^+\rho\sigma^- + \sigma^-\rho\sigma^+ - \frac{1}{2}\Big\{\sigma^-\sigma^+ + \sigma^+\sigma^-, \rho\Big\}\Big) + \\ &\quad + \Big(\sigma^+\rho\sigma^- - \frac{1}{2}\left\{\sigma^-\sigma^+, \rho\right\}\Big), \end{aligned} \tag{17}$$

$$\rho(T) = \rho_{\text{target}}, \tag{18}$$

$$J(u, T) = T \to \min, \tag{19}$$

$$\widehat{\mathbf{H}}_0 = \hbar\omega \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \widehat{\mathbf{V}} = \mu \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

$\gamma > 0$. Control functions v, n are considered as piecewise continuous:

$$u = (v, n) \in PC([0, T]; Q), \quad Q = [v_{\min}, v_{\max}] \times [0, n_{\max}].$$

Ref.: Morzhin O.V., Pechen A.N. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. (Submitted.)

2. Optimization Methods, Approaches. Numerical Experiments

Optimization Methods, Approaches

- Versions of the steepest descent method [steps in the functional space]: Gross P., Neuhauser D., Rabitz H. Optimal control of curve-crossing systems, *J. Chem. Phys.* Vol. 96, 2834 (1992).
- Krotov method [steps in the functional space]: * Kazakov V.A., Krotov V.F. Optimal control of resonant interaction between light and matter, *Autom. Remote Control*. No. 4 (1987).

  * Sklarz S.E., Tannor D.J. Loading a Bose-Einstein condensate onto an optical lattice: An application of optimal control theory to the nonlinear Schrödinger equation, *Phys. Rev. A.* Vol. 66. Issue 5, 053619 (2002).

  * Morzhin O.V., Pechen A.N. Krotov method in optimal control for closed quantum systems. (Review. Submitted.)
- Genetic algorithms: Amstrup B., Toth G.J., Szabo G., Rabitz H., Loerincz A. *J. Phys. Chem.* Vol. 99 (14) (1995).
- GRAPE — Gradient Ascent Pulse Engineering: Khaneja N., Reiss T., Kehlet C., Schulte-Herbrüggen T., Glaser S.J. *J. Magn. Reson.* Vol. 172. Issue 2 (2005).
- CRAB: Caneva T., Calarco T., Montangero S. Chopped random-basis quantum optimization, *Phys. Rev. A.* Vol. 84 (2), 022326 (2011).
- Hybrid schemes: Goerz M.H., Whaley K.B., Koch C.P. Hybrid optimization schemes for quantum control, *EPJ Quantum Technology*. Vol. 2:21 (2015).

Steepest Descent Method

For the problem (1) — (3) considering the Schrödinger equation

$$u^{(k+1)}(t) = u^{(k)}(t; \gamma = \widehat{\gamma}), \quad t \in [0, T], \quad k \geq 0, \tag{20}$$

$$\begin{gathered} \widehat{\gamma} = \arg\min_{\gamma > 0} J\left(\psi^{(k)}(\cdot; \gamma), u^{(k)}(\cdot; \gamma)\right), \\ u^{(k)}(t; \gamma) = u^{(k)}(t) - \gamma J'\left(\psi^{(k)}(\cdot), u^{(k)}(\cdot)\right), \quad t \in [0, T], \end{gathered} \tag{21}$$

where $\chi^{(k)}(\cdot)$ is the solution of the so-called *adjoint system*

$$\frac{d\chi^{(k)}(t)}{dt} = -\frac{i}{\hbar}\left(\mathbf{H}_0 + \sum_{l=1}^{m} \mathbf{H}_l u_l^{(k)}(t)\right)\chi^{(k)}(t), \quad \chi^{(k)}(T) = -\frac{J_T}{\partial\psi}. \tag{22}$$

The parameter γ is used for local variation w.r.t. the current control $u^{(k)}(\cdot)$; $\psi^{(k)}(\cdot; \gamma)$ is the Scrödinger equation solution under $u = u^{(k)}(\cdot; \gamma)$. It's needed to find such value $\widehat{\gamma}$ that allows to improve the current control $u^{(k)}(\cdot)$.

Gross P., Neuhauser D., Rabitz H. Optimal control of curve-crossing systems, *J. Chem. Phys.* Vol. 96, 2834 (1992).

Krotov Method for Open Quantum System

For the considered above optimization problem with Lindblad equation we can use the first-order (i.e. with linear function $\varphi = \mathrm{Tr}\{\rho B(t)\}$) Krotov method:

$$u^{(k+1)}(t) = u^{(k)}(t) + \frac{S(t)}{\lambda_u} \mathrm{Im} \left\{ \mathrm{Tr} \left[B^{(k)}(t) \frac{\partial \mathcal{L}(\rho)}{\partial u} \Big|_{\rho^{(\mathbf{k+1})}} \right] \right\}, \qquad (23)$$

where $S(t)$ is some shape function.

Koch C.P. Controlling open quantum systems: Tools, achievements, and limitations, *J. Phys.: Condens. Matter.* Vol. 28, 213001 (2016).

Control's Parametrization

Using Piecewise-Constant Functions

Control function u is considered as a piecewise–constant function:

$$u(t) \equiv c_j, \quad t \in [t_j, t_{j+1}), \quad j = 0, ..., N-1,$$
$$t_0 = 0, \quad t_N = T, \quad t_{N-1} = T - T/N, \tag{24}$$

where c_j $(j = \overline{0, N_T - 1})$ are parameters with restricted values. For minimizing the objective function $\mathcal{F}(c_j \mid j = \overline{0, N_T - 1})$ one can use, for example, gradient algorithms (GRAPE – Gradient Ascent Pulse Engineering), genetic algorithms.

Using Trigonometric Functions

According to CRAB, the function u is considered as

$$u(t) = u_{\text{guess}}(t) \left(1 + S(t) \sum_j \left(a_j \sin(\omega_j t) + b_j \cos(\omega_j t) \right) \right), \tag{25}$$

where $u_{\text{guess}}(t)$ and $S(t)$ are some given guess and shape functions. It is needed to minimize the corresponding objective function $\mathcal{F}$. One can use the Nelder–Mead method here.

Formulating Optimal Control Problem in the Bloch Ball

For the problem (12) — (15), using

$$\rho = \frac{1}{2}\left(I_2 + \sum_{j=1}^{3} x_j \sigma_j\right) = \frac{1}{2}\begin{pmatrix} 1+x_3 & x_1 - ix_2 \\ x_1 + ix_2 & 1 - x_3 \end{pmatrix},$$

we obtain

$$\frac{dx_1}{dt} = -\frac{\gamma}{2}x_1 + \omega x_2 - \gamma x_1 n, \tag{26}$$

$$\frac{dx_2}{dt} = -\omega x_1 - \frac{\gamma}{2}x_2 - 2\kappa x_3 v - \gamma x_2 n, \tag{27}$$

$$\frac{dx_3}{dt} = 2\kappa x_2 v - \gamma x_3 + \gamma - 2\gamma x_3 n, \tag{28}$$

$$x_j(0) = x_{j,0}, \tag{29}$$

$$x_j(T) = x_{j,\mathrm{target}}, \tag{30}$$

where $j = 1, 2, 3$, $\kappa = \mu/\hbar$. This system is considered together with

$$J(u, T) = T \to \min.$$

Optimization Approach

A) Consider a series of optimal control problems P_j, $j = 1, 2, \dots K$, where each problem has no terminal constraint and is considered with some final time $T = T_j \in \{T_1, T_2, \dots, T_K\}$. Cost criterion for each problem P_j is

$$J_j(u) = \|x(T_j) - x_{\text{target}}\|^2 \to \min . \qquad (31)$$

The goal is to obtain the minimal possible T_j for which $J_j = 0$.

B) For each problem P_j, we can apply, for example, projected gradient method. Here we consider this method in the following version:

$$u^{(k)}(t;\alpha^{(k)}) = \mathrm{Pr}_Q\left(u^{(k)}(t) + \alpha^{(k)}\mathcal{K}(p^{(k)}(t), x^{(k)}(t))\right), \qquad (32)$$

$$u^{(k)}(t;\alpha^{(k)},\beta) = u^{(k)}(t) + \beta\left(u^{(k)}(t;\alpha^{(k)}) - u^{(k)}(t)\right), \qquad (33)$$

$$\beta^{(k)} = \arg\min_{\beta\in(0,1]} f(\beta) = \arg\min_{\beta\in(0,1]} J_i(u^{(k)}(\cdot;\alpha^{(k)},\beta)), \qquad (34)$$

$$u^{(k+1)}(t) = u^{(k)}(t;\alpha^{(k)},\beta^{(k)}), \qquad (35)$$

where $\alpha^{(k)} > 0$ is fixed for all iterations.

On the Bloch Sphere: Non-Uniqueness of Optimal Control

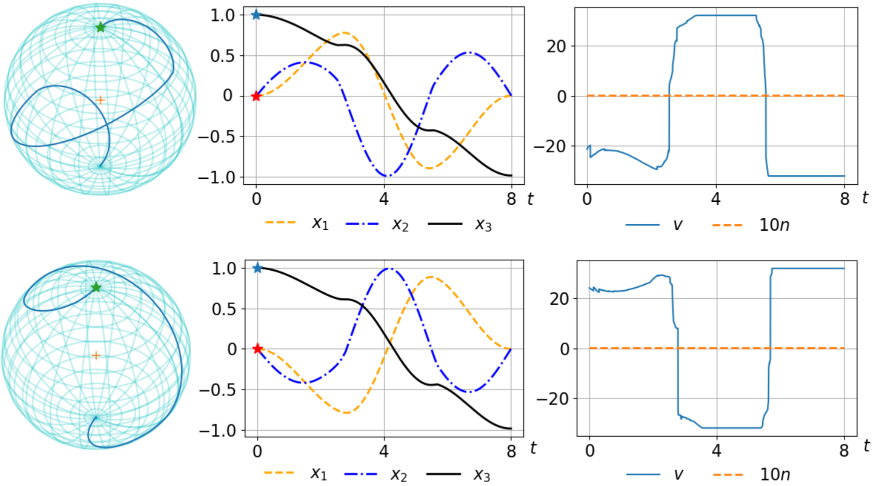


Figure: Movement from $(0, 0, 1)$ to $(0, 0, -1)$ on the Bloch sphere.

On the Bloch Sphere: There and Back

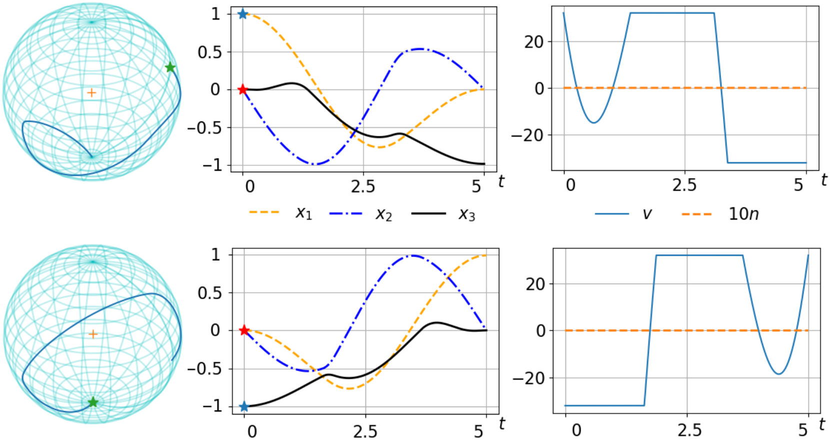


Figure: Movements: from $(1, 0, 0)$ to $(0, 0, -1)$ (top); and back to the starting point (bottom)

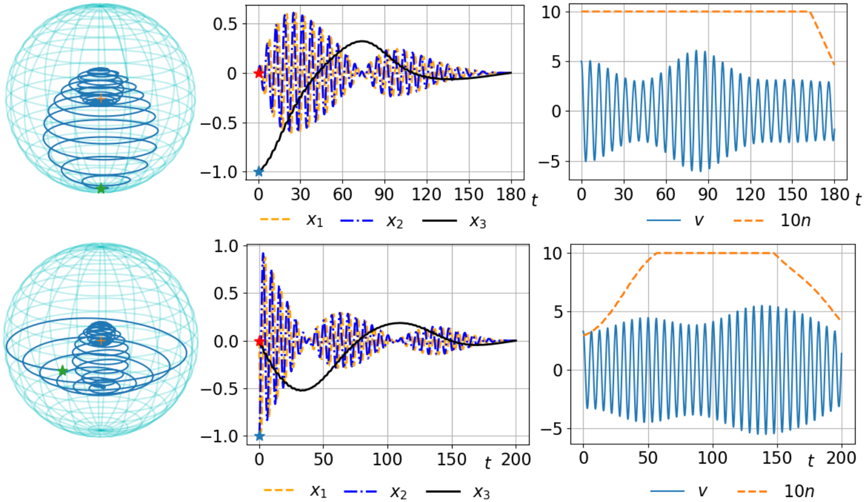


Figure: Movements: from $(0, 0, -1)$ to $(0, 0, 0)$ (top); from $(0, -1, 0)$ to $(0, 0, 0)$ (bottom)

Inside the Bloch Ball: Time Effect

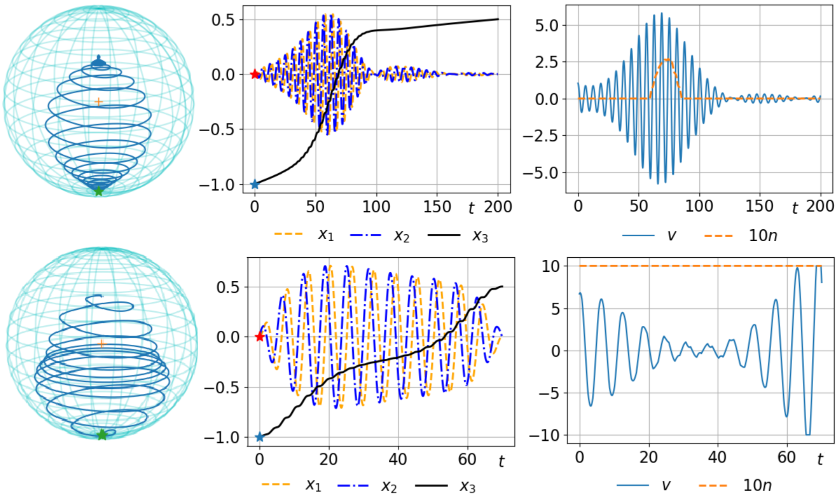


Figure: Movements from $(0, 0, -1)$ to $(0, 0, 0.5)$: $T = 200$ (top); $T = 70$ (bottom)

Inside the Bloch Ball: Time Effect (Second Example)

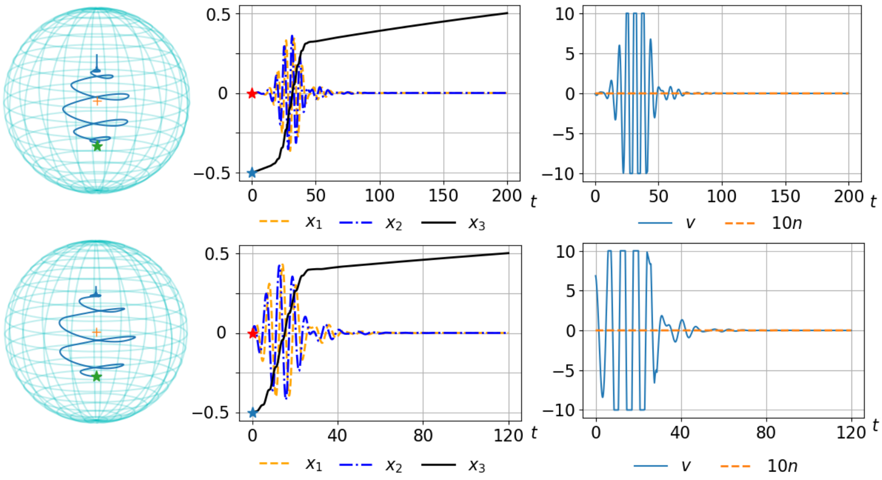


Figure: Movements from $(0, 0, -0.5)$ to $(0, 0, 0.5)$: $T = 200$ (top); $T = 120$ (bottom)

Conclusions

- Control of quantum systems is needed for modern and future technologies.
- Optimization algorithms are very important for modeling of quantum control.
- Three directions:

  – working in the functional space of controls with usage of gradient, Krotov methods, etc;

  – reducing to finite-dimensional optimization problems using control's parametrization;

  – multimethod schemes.
- Articles:

Morzhin O.V., Pechen A.N. Krotov method in optimal control for closed quantum systems. (Review. Submitted.)

Morzhin O.V., Pechen A.N. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. (Submitted.)

Conclusions

- Control of quantum systems is needed for modern and future technologies.
- Optimization algorithms are very important for modeling of quantum control.
- Three directions:

  – working in the functional space of controls with usage of gradient, Krotov methods, etc;

  – reducing to finite-dimensional optimization problems using control's parametrization;

  – multimethod schemes.
- Articles:

  Morzhin O.V., Pechen A.N. Krotov method in optimal control for closed quantum systems. (Review. Submitted.)

  Morzhin O.V., Pechen A.N. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. (Submitted.)

Conclusions

- Control of quantum systems is needed for modern and future technologies.
- Optimization algorithms are very important for modeling of quantum control.
- Three directions:

  – working in the functional space of controls with usage of gradient, Krotov methods, etc;

  – reducing to finite-dimensional optimization problems using control's parametrization;

  – multimethod schemes.
- Articles:

  Morzhin O.V., Pechen A.N. Krotov method in optimal control for closed quantum systems. (Review. Submitted.)

  Morzhin O.V., Pechen A.N. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. (Submitted.)

Conclusions

- Control of quantum systems is needed for modern and future technologies.
- Optimization algorithms are very important for modeling of quantum control.
- Three directions:

  – working in the functional space of controls with usage of gradient, Krotov methods, etc;

  – reducing to finite-dimensional optimization problems using control's parametrization;

  – multimethod schemes.
- Articles:

  Morzhin O.V., Pechen A.N. Krotov method in optimal control for closed quantum systems. (Review. Submitted.)

  Morzhin O.V., Pechen A.N. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. (Submitted.)