Optimization of coherent and incoherent controls and estimation of reachable sets for an open two-level quantum system

O. V. Morzhin[1], A. N. Pechen[2]

Keywords: quantum control, coherent control, incoherent control

MSC2010 codes: 81Q93, 34H05, 49Mxx

Control of quantum systems, e.g., individual atoms, molecules is an important direction in modern quantum technologies [1–5]. Typically in experimental situations controlled systems are open, i.e., interacting with the environment. Environment is often considered as having deleterious effects on the dynamics. However, it also can be used for controlling the system. A powerful method of incoherent control was found and studied in [6]. In this case, spectral density of the environment, i.e., distribution of particles of the environment in their momenta and internal degrees of freedom, is used as the control function to manipulate the system. This spectral density is often considered as thermal (Planck distribution), but in general it can be any non-equilibrium non-negative function, possibly depending on time, of momenta and internal degrees of freedom of environmental particles. In [6], general method of incoherent control using this spectral density was obtained, including in combination with coherent control, either subsequent of simultaneous. The method was developed for any multilevel systems. Numerical simulations were performed for an explicit example of four level systems using global search optimization by genetic algorithms. Non-selective quantum measurements were also found to be a powerful tool for incoherent control [7].

Initially for this incoherent method it was not clear to what degree it allows for manipulating the system. In [8], a significant advance was achieved where it was shown that combination of coherent and incoherent controls allows to approximately steer *any* initial density matrix to *any* given target density matrix. This property approximately realizes controllability of open quantum systems in the set of all density matrices — the strongest possible degree of quantum state control. This result has several important features. (1) It is obtained with a physical class of GKSL master equations well known in quantum optics and derived in the weak coupling limit. (2) It was obtained for almost all values of parameters of this class of master equations and for multi-level quantum systems of arbitrary dimension. (3) For incoherent controls in this scheme an explicit analytic solution (not numerical) was obtained. (4) The scheme is robust to variations of the initial state — the optimal control steers simultaneously *all* initial states into the target state, thereby physically realizing all-to-one Kraus maps previously theoretically exploited for quantum control [9].

In [10–14], this method was applied to the example of two-level quantum systems controlled by scalar coherent v and incoherent n controls from various points of view, including different objective criteria and optimization methods, analysis of reachable and controllability sets, use of machine learning. Density matrix of the system $\rho(t) \in \mathbb{C}^{2\times 2}$ is a Hermitian positive semi-definite matrix, $\rho(t) = \rho^\dagger(t) \geq 0$, with unit trace, $\mathrm{Tr}\rho(t) = 1$. Following [6], master equation for density matrix is

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[\mathbf{H}_0 + \mathbf{V}v, \rho(t)] + \mathcal{L}_{n(t)}(\rho(t)), \quad \rho(0) = \rho_0. \tag{1}$$

Here $[A, B]$ denote the commutator $[A, B] = AB + BA$ of operators A, B; $\hbar$ is the Planck's constant. Without loss of generality, $\mathbf{H}_0 = \hbar\omega \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ and $\mathbf{V} = \mu \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, where $\omega > 0$, $\mu \in \mathbb{R}$,

[1]Steklov Mathematical Institute of Russian Academy of Sciences, Department of Mathematical Methods for Quantum Technologies, Russia, Moscow. Email: morzhin.oleg@yandex.ru

[2]Steklov Mathematical Institute of Russian Academy of Sciences, Department of Mathematical Methods for Quantum Technologies, Russia, Moscow. National University of Science and Technology "MISIS", Russia, Moscow. Moscow Institute of Physics and Technology, Russia, Dolgoprudny. Email: apechen@gmail.com

$\mu \neq 0$. The superoperator of dissipation $\mathcal{L}_{n(t)}$ is

$$\mathcal{L}_{n(t)}(\rho(t)) = \gamma\,(n(t)+1)\left(\sigma^- \rho(t)\sigma^+ - \frac{1}{2}\left\{\sigma^+\sigma^-, \rho(t)\right\}\right) \\ + \gamma n(t)\left(\sigma^+ \rho(t)\sigma^- - \frac{1}{2}\left\{\sigma^-\sigma^+, \rho(t)\right\}\right), \qquad \gamma > 0$$

It describes the controlled interactions between the quantum system and its environment (reservoir). Here $\{A, B\}$ denotes the anti-commutator $\{A, B\} = AB - BA$ of two operators A, B; matrices $\sigma^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, $\sigma^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ define the transitions between the two energy levels. The following constraint follows from physical meaning of incoherent control as spectral distribution of particles:

$$n(t) \geq 0 \qquad \forall t \geq 0.$$

The optional constraints $v(t) \in [v_{\min}, v_{\max}]$, $n(t) \in [0, n_{\max}]$ $\forall t \geq 0$ can be used with some bounds $v_{\min}$, $v_{\max}$, and $n_{\max}$. We denote $u = (v, n)$.

In [10], the optimal control problem for steering the system (1) to a given target density matrix ρ_{target} in minimal final time T was considered with piecewise continuous controls v, n. For this time-minimal control problem, we consider the problems

$$J_i(u) = \|\rho(T_i) - \rho_{\text{target}}\|^2_{\text{HS}} \to \inf, \qquad i = 1, 2, \ldots, N,$$

for a series of decreasing final times $\{T_i\}_{i=1}^N$. "HS" means the Hilbert–Schmidt norm.

In [11], the optimal control problem for maximizing the overlap $\langle \rho(T), \rho_{\text{target}} \rangle_{\text{HS}}$ between the final density matrix $\rho(T)$ and given target density matrix ρ_{target} for the system (1) together with minimization of T was considered with piecewise continuous controls v, n. The problems

$$I_i(u) = \langle \rho(T_i), \rho_{\text{target}} \rangle_{\text{HS}} \to \sup, \qquad i = 1, 2, \ldots, N,$$

are considered for a series of decreasing final times $\{T_i\}_{i=1}^N$.

In [12, 13], the system (1) was considered with piecewise constant controls under various constraints on controls' magnitudes and variations. The article [12] considers a series of time-minimal control problems using Bloch vectors for representing system quantum states, and contains a design of a machine learning scheme based on the kNN method and neural networks (MLPs), which shows useful results for generating suboptimal final time and controls v, n for a given initial density matrix in the numerical experiments. The scheme uses the training dataset formed by the optimization results obtained via the differential evolution and dual annealing methods, implementations of which are available in SciPy. For training MLPs, scikit-learn library was used.

In [13, 14], various tools (support hyperplanes (see [15]), sections (see [16]), etc.) were applied for numerical estimation of reachable and controllability sets in terms of the Bloch parametrization. The work [13] includes also the exact description of reachable and controllability sets for some class of controls. In the framework of the approach using support hyperplanes, [13] notes an optimal control problem, where $v = 0$ and $n = 0$ satisfy the Pontryagin maximum principle [17] but not optimal. In addition, for this optimal control problem some comparative numerical results were obtained using the dual annealing method, Krotov method (see [4, 5, 18]), and Gradient Ascent Pulse Engineering (GRAPE) with one- and- two-step gradient projection methods (see [19, 20]) for illustrating, first, how zero controls v, n are far from the optimized controls and, second, the importance of adjusting the methods' parameters.

Acknowledgments. This talk presents the work partially funded by the Russian Science Foundation (project No. 17-11-01388).

References

[1] S.J. Glaser, U. Boscain, T. Calarco, C.P. Koch, W. Köckenberger, R. Kosloff, I. Kuprov, B. Luy, S. Schirmer, T. Schulte-Herbrüggen, D. Sugny, F.K. Wilhelm. Training Schrödinger's cat: quantum optimal control. Strategic report on current status, visions and goals for research in Europe. // Eur. Phys. J. D. 2015. V. 69. No. 12. P. 279

[2] C. Brif, R. Chakrabarti, H. Rabitz. Control of quantum phenomena: past, present and future. // New J. Phys. 2010. V. 12. No 7. P. 075008.

[3] K.W. Moore, A. Pechen, X.-J. Feng, J. Dominy, V.J. Beltrani, H. Rabitz. Why is chemical synthesis and property optimization easier than expected? // Physical Chemistry Chemical Physics. 2011. V. 13(21). P. 10048–10070.

[4] C.P. Koch. Controlling open quantum systems: Tools, achievements, and limitations. // J. Phys.: Condens. Matter. 2016. 28:21. P. 213001.

[5] O.V. Morzhin, A.N. Pechen. Krotov method for optimal control of closed quantum systems. // Russian Math. Surveys. 2019. V. 74. No. 5. P. 851–908.

[6] A. Pechen, H. Rabitz. Teaching the environment to control quantum systems. // Phys. Rev. A. 2006. V. 73. No. 6. P. 062102.

[7] A. Pechen, N. Il'in, F. Shuang, H. Rabitz. Quantum control by von Neumann measurements. // Phys. Rev. A. 2006. V. 74. P. 052102

[8] A. Pechen. Engineering arbitrary pure and mixed quantum states. // 2011. Phys. Rev. A. V. 84. No. 4. P. 042106

[9] R. Wu, A. Pechen, C. Brif, H. Rabitz. Controllability of open quantum systems with Kraus-map dynamics. //J. Phys. A. 2007. V. 40. No. 21. P. 5681–5693

[10] O.V. Morzhin, A.N. Pechen. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. // Int. J. Theor. Phys. 2019.

[11] O.V. Morzhin, A.N. Pechen. Maximization of the overlap between density matrices for a two-level open quantum system driven by coherent and incoherent controls. // Lobachevskii J. Math. 2019. V. 40. No. 10. P. 1532–1548

[12] O.V. Morzhin, A.N. Pechen. Machine learning for finding suboptimal final times and coherent and incoherent controls for an open two-level quantum system. // Lobachevskii J. Math. 2020. V. 41. No. 12. P. 2353–2369.

[13] O.V. Morzhin, A.N. Pechen. On reachable and controllability sets for time-minimal control of an open two-level quantum system // Proc. Steklov Inst. Math. 2021. (In press).

[14] O.V. Morzhin, A.N. Pechen. Numerical estimation of reachable and controllability sets for a two-level open quantum system driven by coherent and incoherent controls. // AIP Conf. Proceedings (Submitted).

[15] F.L. Chernousko: State Estimation for Dynamic Systems. — Boca Raton, Ann Arbor, London, Tokyo, CRC Press. 1993.

[16] O.V. Morzhin, A.I. Tyatyushkin. An algorithm of the method of sections and program tools for constructing reachable sets of nonlinear control systems. // J. Comput. Syst. Sci. Int. 2008. V. 47. No. 1 P. 1–7.

[17] L.S. Pontryagin, V.G. Boltyanskii, R.V. Gamkrelidze, E.F. Mishchenko. The Mathematical Theory of Optimal Processes (transl. from Russian). — New York, London, Interscience Publishers John Wiley & Sons, Inc. 1962.

[18] V.F. Krotov: Global Methods in Optimal Control Theory. — New York, Marcel Dekker. 1996.

[19] D.P. Bertsekas: Nonlinear Programming. 3rd ed. – Athena Scientific, Belmont. 2016.

[20] A.S. Antipin. Minimization of convex functions on convex sets by means of differential equations. // Diff. Equations. 1994. V. 30. No. 9. P. 1365–1375 .