Optimization methods for open quantum systems driven by coherent and incoherent controls

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

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Control of quantum systems, e.g., individual atoms, molecules is an important direction in modern quantum technologies [1–5]. In mathematical modeling of such control for a closed or open (interacting with the environment) quantum system, various numerical optimization schemes are used including Pontryagin maximum principle, steepest descent, Krotov, Zhu–Rabitz, Maday–Turinici methods, GRadient Ascent Pulse Engineering (GRAPE), zeroth order stochastic optimization methods, Chopped Random-Basis (CRAB), etc.; the survey [6] gives a number of the corresponding bibliographic references and is mainly devoted to Krotov method for closed quantum systems. An important application of numerical optimization is to help in theoretical analysis of certain properties of a quantum system, as, e.g., the article [7] shows.

This talk is devoted to controls of some kind of open quantum systems. Typically in experimental situations controlled systems are open. 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 [8]. 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 [8], 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 [9].

Initially for this incoherent method it was not clear to what degree it allows for manipulating the system. In [10], 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 Gorini–Kossakowski–Sudarshan–Lindblad (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 [11].

Based on the articles [8, 10], the works [12–20] consider one- and two-qubit open quantum systems driven by coherent and incoherent controls of various classes. Consider N-order density matrix ρ, i.e. $\rho \in \mathbb{C}^{N\times N}$ is a Hermitian positive semi-definite matrix, $\rho = \rho^\dagger \geq 0$, with unit

[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

trace, Tr$\rho = 1$. Its evolution is determined by the GKSL master equation, where, in general, coherent control u enters into the Hamiltonian and incoherent control n inters into both the Hamiltonian (via Lamb shift) and the dissipative superoperator $\mathcal{L}_{n(t)}$:

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}\left[H_S + \varepsilon H_{\mathrm{eff},n(t)} + V_{u(t)}, \rho(t)\right] + \varepsilon \mathcal{L}_{n(t)}(\rho(t)), \quad \rho(0) = \rho_0, \tag{1}$$

where $[A, B]$ denote the commutator $[A, B] = AB - BA$ of operators A, B; H_S and $H_{\mathrm{eff},n(t)}$ are correspondingly the free and effective Hamiltonians; $V_{u(t)}$ describes interactions between the quantum system and coherent control. The articles [12 – 18] are devoted to analyzing various aspects of the one-qubit case, i.e. for $N = 2$, where $H_{\mathrm{eff},n(t)}$ is absent and $\varepsilon = 1$ is considered. The two-qubit case, i.e. for $N = 4$, with certain $H_{\mathrm{eff},n(t)}$ and arbitrary $\varepsilon > 0$ is considered in [19, 20]. The detailed formulations of these quantum systems are given in these articles.

For the system (1), various objective criteria were used under various classes of coherent and incoherent controls. For example, the articles [12, 15] are devoted to minimal time generation of a given target density matrix for the one-qubit case using (a) reduction to a sequance of the problems for minimizing the Hilbert–Schmidt distance between the final and target density matrices with some fixed final times (two-parameter one-step gradient projection method (GPM) in the functional space of controls was used) or (b) certain objective function taking into account the requirements to minimize the distance and final time (finite-dimensional stochastic optimization and machine learning were used). For the two-qubit case, the works [19, 20] consider the problem of minimizing the Hilbert–Schmidt distance for a given final time via final-dimensional optimization, where stochastic optimization in [19], GRAPE and one/two-step GPM (without projection, the two-step version of GPM is Polyak heavy ball method) were used in [20]. For the one-qubit case, the articles [13, 14] are devoted to maximization correspondingly of the Hilbert–Schmidt scalar product (i.e. mean) and Uhlmann–Jozsa fidelity for a given target density matrix, where various numerical optimization methods, Pontryagin maximum principle, and Gabasov second order necessary condition for optimality were used. The articles [16–18] are devoted to analyzing reachable and controllability sets of the one-qubit quantum system under various classes of controls including use of optimization methods. The results of [12–20] are various including conclusions about the optimization methods' effectiveness, structures of optimized controls, reachable and controllability aspects, etc.

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