Quantum control landscapes

A. N. Pechen[1]

Keywords: quantum control, control landscape, qubit, quantum gates

MSC2010 codes: 81P68, 81Q93, 46N50

Control of quantum systems, e.g., individual atoms, molecules is an important direction in modern quantum technologies [1–5]. Consider coherent control of an N–level quantum system which is isolated from the environment. Its dynamics is described by Schrödinger equation:

$$i\frac{dU_t^f}{dt} = (H_0 + f(t)V)U_t^f, \qquad U_{t=0}^f = \mathbb{I}.$$

Here H_0 and V are the free and interaction Hamiltonians (Hermitian $N \times N$-matrices such that $[H_0, V] \neq 0$), and $f \in L_2([0,T],\mathbb{R})$ is a coherent control.

Let O be a quantum observable (system's Hermitian operator) and $W \in SU(N)$ be a target unitary operator. Typical quantum control objectives correspond to maximization of average value of O and generation of target process W and are characterized by objective functionals

$$\begin{aligned} J_O[f] &= \mathrm{Tr}(OU_T^f\rho_0 U_T^f)| \to \max . \\ J_W[f] &= \frac{1}{4}|\mathrm{Tr}(W^\dagger U_T^f)|^2 \to \max . \end{aligned}$$

Globally optimal controls realize global maximum of the objective. Trap is a control which is optimal only locally but not globally. To establish whether traps exist or not for a given control objective is a highly important practical problem, since they determine the level of difficulty for finding globally optimal controls in numerical and laboratory experiment [5-7].

In [5] it was proposed that quantum control objectives are typically free of traps. However, this property was proved only for $N = 2$ [8,9] and for control of transmission (that corresponds to $N = \infty$) [10]. Examples of trapping behavior were found for systems with $N \geq 3$ [6,7].

In [8,9] it was shown that if time T is large enough then the objective functional J_W for a qubit has not traps. To explicitly formulate these results, define the special constant control f_0 and the special time T_0:

$$\begin{aligned} f_0 &:= \frac{-\mathrm{Tr}H_0\mathrm{Tr}V + 2\mathrm{Tr}(H_0V)}{(\mathrm{Tr}V^2)^2 - 2\mathrm{Tr}(V^2)}, \\ T_0 &:= \frac{\pi}{\|H_0 - \mathbb{I}\mathrm{H}_0/2 + f_0(V - \mathbb{I}\mathrm{Tr}V/2)\|}. \end{aligned}$$

Theorem 1. For $N = 2$, if $\mathrm{Tr}V = 0$ and $T \geq T_0$, then all maxima and minima of the objective functionals $\mathcal{J}_O[f]$ and $J_W[f]$ are global. Any control $f \neq f_0$ can not be a trap for any $T > 0$.

In [10] it was proved that control of quantum transmission of a particle with energy E through potential V is free of traps. For fixed E, consider $T_E[V]$ as objective functional of the control potential V. The control goal is to maximize transmission.

Theorem 2. The only extremum of the transmission coefficient $T_E[V]$ is the value $T_E = 1$, i.e.,

$$\frac{\delta T_E}{\delta V} = 0 \Leftrightarrow T_E[V] = 1$$

[1]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

In [11,12], small-time control landscapes were studied for the control objective J_W. The following result was proved [11].

Theorem 3. Let $W \in SU(2)$ be a single qubit quantum gate. If $[W, H_0 + f_0V] \neq 0$ then for any $T > 0$ traps do not exist. If $[W, H_0 + f_0V] = 0$ then any control, except possibly $f \equiv f_0$, is not trap for any $T > 0$ and the control f_0 is not trap for $T > T_0$.

In [12] it is shown that the control f_0 is not a trap in the case $T \leq T_0$ and $[W, H_0 + f_0V] = 0$. One can show that it is sufficient to consider $H_0 = \sigma_z$, $V = v_x\sigma_x + v_y\sigma_y$ and $W = e^{i\varphi_W\sigma_z}$ without loss of generality. Here $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices, $v_x, v_y \in \mathbb{R}$ such that $v = \sqrt{v_x^2 + v_y^2} > 0$, and $\varphi_W \in (0, \pi]$. In this case, the special time is $T_0 = \frac{\pi}{2}$ and the special control is $f_0 = 0$. For fixed φ_W and T the value of the objective evaluated at f_0 is

$$J_W[f_0] = \cos^2(\varphi_W + T). \tag{1}$$

The control $f_0 = 0$ is a critical point, i.e., gradient of the objective evaluated at this control is zero. The Taylor expansion of the functional J_W at f_0 up to the second order has the form:

$$J_W[f_0 + \delta f] = J_W[f_0] + \frac{1}{2}\int_0^T\int_0^T \mathrm{Hess}(t,s)\delta f(t)\delta f(s)dtds + o(\|\delta f\|_{L_2}^2), \quad \delta f \to 0,$$

where the integral kernel of Hessian has the form (see [12]):

$$\mathrm{Hess}(s,t) = -2v^2\cos(\varphi_W + T)\cos(\varphi_W + T - 2|t-s|).$$

We study the spectrum of this integral operator. For this purpose, we consider the following cases:

- (φ_W, T) belongs to the triangle domain
$$\mathcal{D}_1 := \left\{(\varphi_W, T) \ : \ 0 < T < \frac{\pi}{2}, \quad \frac{\pi}{2} \leq \varphi_W < \pi - T\right\};$$
- (φ_W, T) belongs to the triangle domain
$$\mathcal{D}_2 := \left\{(\varphi_W, T) \ : \ 0 < T \leq \frac{\pi}{2}, \quad \pi - T < \varphi_W \leq \pi, \quad (\varphi_W, T) \neq (\frac{\pi}{2}, \pi)\right\};$$
- (φ_W, T) belongs to the square domain without the diagonal
$$\mathcal{D}_3 := \left\{(\varphi_W, T) \ : \ 0 < T \leq \frac{\pi}{2}, \quad 0 < \varphi_W < \frac{\pi}{2}, \varphi_W + T \neq \frac{\pi}{2}\right\}.$$

Remark 1. It is easy to see from (1) that if $(\varphi_W, T) \in (0, \frac{\pi}{2}] \times (0, \pi] \setminus (\mathcal{D}_1 \cup \mathcal{D}_2 \cup \mathcal{D}_3)$ then f_0 is a point of global extrema of the objective functional J_W.

Theorem 4. If $(\varphi_W, T) \in \mathcal{D}_1 \cup \mathcal{D}_2 \cup \mathcal{D}_3$ then the Hessian of the objective functional J_W at $f_0 = 0$ is an injective compact operator on $L_2([0, T], \mathbb{R})$. Moreover,

1. If $(\varphi_W, T) \in \mathcal{D}_1$, then Hessian at f_0 is strictly negative.
2. If $(\varphi_W, T) \in \mathcal{D}_2 \cup \mathcal{D}_3$ then Hessian at f_0 has both negative and positive eigenvalues. In this case, the special control $f_0 = 0$ is a saddle point for the objective functional.

The second case was previously proved using a different method [11]. The first case is a new result of [12], where it was rigorously proved that in this case f_0 is either a global maximum point or a trap. In [12], also numerical optimization methods were used such as Gradient Ascent Pulse Engineering (GRAPE), differential evolution, and dual annealing to show that the special control is a point of global maximum if $(\varphi_W, T) \in \mathcal{D}_1$. A rigorous proof of this finding remains an open problem. The numerical results also shown that for $\frac{\pi}{2} \leq \varphi_W \leq \pi$ and $0 < T \leq \frac{\pi}{2}$ achieving the objective functional value 1, i.e., providing exact generation of phase shift gate, requires a final time T being not less than the minimal time $T_{\min} = \pi - \varphi_W$.

Acknowledgments. This talk presents work partially funded by Russian Federation represented by the Ministry of Science and Higher Education (grant number 075-15-2020-788).

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. 69:12 (2015), 279

[2] C. Brif, R. Chakrabarti, H. Rabitz. Control of quantum phenomena: past, present and future // New J. Phys. 2010. V. 12. No. 7. 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. No. 21. P. 10048–10070

[4] C.P. Koch. Controlling open quantum systems: Tools, achievements, and limitations // J. Phys.: Condens. Matter. 2016. V. 28 No. 21. 213001

[5] H.A. Rabitz, M.M. Hsieh, C.M. Rosenthal. Quantum optimally controlled transition landscapes // Science. 2004. 303:5666. 1998–2001

[6] A.N. Pechen, D.J. Tannor. Are there traps in quantum control landscapes? // Phys. Rev. Lett. 2011. 106 120402

[7] P. de Fouquieres, S.G. Schirmer. A closer look at quantum control landscapes and their implication for control optimization // Infin. Dimens. Anal. Quantum Probab. Relat. Top. 2013 16:3 1350021

[8] A. Pechen, N. Il'in. Trap-free manipulation in the Landau-Zener system // Phys. Rev. A. 2012. 86 052117

[9] A.N. Pechen, N.B. Il'in. Coherent control of a qubit is trap-free // Proc. Steklov Inst. Math. 2014. 285:1 P. 233–240

[10] A. N. Pechen, D. J. Tannor. Control of quantum transmission is trap-free // Canadian Journal of Chemistry. 2014. 92:2 P. 157–159

[11] N.B. Il'in, A.N. Pechen. On extrema of the objective functional for short-time generation of single-qubit quantum gates // Izvestiya: Mathematics. 2016. 80:6 P. 1200–1212

[12] B.O. Volkov, O.V. Morzhin, A.N. Pechen. Quantum control landscape for ultrafast generation of single-qubit phase shift quantum gates // J. Phys. A: Math. Theor. Accepted.