On extrema of the objective functional for short-time generation of single-qubit quantum gates

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Abstract. We study the extrema of the objective functional in the problem of generation of quantum gates (logical elements for quantum computations) for two-level systems with short duration of the control. We consider the problem of the existence of local but not global extrema, the so-called traps. The absence of traps was previously proved for a sufficiently long duration of the control. We prove that traps are absent for an arbitrarily small duration of the control for almost all target unitary operators and Hamiltonians. For the remaining target unitary operators and Hamiltonians we obtain a new lower bound for the duration of the control which guarantees the absence of traps.

Keywords: quantum control, qubit.

Introduction

In this paper we study the problem of controlling a qubit (that is, a two-level quantum system) using coherent control pulses (electromagnetic fields). A qubit is one of the basic elements in the realization of quantum computing and the creation of a quantum computer. An important problem is to generate single-qubit gates (logical elements for quantum computation) [1].

The dynamics of a qubit interacting with a coherent control $f(t)$ under the assumption of sufficiently good isolation of the qubit from the environment is described by the Schrödinger equation for a unitary evolution $U_t$ (a unitary $2 \times 2$ matrix):

$$i \frac{dU_t}{dt} = (H_0 + f(t)V)U_t, \quad U_{t=0} = I.$$  \hspace{1em} (1)

Here $H_0$ and $V$ are Hermitian $2 \times 2$ matrices. To make the control problem non-trivial, we assume that $[H_0, V] \neq 0$. The reduced dynamics of the qubit in the presence of an environment is described by various master equations ([2]–[4]) and by a quantum channel instead of a unitary transformation [5], [6]. The control $f$ belongs to some set $\mathcal{U}$ of admissible controls, $f \in \mathcal{U}$. In applications one considers sets of admissible controls $\mathcal{U} = L^1([0, T]; \mathbb{R})$, $\mathcal{U} = L^2([0, T]; \mathbb{R})$ and others. Here $T > 0$ is the fixed duration of the control. The problem of optimal performance has also been considered [7]. We consider the set of controls $\mathcal{U} = L^1([0, T]; \mathbb{R})$. 

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The matrix entries \([U_t]_{ik}\) are assumed to be absolutely continuous functions on the interval \([0, T]\), \([U_t]_{ik} \in AC[0, T]\). In this case the equation (1) has a unique solution for every control \(f \in U\) [8].

An important problem in quantum information theory is the generation of quantum gates (special unitary \(2 \times 2\) matrices) \(W \in SU(2)\), that is, finding a control \(f\) such that \(U_T = W\), perhaps up to a phase factor. This problem can be formulated as the problem of finding a control \(f\) which maximizes the objective functional

\[
\mathcal{J}_W[f] = \frac{1}{4} |\text{Tr}(W^\dagger U_T)|^2. \tag{2}
\]

The objective functional \(\mathcal{J}_W\) reaches its maximum value \(\mathcal{J}_W^{\text{max}} = 1\) on a unitary matrix of the form \(U_T = W e^{i\omega}\), where \(\omega \in \mathbb{R}\) is an arbitrary phase. The global minimum of the objective \(\mathcal{J}_W\) is equal to zero, \(\mathcal{J}_W^{\text{min}} = 0\). Examples of the objective matrix \(W\) which are important for applications include the Hadamard gate \(W = \mathbb{H}\),

\[
\mathbb{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{3}
\]

the phase shift gate \(W = U_\phi\), where \(\phi \in (0, 2\pi)\),

\[
U_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \tag{4}
\]

and others.

In this paper we consider the problem of the possible existence of local but not global maxima for the objective functional \(\mathcal{J}_W\) for short \(T\). Such local maxima are called traps [9]–[13]. We prove the absence of traps for almost all objective unitary operators and Hamiltonians for an arbitrarily small duration of the control. For the remaining set of objective unitary operators and Hamiltonians we obtain a new lower bound for the duration of the control that guarantees the absence of traps.

§ 1. The absence of traps for controlling a qubit over long times

If traps were to exist they would become an obstacle in the search for globally optimal control by local search algorithms. In [9], [10] the absence of traps was conjectured for typical control problems for systems which are isolated from the environment, that is, for closed quantum systems [14], [15]. In [16]–[18] the absence of traps was proved for closed two-level quantum systems in the case of sufficiently long \(T\).

Define the special control \(f_0\) and time \(T_0\):

\[
f_0 := -\frac{\text{Tr} H_0 \text{Tr} V + 2 \text{Tr}(H_0 V)}{(\text{Tr} V)^2 - 2 \text{Tr} V^2}, \tag{5}
\]

\[
T_0 := \frac{\pi}{\|H_0 - \mathbb{I} \text{Tr} H_0/2 + f_0 V\|}. \tag{6}
\]

Here and below the norm of a matrix \(A\) is the operator norm

\[
\|A\| = \sup_{\|a\|=1} \|Aa\|.
\]
Note that $T_0 < \infty$ because if $H_0 = \mathbb{I} \text{Tr} H_0/2 - f_0 V$, then $[H_0, V] = 0$ contrary to the assumption of non-triviality of the Hamiltonian.

If $\text{Tr} H_0 \neq 0$ and $\text{Tr} V \neq 0$, then replacing $H_0$ and $V$ by $\tilde{H}_0 = H_0 - \text{Tr} H_0/2$ and $\tilde{V} = V - \text{Tr} V/2$, we can bring the free Hamiltonian into a form with $\text{Tr} \tilde{H}_0 = 0$ and $\text{Tr} \tilde{V} = 0$. This does not affect the existence of traps because the evolution operators $U_T$ and $\tilde{U}_T$ determined by the solutions of (1) for the pairs $(H_0, V)$ and $(\tilde{H}_0, \tilde{V})$ respectively are related by $\tilde{U}_T = U_T e^{-i\lambda(T)\mathbb{I}}$. Here $\lambda(T) = (T \text{Tr} H_0 + Tr V \int_0^T f(t) \, dt)/2$. Hence $U_T$ differs from $\tilde{U}_T$ by a phase, and the objective value does not change:

$$|\text{Tr}(W^{\dagger} U_T)|^2 = |e^{-i\lambda(T)} \text{Tr}(W^{\dagger} U_T)|^2 = |\text{Tr}(W^{\dagger} U_T)|^2.$$  

In what follows we assume without loss of generality that the matrices $H_0$ and $V$ are traceless, unless otherwise stated. We will also use the Pauli matrices $\sigma_x$, $\sigma_y$ and $\sigma_z$:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (7)$$

The following statement was proved in [17].

**Theorem 1.** If $[H_0, V] \neq 0$ and $T \geq T_0$, then all maxima of the objective functional $\mathcal{J}_W$ are global. No control $f \neq f_0$ is a trap for any $T > 0$.

It follows from the results in [17] that for small $T$ only the special control $f = f_0$ may be a trap. We shall show that for almost all $W$ the control $f_0$ is not a trap for any $T > 0$.

**§ 2. The absence of traps for small $T$**

By Theorem 1, the only potential trap is $f = f_0$. Therefore, to study the possibility of the existence of traps for small $T$ it suffices to consider the behaviour of the objective at this point.

Theorem 2 states the absence of traps for the objective $\mathcal{J}_W$ for almost all $W$. Let $d = \|H_0 + f_0 V - \mathbb{I} \text{Tr} H_0/2 - f_0 \mathbb{I} \text{Tr} V/2\|$. Note that any matrix $W$ with $[H_0 + f_0 V, W] = 0$ is of the form

$$W = e^{i\alpha_W (H_0 + f_0 V) + i\beta_W}, \quad \alpha_W \in \left(0, \frac{\pi}{d}\right], \quad \beta_W \in [0, 2\pi). \quad (8)$$

**Theorem 2.** Suppose that $[H_0, V] \neq 0$ in (1). Let $[H_0 + f_0 V, W] \neq 0$. Then for any $T > 0$ all maxima of the objective functional $\mathcal{J}_W$ are global. Let $[H_0 + f_0 V, W] = 0$. If $\alpha_W \in (0, \pi/(2d))$, then all maxima of $\mathcal{J}_W$ are global for any $T > 0$. If $\alpha_W \in [\pi/(2d), \pi/d]$, then all maxima of $\mathcal{J}_W$ are global for any $T > \pi/d - \alpha_W$.

The proof of Theorem 2 is based on Lemmas 1–4. We will use the Taylor expansion of $\mathcal{J}_W$ up to second-order terms [19].
Lemma 1. There is an asymptotic expansion

\[ J_W[f + \delta f] = J_W[f] + \int_0^T \frac{\delta J_W}{\delta f(t)} \delta f(t) \, dt 
+ \frac{1}{2} \int_0^T \int_0^T \frac{\delta^2 J_W}{\delta f(t_2) \delta f(t_1)} \delta f(t_1) \delta f(t_2) \, dt_1 \, dt_2 + o(\|\delta f\|_{L^1}^2). \] (9)

Here

\[ \frac{\delta J_W}{\delta f(t)} = \frac{1}{2} \text{Im}(\text{Tr} Y^\dagger \text{Tr}(YV_t)) \], \quad Y = W^\dagger U, \quad V_t = U_t^\dagger VU_t, \] (10)

\[ \frac{\delta^2 J_W}{\delta f(t_2) \delta f(t_1)} = \begin{cases} 
\frac{1}{2} \text{Re}(\text{Tr}(YV_{t_1}) \text{Tr}(Y^\dagger V_{t_2}) - \text{Tr}(YV_{t_2} V_{t_1}) \text{Tr} Y^\dagger), & t_2 \geq t_1, \\
\frac{1}{2} \text{Re}(\text{Tr}(YV_{t_2}) \text{Tr}(Y^\dagger V_{t_1}) - \text{Tr}(YV_{t_1} V_{t_2}) \text{Tr} Y^\dagger), & t_2 < t_1.
\end{cases} \] (11)

The linear map \( A: L^1([0, T]; \mathbb{R}) \mapsto \mathbb{R} \) given by

\[ Ag = \int_0^T \frac{\delta J_W}{\delta f(t)} g(t) \, dt \] (12)

is the Fréchet differential of the map \( f \to J_W[f] \).

Proof. The evolution operator \( U_t^f \) induced by the control \( f \) satisfies the Schrödinger equation

\[ i \frac{dU_t^f}{dt} = (H_0 + fV)U_t^f. \] (13)

The evolution operator \( U_t^{f+g} \) induced by the control \( f + g \) satisfies the equation

\[ i \frac{dU_t^{f+g}}{dt} = (H_0 + fV)U_t^{f+g} + gUU_t^{f+g}. \] (14)

By putting \( U_t^{f+g} = U_t^f Z_t \) in (14), we obtain

\[ i \frac{dZ_t}{dt} = gV_t Z_t, \quad V_t = U_t^f VU_t^f. \] (15)

We now represent (15) in the integral form

\[ Z_t = I - i \int_0^t V_{t_1} Z_{t_1} g(t_1) \, dt_1. \] (16)

Iterating the expression (16) and multiplying by \( U_t^f \) on the left, we obtain

\[ U_t^{f+g} = U_T^f - i \int_0^T U_T^f V_t g(t) \, dt - \int_0^T \int_0^{t_1} U_T^f V_{t_1} V_{t_2} g(t_1) g(t_2) \, dt_2 \, dt_1 \\
+ i \int_0^T \int_0^{t_1} \int_0^{t_2} U_T^f V_{t_1} V_{t_2} Z_{t_3} g(t_1) g(t_2) g(t_3) \, dt_3 \, dt_2 \, dt_1. \] (17)
Since $\|U_T^f\| = \|Z_t\| = 1$ and $\|V_t\| = \|V\|$, we obtain the following estimate for the last summand in (17):

$$\left\| \int_0^T \int_0^{t_1} \int_0^{t_2} U_T^f V_t_1 V_t_2 Z_{t_3} g(t_1) g(t_2) g(t_3) \ dt_3 \ dt_2 \ dt_1 \right\| \leq \|g\|_{L^1([0,T];\mathbb{R})}^3 \|V\|^2. \ (18)$$

For the first- and second-order variations we have

$$\left\| \int_0^T U_T^f V_t g(t_1) \ dt_1 \right\| \leq \|g\|_{L^1([0,T];\mathbb{R})} \|V\|, \quad \tag{19}$$
$$\left\| \int_0^T \int_0^{t_1} U_T^f V_t_1 V_t_2 g(t_1) g(t_2) \ dt_2 \ dt_1 \right\| \leq \|g\|_{L^1([0,T];\mathbb{R})}^2 \|V\|^2. \quad \tag{20}$$

Substituting (17) into the objective

$$J_W[f + \delta f] = \frac{1}{4} \text{Tr}(W^+ U_T^{f+\delta f}) \text{Tr}(W U_T^{f+\delta f}), \quad \tag{21}$$

we obtain the asymptotic expansion (9). Since $\delta J_W/\delta f(t)$ and $\delta^2 J_W/\delta f(t_2)\delta f(t_1)$ are bounded functions, we obtain from (9) that

$$J_W[f + g] = J_W[f] + Ag + o(\|g\|_{L^1}),$$
$$Ag = \int_0^T \frac{\delta J_W}{\delta f(t)} g(t) \ dt.$$  

Therefore the bounded linear operator $A: L^1([0,T];\mathbb{R}) \mapsto \mathbb{R}$ is the Fréchet differential of the map $f \mapsto J_W[f]. \ □$

Necessary conditions for the point $f = f_0$ to be a maximum or a minimum of the objective functional $J_W$ are given by the vanishing of the gradient $\delta J_W/\delta f|_{f=f_0} = 0$ and the semi-definiteness of the quadratic form

$$\int_0^T \int_0^T \text{Hess}(\tau_2, \tau_1) f(\tau_2) f(\tau_1) \ d\tau_1 \ d\tau_2 \geq 0, \quad \text{where} \quad \text{Hess}(t_1, t_2) = \frac{\delta^2 J_W}{\delta f(t_2)\delta f(t_1)} \bigg|_{f=f_0}.\nonumber$$

A sufficient condition for the control $f = f_0$ to be a saddle point is given by the vanishing of the gradient $\delta J_W/\delta f|_{f=f_0} = 0$ and the indefiniteness of the quadratic form

$$\int_0^T \int_0^T \text{Hess}(\tau_2, \tau_1) f(\tau_2) f(\tau_1) \ d\tau_1 \ d\tau_2.$$  

To analyze the properties of the control problem in a neighbourhood of the special control $f_0$, it is convenient to choose a special basis in the space of $2 \times 2$ matrices where the equation (1) takes a simpler form. Recall that we can set $\text{Tr} H_0 = \text{Tr} V = 0$ without loss of generality. Therefore there exists a unitary matrix $S$ such that $S(H_0 + f_0 V) S^\dagger = h z, \text{where} \ h = \|H_0 + f_0 V\|$ and $S V S^\dagger = v_x \sigma_x + v_y \sigma_y + v_z \sigma_z$. Note that $v_z = 0$ because $v_z = \text{Tr}(S V S^\dagger \sigma_z)/2 = \text{Tr}[V(H_0 + f_0 V)]/2h = 0$ since
We will consider maximization of the objective functional \( \max J(\phi) \) belonging to the domain \( 0 \leq \psi \leq \pi \). The angles \( \phi, \psi, \theta \) and the phase \( \omega \) appear in pairs, so that the gradient and the Hessian are phase-invariant. The expression for the objective at the point \( g = 0 \) takes the form

\[
\delta J_W[0] = \frac{1}{4} |\text{Tr}Y|^2 = \cos^2 \varphi \cos^2 \theta.
\]

We introduce the notation

\[
L(X) := \frac{1}{2} \text{Im}(\text{Tr}Y^\dagger \text{Tr}(YX)).
\]

If \( g = 0 \) is an extremum for \( (22) \), then the gradient of the objective functional must vanish identically at this point:

\[
\frac{\delta J_W}{\delta f(t)} \bigg|_{g=0} = v \cos(2t - \phi)L(\sigma_x) - v \sin(2t - \phi)L(\sigma_y) = 0 \quad \forall t \in [0, T].
\]
The equality (27) can be satisfied only if \( L(\sigma_x) = 0 \) and \( L(\sigma_y) = 0 \). This imposes the following restrictions on the angles \( \varphi, \psi \) and \( \theta \) at the extremal points:

\[
\begin{align*}
L(\sigma_x) &= 2 \cos \varphi \cos \theta \sin \theta \sin \psi = 0, \quad (28) \\
L(\sigma_y) &= 2 \cos \varphi \cos \theta \sin \theta \cos \psi = 0. \quad (29)
\end{align*}
\]

If \( \cos \varphi \cos \theta = 0 \), then according to (25) the objective reaches its global minimum \( J_W = 0 \). If \( \cos \varphi \cos \theta \neq 0 \), then (28) and (29) hold only when \( \sin \theta = 0 \). Under this condition, \( \cos \theta = \pm 1 \) and we have \( Y = e^{i\sigma_z \varphi} \) up to a phase factor. Then

\[
W = U_T Y^\dagger = e^{-i \sigma_z T} Y^\dagger = e^{-i \sigma_z (T+\varphi)}. \quad (30)
\]

Thus, in this case \([W, \sigma_z] = 0\) contrary to the hypothesis of the lemma. □

Recall that the special time for the system (22) is \( T_0 = \pi \) and there are no traps for \( T \geq T_0 \) by Theorem 1. Lemma 2 states that if \([W, \sigma_z] \neq 0\), then traps are absent for any \( T > 0 \). Here we show that if \([W, \sigma_z] = 0\), then one can decrease the lower bound for the time \( T \) for which there are no traps.

**Lemma 3.** For \( T \geq \pi/2 \) and any \( W \), the control \( g = 0 \) is not a trap for the maximization of the objective functional \( J_W \) for the system (22).

**Proof.** When \( \sin \theta = 0 \), the Hessian has the form

\[
\text{Hess}(t_2, t_1) = -2v^2 \cos \varphi \cos(2|t_2 - t_1| + \varphi). \quad (31)
\]

We introduce an auxiliary function,

\[
\delta_\varepsilon(t) = \begin{cases} 
0, & |t| \geq \frac{\varepsilon}{2} \\
\frac{1}{\varepsilon}, & |t| < \frac{\varepsilon}{2}
\end{cases} \quad (32)
\]

Then for all \( f \in C[0, T] \) and \( t \in (\varepsilon/2, T - \varepsilon/2) \) we have

\[
\int_0^T \delta_\varepsilon(\tau - t)f(\tau) \, d\tau = f(t) + O(\varepsilon). \quad (33)
\]

Let

\[
f_\varepsilon(t) = \lambda \delta_\varepsilon(t - t_1) + \mu \delta_\varepsilon(t - t_2), \quad \frac{\varepsilon}{2} < t_1 < t_2 < T - \varepsilon/2, \quad \varepsilon < t_2 - t_1.
\]

Substituting the function \( f_\varepsilon(t) \) into the expression for the second variation of the objective functional, we obtain

\[
(f, \text{Hess } f) = \int_0^T \int_0^T \text{Hess}(\tau_2, \tau_1)f(\tau_2)f(\tau_1) \, d\tau_1 \, d\tau_2
\]

\[
= -2v^2 \cos \varphi G(\lambda, \mu) + O(\varepsilon), \quad (34)
\]

where

\[
G(\lambda, \mu) = \lambda^2 \cos \varphi + 2\lambda \mu \cos(2|t_2 - t_1| + \varphi) + \mu^2 \cos \varphi. \quad (35)
\]
The bilinear form $G(\lambda, \mu)$ is indefinite if and only if its discriminant $D$ is positive:

$$D = D(|t_2 - t_1|) = \cos^2(2|t_2 - t_1| + \varphi) - \cos^2 \varphi > 0. \quad (36)$$

If $\cos^2 \varphi = 0$ or $\cos^2 \varphi = 1$, then the objective functional has the global extremum $J_W = 0$ or $J_W = 1$. Hence traps may correspond only to those angles $\varphi$ for which $0 < \cos^2 \varphi < 1$. Then $D$ as a function of the difference $|t_2 - t_1|$ takes positive values at some points in the interval $[0, \pi/2]$ and, because it has period $\pi/2$, its maximum values are positive and its minimum values are negative. Let $t_1, t_2 \in [0, \pi/2]$ be such that $G(\lambda, \mu)$ is an indefinite form. For such $t_1$ and $t_2$ choose $\lambda_1, \lambda_2, \mu_1$ and $\mu_2$ in such a way that $G(\lambda_1, \mu_1) > 0$ and $G(\lambda_2, \mu_2) < 0$. Let

$$f_{1, \varepsilon}(t) = \lambda_1 \delta_{\varepsilon}(t - t_1) + \mu_1 \delta_{\varepsilon}(t - t_2),$$

$$f_{2, \varepsilon}(t) = \lambda_2 \delta_{\varepsilon}(t - t_1) + \mu_2 \delta_{\varepsilon}(t - t_2),$$

where $\varepsilon$ is such that the signs of $(f_{j, \varepsilon}, \text{Hess} f_{j, \varepsilon}), \ j = 1, 2$, coincide with those of $\lim_{\varepsilon \to 0}(f_{j, \varepsilon}, \text{Hess} f_{j, \varepsilon})$. Then $(f_{1, \varepsilon}, \text{Hess} f_{1, \varepsilon})$ and $(f_{2, \varepsilon}, \text{Hess} f_{2, \varepsilon})$ will have opposite signs, that is, the Hessian at the point $f = 0$ is indefinite. □

Consider a matrix $W$ of the form

$$W = e^{i\sigma_{\varphi} W} \quad (37)$$

Note that we can put $\varphi_W \in (0, \pi]$. Otherwise $\varphi_W = \varphi_W' + \pi k$, $\varphi_W' \in [0, \pi]$ and

$$W = e^{i\sigma_{\varphi} W} = e^{i\sigma_{\varphi_W} W}(-1)^k = W' e^{i\pi k},$$

which differs by an irrelevant phase factor. The corresponding matrix $Y$ has the form

$$Y = e^{-i\sigma_{\varphi} (\varphi_W + T)}, \quad (38)$$

that is, $\varphi = -\varphi_W - T$.

**Lemma 4.** If $\varphi_W \in (0, \pi/2)$, then for every $T > 0$ the control $g = 0$ is not a trap for the maximization of the objective functional $J_W$ for the system (22). If $\varphi_W \in [\pi/2, \pi)$, then for every $T > \pi - \varphi_W$ the control $g = 0$ is not a trap for the maximization of the objective functional $J_W$ for the system (22).

**Proof.** The Hessian of the objective functional $J_W[f]$ at the point $g = 0$ has the form (34), where the bilinear form $G(\lambda, \mu)$ is defined by (35). The Hessian is definite if the discriminant $D$, which is defined by (36), is positive. We claim that there exist $t_1 > 0$ and $t_2 < T$ such that $D > 0$.

Indeed, the expression (36) for $D$ can be rewritten as

$$D = \sin(2(\varphi_W + T - |t_2 - t_1|) \sin 2|t_2 - t_1|). \quad (39)$$

If $\varphi_W \in (0, \pi/2)$, then for any $T, \pi/2 > T > 0$, chose $|t_2 - t_1| = T - \varepsilon$, where $\varepsilon$ is so small that $(\varphi_W + \varepsilon) \in (0, \pi/2)$ and $T - \varepsilon > 0$. Then

$$D = \sin(2(\varphi_W + \varepsilon) \sin 2(T - \varepsilon)) > 0 \quad (40)$$

because $(\varphi_W + \varepsilon) \in (0, \pi/2)$ and $T < \pi/2$. 

If $\varphi_W \in [\pi/2, \pi)$, then to obtain $D > 0$ it suffices to have the inequalities

$$\pi < \varphi_W + T - |t_2 - t_1| < \frac{3\pi}{2}, \quad |t_2 - t_1| < \frac{\pi}{2}.$$  \hfill (41)

For any $T$ satisfying

$$\pi < \varphi_W + T < \frac{3\pi}{2},$$  \hfill (42)

choose a small $\varepsilon$ such that

$$\pi < \varphi_W + T - \varepsilon < \frac{3\pi}{2}.$$  \hfill (43)

Choose $t_1$ and $t_2$ such that $|t_2 - t_1| = \varepsilon$. Then the first inequality in (41) holds for such $\varepsilon$ by (43). The right inequality $T < \pi/2 - \varphi_W$ in (42) is a consequence of the inequality $T < \pi/2$, but for $T \geq \pi/2$ traps are absent by Lemma 3. Hence for $\varphi_W \in [\pi/2, \pi]$ and $T > \pi - \varphi_W$ there exist $t_1$ and $t_2$ such that $D > 0$. □

**Proof of Theorem 2.** We make the inverse transformation $U \rightarrow S^\dagger US, W \rightarrow S^\dagger WS$ from the system (22) to the system (1), replace $t$ by $th$ and take into account that $g(t) = f(t) - f_0$. In this case $T \rightarrow Th$ and $\varphi_W \rightarrow \alpha W h$. Then the theorem follows from Lemmas 2–4. □

§ 3. **Numerical analysis of the behaviour of the objective functional in the neighbourhood of the special control $f_0$**

The absence of traps for the objective functional $J_W$ for the system (22) when $T > \pi/2$ can be illustrated by numerical analysis. Fig. 1 shows the plots for the objective value $J_0 = J_W[0]$ calculated at the special control $f = 0$ and for the probability $P$ that a random control $f$ in a sufficiently small neighbourhood of the special control satisfies the inequality $J_W[f] < J_0$, both as functions of $(\alpha, \varphi_W)$. Here $\alpha$ is the angle between the vector $v = \text{Tr}(\sigma V)/2$ and the axis $Ox$, and the angle $\varphi_W$ parametrizes the matrix

$$W = \begin{pmatrix} e^{i\varphi_W} & 0 \\ 0 & e^{-i\varphi_W} \end{pmatrix}. \hfill (44)$$

This matrix determines the phase-shift gate $U_\phi = e^{-i\phi/2}W$, where $\varphi_W = -\phi/2$. At each point $(\alpha, \varphi_W)$ the probability $P(\alpha, \varphi_W)$ is estimated as the share of realizations of the inequality $J_W[f] < J_0$ for values of the objective functional $J_W$ calculated for $M = 10^3$ randomly chosen controls in the neighbourhood of the special control $f = 0$:

$$P(\alpha, \varphi_W) = \frac{\#(f: J_W[f] < J_0)}{M}. \hfill (45)$$

The random controls are chosen as piecewise-constant functions $f = \sum_{i=1}^{100} a_i \chi_i$, where $\chi_i$ is the characteristic function of the interval $[(i - 1)T/100, iT/100]$, and each $a_i$ has normal distribution with unit variance. Fig. 1 shows that for $T > \pi/2$ the maxima of the probability $P = P(\alpha, \varphi_W)$ coincide with the points where
Figure 1. The plots of the objective value \( J_0 = J_W[0] \) calculated at the special control \( f = 0 \) and of the probability \( P \) that the random control \( f \) in a sufficiently small neighbourhood of the special control satisfies the inequality \( J_W[f] < J_0 \). Left: \( T = \pi/3 \). Right: \( T = 2\pi/3 \). At each point \((\alpha, \varphi_W)\) the probability \( P \) is estimated as the share \( N_{J_W<J_0} \) of realizations of the inequality \( J_W < J_0 \) among the values of the objective functional \( J_W \) calculated at \( M = 10^3 \) randomly chosen controls. The random controls are chosen as piecewise-constant functions \( f = \sum_{i=1}^{100} a_i \chi_i \), where \( \chi_i \) is the characteristic function of the interval \( [(i-1)T/100, iT/100] \) and each \( a_i \) has normal distribution with unit variance.

\( J_0(\alpha, \varphi_W) = 1 \), that is, where \( f = 0 \) is a global maximum and, therefore, there are no traps at these points. At the remaining points we have \( P < 1 \) and, therefore, there are also no traps. The probability \( P \) in Fig. 1 does not depend on the angle \( \alpha \), that is, on the direction of the vector \( v = \text{Tr}(\sigma V)/2 \). This is because the values of the objective functional do not depend on this vector, as stated in the following lemma.

**Lemma 5.** Let \([W, \sigma_z] = 0\). Then for any vectors \( v \) and \( v' \) determined by the interaction Hamiltonians \( V = (v_x \sigma_x + v_y \sigma_y) \) and \( V' = (v'_x \sigma_x + v'_y \sigma_y) \) in the equation (22), the values of the objective functional \( J^v_W[f] \) and \( J^{v'}_W[f] \) calculated for \( V \) and \( V' \) at the point \( f \) coincide:

\[ J^v_W[f] = J^{v'}_W[f]. \]

**Proof.** Suppose that \( U^v_T[f] \) and \( U^{v'}_T[f] \) satisfy the equation (22) with Hamiltonians \( V = v_x \sigma_x + v_y \sigma_y \) and \( V' = v'_x \sigma_x + v'_y \sigma_y \) respectively. Since

\[ e^{-i\sigma_z \theta/2}(v_x \sigma_x + v_y \sigma_y) e^{i\sigma_z \theta/2} = v'_x \sigma_x + v'_y \sigma_y, \]

we have

\[ J^v_W[f] = J^{v'}_W[f]. \]
where \( \vartheta = \alpha' - \alpha \) is the angle between the vectors \( \mathbf{v}' \) and \( \mathbf{v} \), we see that the matrix
\[
Z_t = e^{-i\sigma_z \vartheta/2} U_t^\dagger \mathbf{v}' f e^{i\sigma_z \vartheta/2}
\]
satisfies (22) with the potential \( V' = v'_x \sigma_x + v'_y \sigma_y \). Since \( Z_0 = I \), we have
\[
Z_t = e^{-i\sigma_z \vartheta/2} U_t^\dagger \mathbf{v}' f = U_t^\dagger \mathbf{v}'.f.
\]
Then
\[
\mathcal{J}_W[f] = \frac{1}{4} \left| \text{Tr}(W^\dagger U_t \mathbf{v}'.f) \right|^2 = \frac{1}{4} \left| \text{Tr}(e^{-i\sigma_z \vartheta/2} W^\dagger e^{i\sigma_z \vartheta/2} U_t \mathbf{v}'.f) \right|^2 = \mathcal{J}_W'[f]
\]
(47) because in this case \([W, \sigma_z] = 0\) and, therefore,
\[
e^{-i\sigma_z \vartheta/2} W^\dagger e^{i\sigma_z \vartheta/2} = W^\dagger. \quad \Box
\]

Fig. 2 shows the probability \( P = P(\alpha) \) that \( J_0 > J_H[f] \), where the matrix
\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}
\]
(48) describes the Hadamard gate. It is clear from Fig. 2 that \( P(\alpha) \approx 1/2 \). Hence there are no traps for any \( \alpha \). This is compatible with Theorem 2 because \([H, \sigma_z] \neq 0\).

![Figure 2](image_url)

Figure 2. The probability \( P \) that \( J_H < J_0 \) for \( T = \pi/3 \). At each point \( \alpha \) the probability \( P \) is estimated as the share \( N_{J_H < J_0} \) of realizations of the inequality \( J_H < J_0 \) among the values of the objective functional \( J_H \) calculated at \( M = 10^3 \) random controls. The random controls are chosen as piecewise-constant functions \( f = \sum_{i=1}^{100} a_i \chi_i \), where \( \chi_i \) is the characteristic function of the interval \( [(i-1)T/100, iT/100] \) and each \( a_i \) has normal distribution with unit variance.
Conclusion

We have proved Theorem 2 about the absence of traps in the problem of maximizing the objective functional

$$\mathcal{J}_W[f] = \frac{1}{4} |\text{Tr}(W^\dagger U_T)|^2$$

for a qubit for small $T$ and almost all $W$. If $[H_0 + f_0 V, W] \neq 0$, then for any $T > 0$ all maxima of the objective functional $\mathcal{J}_W$ are global. If $[H_0 + f_0 V, W] = 0$, then the matrix $W$ has the form (8). In this case if

$$\alpha_W \in \left(0, \frac{\pi}{2d}\right),$$

$$d = \left\|H_0 + f_0 V - \frac{1}{2} \text{Tr} H_0 - \frac{1}{2} f_0 \text{Tr} V\right\|,$$

then all maxima of the objective functional $\mathcal{J}_W$ are global for any $T > 0$. If $\alpha_W \in \left[\frac{\pi}{2d}, \frac{\pi}{d}\right]$ then all maxima of the objective functional $\mathcal{J}_W$ are global for any $T > \pi/d - \alpha_W$.

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