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Time-optimal control of quantum systems: a solution to the quantum Zermelo problem

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Time-optimal control of quantum systems: a solution to the quantum Zermelo problem

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Abstract. In the present manuscript, we introduce the quantum counterpart of the well known classical navigation problem posed by Zermelo and provide a simple resolution in terms of a control Hamiltonian with constant maximum variance. This Hamiltonian yields a time-optimal control of general quantum systems. In developing this theory, we encounter some relevant conditions on the elapsed time of the journey between initial and final states and the energy resource provided by the control Hamiltonian. Later, we demonstrate the feasibility of our results in the context of two and three-level systems and highlight their applicability as quantum gates. Finally, along with the conclusions, we provide some comments about the ubiquitous case of the harmonic potential, which is work in progress.

Keywords: quantum control, single qubit, qutrit, quantum gate, time-dependent Schrödinger equation.

1 Introduction

Quantum technologies are nowadays at the cutting-edge of science. Many advances have been made to understand controlled quantum dynamics and be aware of its limits. In this context, special attention has been focused on time-optimal manipulation of quantum states [1, 2]. Among this kind of problems, there are an important class related to the time-optimal quantum evolution under the influence of external fields or potentials that cannot be suppressed. Such problems are really important because in real laboratories one cannot get rid of certain external influences. From a classical point of view, this problem was first posed by Zermelo [3, 4]. The classical Zermelo navigation problem aims at finding the time-optimal control of a ship, that is supposed to act constantly on it, in order to reach its destination in the least time. Moreover, the ship is undergoing the local action of the sea current and wind, which are uncontrollable. The quantum counterpart of the Zermelo problem was solved by Brody and Meier [5] by a geometric means.

In this work, we present a solution to the quantum Zermelo problem that is obtained by a different procedure. In particular, our derivation does not rely on geometric arguments,

but on rather simple physical arguments. To this end, in section 2 we firstly reformulate the Zermelo problem in the quantum realm and devise a simple and concise protocol that warrants the evolution from some initial state to some final state in the least time. The resulting time-dependent Schrödinger equation has been implemented numerically by two different algorithms: the Runge-Kutta method of fourth order and the Crank-Nicolson method. Secondly, in section 3 we apply the time-optimal control previously developed to two-level quantum systems. This is, for instance, the case of two-level atoms interacting with a classical field and of spin 1/2 in a magnetic field. We also explore the possibility of applying this technique to implement quantum gates that act on qubits in an optimal-time manner. Sections 4 is devoted to three-level systems or qutrits, that are also useful in quantum information and, in contrast to qubits, are more robust against decoherence. Finally, in section 5, we briefly summarize some conclusions gained during this work and provide a few comments on future directions.

2 Theoretical framework

2.1 Formulation of the quantum Zermelo problem

The quantum analog of the classical Zermelo navigation problem aims at finding the time-optimal evolution from a initial state $|\psi(t=0)\rangle = |\psi_i\rangle$ to a desired final state $|\psi(t=\tau)\rangle = |\psi_f\rangle$ in the least time τ. The problem posed by Zermelo considers a time-independent background Hamiltonian that cannot be controlled and a time-dependent part that constitutes the control over the system that we want to optimize; hence, we can write:

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_c(t)\,, \tag{1}$$

where $\hat{H}_c(t)$ is the control Hamiltonian. Throughout this manuscript we use natural units, where $\hbar = 1$.

At first glance, the form of $\hat{H}(t)$ suggests to work in the interaction picture. Besides, the fact that in the quantum Zermelo problem we can only manipulate $\hat{H}_c(t)$ reinforces the necessity to switch to this picture. In this new frame, we define $|\psi'(t)\rangle = \hat{\mathcal{U}}_0^\dagger(t)|\psi(t)\rangle$ with $\hat{\mathcal{U}}_0 = \exp(-i\hat{H}_0 t)$. These states obey the following Schrödinger equation:

$$i\frac{d}{dt}|\psi'(t)\rangle = \hat{H}_c'(t)|\psi'(t)\rangle\,, \tag{2}$$

with $\hat{H}_c'(t) = \hat{\mathcal{U}}_0^\dagger(t)\hat{H}_c(t)\hat{\mathcal{U}}_0(t)$.

Note that due to the fact that the time evolution operator is unitary, $\mathrm{tr}(\hat{H}_c'^2(t)) = \mathrm{tr}(\hat{H}_c^2(t))$. Moreover, the transformed control Hamiltonian evolves in time according to

$$\hat{H}_c'(t) = \hat{\mathcal{U}}_c(t)\hat{H}_c'(0)\hat{\mathcal{U}}_c^\dagger(t) = \hat{\mathcal{U}}_c(t)\hat{H}_c(0)\hat{\mathcal{U}}_c^\dagger(t)\,, \tag{3}$$

where the time evolution operator is of the form:

$$\hat{\mathcal{U}}_c(t) = \mathcal{T}\exp\left(-i\int_0^t \hat{H}_c'(t')dt'\right). \tag{4}$$

Above, we have introduced the time ordered product, since the Hamiltonian does not need to commute at different times. Any state vector can thus be written as $|\psi(t)\rangle = \hat{\mathcal{U}}_0(t)\hat{\mathcal{U}}_c(t)|\psi_i\rangle$.

As stated earlier, our concern is to achieve an optimal-time evolution of the state $|\psi(t)\rangle$. In this sense, Anandan and Aharonov [6] showed that the variance of the Hamiltonian is directly proportional to the speed of the quantum evolution. Then, in order to maximize the variance

$$(\Delta\hat{H}'_c(t))^2 = \langle\psi'(t)|\hat{H}'^2_c(t)|\psi'(t)\rangle - (\langle\psi'(t)|\hat{H}'_c(t)|\psi'(t)\rangle)^2 \,, \tag{5}$$

the second term on the right hand side must vanish for all t. This is accomplished if we assume that

$$\langle\psi'(t)|\frac{d|\psi'(t)\rangle}{dt} = 0 \,, \tag{6}$$

which is also valid for its complex conjugate. Strikingly, it seems reasonably to impose this condition (the time derivative of the state being orthogonal to the state itself) if we want to optimize the change of the state over time. We can easily visualize this idea if we consider the particular case of the Bloch sphere for a qubit: hence, we are claiming that the vector corresponding to the time variation of the state lies on the tangent space of the aforementioned sphere. Under this condition, we ensure that the journey to the target state is minimized. Furthermore, the first term on the right hand side of Eq. (5) is

$$\langle\psi'(t)|\hat{H}'^2_c(t)|\psi'(t)\rangle = \langle\psi_i|\hat{H}^2_c(0)|\psi_i\rangle = \frac{d\langle\psi'_i|}{dt}\frac{d|\psi'_i\rangle}{dt} = \left|\frac{d\psi'_i}{dt}\right|^2 \,, \tag{7}$$

where we have used Eq. (3) and $|\psi(t)\rangle = \hat{\mathcal{U}}_0(t)\hat{\mathcal{U}}_c(t)|\psi_i\rangle$. In addition, using Eq. (2) we can also write:

$$\langle\psi'(t)|\hat{H}'^2_c(t)|\psi'(t)\rangle = \left|\frac{d\psi'(t)}{dt}\right|^2 \,, \tag{8}$$

where $d|\psi'_i\rangle/dt$ is short for the time-derivative of $|\psi'(t)\rangle$ evaluated at $t = 0$. We end up, combining both results:

$$\left|\frac{d\psi'(t)}{dt}\right|^2 = \left|\frac{d\psi'_i}{dt}\right|^2 = k \,, \tag{9}$$

with k a constant, whose interpretation will be clarified immediately.

At this point, we can already constrain the control Hamiltonian to be of the form

$$\hat{H}'_c(t) = i\left[\frac{d|\psi'(t)\rangle}{dt}\langle\psi'(t)| - |\psi'(t)\rangle\frac{d\langle\psi'(t)|}{dt}\right] , \tag{10}$$

which is hermitian. Notice that, since the trace is a linear mapping, we find $\mathrm{tr}(\hat{H}'_c(t)) = 0$, so $\hat{H}'_c(t)$ is traceless (bearing in mind Eq. (6)). The structure of the transformed Hamiltonian above, also allows us to calculate the trace of $\hat{H}'^2_c(t)$ easily:

$$\begin{aligned}\mathrm{tr}(\hat{H}'^2_c(t)) &= \mathrm{tr}\left(\frac{d|\psi'(t)\rangle}{dt}\frac{d\langle\psi'(t)|}{dt}\right) + \frac{d\langle\psi'(t)|}{dt}\frac{d|\psi'(t)\rangle}{dt}\mathrm{tr}\Big(|\psi'(t)\rangle\langle\psi'(t)|\Big) \\ &= 2\left|\frac{d\psi'(t)}{dt}\right|^2 = 2k \,,\end{aligned} \tag{11}$$

where the last equality follows from Eq. (9). Physically, the value of the constant k is thus connected with the energy at hand for performing the control.

In what follows, our purpose is to find a closed form for the Hamiltonian (10) that solves the quantum Zermelo problem. It turns out that the conditions established by Eqs. (6) and (11) are satisfied at any time t by the ansatz state:

$$|\psi'(t)\rangle = \cos\left(\sqrt{k/2}\,t\right)|\psi_i'\rangle + \sqrt{2/k}\sin\left(\sqrt{k/2}\,t\right)\frac{d|\psi_i'\rangle}{dt}\,, \tag{12}$$

with time-derivative given by

$$\frac{d|\psi'(t)\rangle}{dt} = -\sqrt{k/2}\sin\left(\sqrt{k/2}\,t\right)|\psi_i'\rangle + \cos\left(\sqrt{k/2}\,t\right)\frac{d|\psi_i'\rangle}{dt}\,. \tag{13}$$

Notice that $|\psi_i'\rangle = |\psi_i\rangle$ since $\hat{\mathcal{U}}_0(t=0) = \mathbb{1}$. At this point, it is convenient to introduce the transformed target state:

$$|\psi_f'\rangle = \hat{\mathcal{U}}_0^\dagger(\tau)|\psi_f\rangle = \hat{\mathcal{U}}_0^\dagger(\tau)\hat{\mathcal{U}}_0(\tau)\hat{\mathcal{U}}_c(\tau)|\psi_i\rangle = \hat{\mathcal{U}}_c(\tau)|\psi_i\rangle\,. \tag{14}$$

By applying the Gram-Schmidt orthogonalizing process, we construct an orthogonal state to $|\psi_i\rangle$ from $|\psi_f'\rangle$

$$|\varphi_f'\rangle = (\mathbb{1} - |\psi_i\rangle\langle\psi_i|)|\psi_f'\rangle = \frac{\sin\left(\sqrt{k/2}\,\tau\right)}{\sqrt{k/2}}\frac{d|\psi_i'\rangle}{dt}\,, \tag{15}$$

and then, normalizing

$$|\varphi_f'\rangle_N = \frac{|\varphi_f'\rangle}{\left|\varphi_f'\right|} = \frac{(\mathbb{1} - |\psi_i\rangle\langle\psi_i|)\,\hat{\mathcal{U}}_0^\dagger(\tau)|\psi_f\rangle}{\sqrt{1 - \left|\langle\psi_f|\hat{\mathcal{U}}_0(\tau)|\psi_i\rangle\right|^2}} = \sqrt{2/k}\,\frac{d|\psi_i'\rangle}{dt}\,. \tag{16}$$

It is important to remark that the above expression only includes the initial state, the final state, the elapsed time of the evolution and the background Hamiltonian. Thus, we can recast Eqs. (12) and (13) in these terms:

$$|\psi'(t)\rangle = \cos\left(\sqrt{k/2}\,t\right)|\psi_i\rangle + \sin\left(\sqrt{k/2}\,t\right)|\varphi_f'\rangle_N\,, \tag{17}$$

$$\frac{d|\psi'(t)\rangle}{dt} = -\sqrt{k/2}\sin\left(\sqrt{k/2}\,t\right)|\psi_i\rangle + \sqrt{k/2}\cos\left(\sqrt{k/2}\,t\right)|\varphi_f'\rangle_N\,. \tag{18}$$

Finally, in order to obtain the desired Hamiltonian, we substitute these equations into Eq. (10) and then, with the aid of Eq. (17) evaluated at $t=\tau$, we cast $|\varphi_f'\rangle_N$ in terms of $|\psi_f'\rangle$ to find

$$\hat{H}_c'(t) = i\frac{\sqrt{k/2}}{\sin\left(\sqrt{k/2}\,\tau\right)}[|\psi_f'\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_f'|] = \mathcal{K}\,[|\psi_f'\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_f'|]\,, \tag{19}$$

where we have defined the imaginary constant $\mathcal{K}$. Surprisingly, this expression is time-independent. Thus, if we use Eqs. (3) and (4) in combination with the fact that $\hat{H}_c'(t) = \hat{H}_c'$, we conclude that $\hat{H}_c'(t) = \hat{H}_c(0)$ and $\hat{\mathcal{U}}_c(t) = \exp\left(-i\hat{H}_c(0)\,t\right)$. Consequently, the control Hamiltonian evolves as

$$\hat{H}_c(t) = \hat{\mathcal{U}}_0(t)\hat{H}_c'(t)\hat{\mathcal{U}}_0^\dagger(t) = \hat{\mathcal{U}}_0(t)\hat{H}_c(0)\hat{\mathcal{U}}_0^\dagger(t)\,, \tag{20}$$

and, accordingly, the full Hamiltonian for the quantum Zermelo problem acquires the final form

$$\hat{H}(t) = \hat{H}_0 + \mathrm{e}^{-i\hat{H}_0 t}\hat{H}_c(0)\,\mathrm{e}^{i\hat{H}_0 t}\,, \tag{21}$$

in good agreement with the result in [7]. That is, the time optimization in the quantum Zermelo approach is fully determined once we have constructed the control Hamiltonian $\hat{H}_c(0)$. Hence, we have provided a fundamental solution to the quantum version of the problem stated by Zermelo.

2.2 Conditions over τ and k

So far, we have successfully written down an expression for the control Hamiltonian that is needed in order to reach a target state in the least time τ. Now, we want to address which is this value and how it is related to the constant k.

Let us consider the complete orthonormal set of eigenkets of $\hat{H}_0$, namely $\{|j\rangle,\ j = 0, 1, 2, \ldots\}$, and write the initial and final states in this basis; then

$$|\psi_i\rangle = \sum_j \langle j|\psi_i\rangle|j\rangle = \sum_j a_j|j\rangle \quad \text{and} \quad |\psi_f\rangle = \sum_j \langle j|\psi_f\rangle|j\rangle = \sum_j b_j|j\rangle\,. \tag{22}$$

Evaluating Eq. (17) at time $t = \tau$ and applying $\hat{\mathcal{U}}_0(\tau)$ from the left we find:

$$\begin{aligned}|\psi(\tau)\rangle = \Bigg(\cos\left(\sqrt{k/2}\,\tau\right) - \frac{\langle\psi_i|\hat{\mathcal{U}}_0^\dagger(\tau)|\psi_f\rangle\sin\left(\sqrt{k/2}\,\tau\right)}{\sqrt{1-\left|\langle\psi_f|\hat{\mathcal{U}}_0(\tau)|\psi_i\rangle\right|^2}}\Bigg)\hat{\mathcal{U}}_0(t)|\psi_i\rangle \\ + \frac{\sin\left(\sqrt{k/2}\,\tau\right)}{\sqrt{1-\left|\langle\psi_f|\hat{\mathcal{U}}_0(\tau)|\psi_i\rangle\right|^2}}|\psi_f\rangle\,,\end{aligned} \tag{23}$$

from which, since $|\psi(\tau)\rangle = |\psi_f\rangle$, we can extract the following constraints relating k and τ:

$$\cos\left(\sqrt{k/2}\,\tau\right) = \langle\psi_i|\hat{\mathcal{U}}_0^\dagger(\tau)|\psi_f\rangle \ \text{ and } \ \sin\left(\sqrt{k/2}\,\tau\right) = \sqrt{1-\left|\langle\psi_f|\hat{\mathcal{U}}_0(\tau)|\psi_i\rangle\right|^2}\,. \tag{24}$$

For the sake of clarity, let us first calculate the overlap in the above equality as

$$\langle\psi_f|\hat{\mathcal{U}}_0(\tau)|\psi_i\rangle = \sum_j b_j^* a_j \mathrm{e}^{-iE_j\tau} = \mathcal{Z}(\tau)\,, \tag{25}$$

where E_j are the eigenvalues of $\hat{H}_0$. Generally, this overlap is a complex number and we denote this value by $\mathcal{Z}(\tau)$ to emphasize that it depends on the parameter τ. Recall, on the contrary, that τ and k are both real numbers. Consequently, we find that τ and k are related in an intricate manner and both must verify simultaneously the following three restrictions:

$$\begin{aligned}&0 = \mathrm{Im}(\mathcal{Z}^*(\tau))\,,\\ &\cos\left(\sqrt{k/2}\,\tau\right) = \mathrm{Re}(\mathcal{Z}^*(\tau)) \quad \text{and} \quad \sin\left(\sqrt{k/2}\,\tau\right) = \sqrt{1-\mathcal{Z}^*(\tau)\mathcal{Z}(\tau)}\,.\end{aligned} \tag{26}$$

Needless to say that, except for particular cases, these equations have no analytical solution and a numerical technique is required.

We finish this section by considering the simple case of orthogonal initial and final states, i.e. $\langle\psi_f|\psi_i\rangle = 0$, for which we obtain the compact result

$$\tau = \frac{\pi}{\sqrt{2k}}\,, \tag{27}$$

that brings to light the inverse relationship between the energy at our disposal and the least time of the evolution.

3 Two-level system

In this section, we apply the time-optimal control to a two-level system, also known as qubits. This entities are of vital significance in quantum computing, so it is relevant to present the details meticulously.

First of all, let us assume that we have a two-dimensional Hilbert space and our initial and final states of interest are $|\psi_i\rangle = a_0|0\rangle + a_1|1\rangle$ and $|\psi_f\rangle = b_0|0\rangle + b_1|1\rangle$ (remind that $|0\rangle$ and $|1\rangle$ are eigenstates of the background Hamiltonian $\hat{H}_0$). Correspondingly, the background Hamiltonian can be written as $\hat{H}_0 = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|$. If we plug these states into Eqs. (19) and (20), the control Hamiltonian can be cast as the two-dimensional matrix:

$$\hat{H}_c(t) = \mathcal{K}\begin{pmatrix} a_0^* b_0 \mathrm{e}^{i\omega_0\tau} - \text{c.c.} & (a_1^* b_0 \mathrm{e}^{i\omega_0\tau} - b_1^* a_0 \mathrm{e}^{-i\omega_1\tau})\mathrm{e}^{i\omega_{10}t} \\ (a_0^* b_1 \mathrm{e}^{i\omega_1\tau} - b_0^* a_1 \mathrm{e}^{-i\omega_0\tau})\mathrm{e}^{-i\omega_{10}t} & a_1^* b_1 \mathrm{e}^{i\omega_1\tau} - \text{c.c.} \end{pmatrix}, \tag{28}$$

where $\omega_i = E_i$ and $\omega_{10} = E_1 - E_0$, and $\mathcal{K}$ has been defined in Eq. (19).

In the framework worked out in the previous section, this is the control Hamiltonian that brings the initial state to the target state and, not surprisingly, it depends on the expansion coefficients $a_{0,1}$ and $b_{0,1}$. Now, it is desirable to give a proper interpretation in terms of physical quantities.

3.1 Interaction of a two-level atom with an electromagnetic field

The physical situation proposed here is the following: imagine a single atom with two relevant energy levels interacting with an electromagnetic wave, a laser field, for instance. The corresponding electric field can be written (in the dipole approximation) $\vec{E} = E_0\vec{e_z}\cos(\omega t+\phi)$, and the corresponding interaction Hamiltonian is

$$\hat{H}_{\text{int}} = -\hat{d}\cdot\vec{E} = -q\,\hat{r}\cdot\vec{E} = -q\hat{z}E_0\cos(\omega t+\phi)\,, \tag{29}$$

with $\hat{d}$ the dipole moment operator of the atom [8]. We take for granted that the atom has inversion symmetry, then the energy eigenstates must have definite parity, i.e. $\langle 0|\hat{z}|0\rangle = \langle 1|\hat{z}|1\rangle = 0$, and the interaction Hamiltonian can be represented as a matrix with this appearance

$$\hat{H}_{\text{int}} = \begin{pmatrix} 0 & V_{01}\cos(\omega t+\phi) \\ V_{01}^*\cos(\omega t+\phi) & 0 \end{pmatrix}, \tag{30}$$

where $V_{01} = -qE_0\langle 0|\hat{z}|1\rangle$.

If the initial state is the ground state of the atom $|\psi_i\rangle = |0\rangle$ and the goal is to excite it to the first excited state $|1\rangle$. Under this circumstances, the control Hamiltonian in Eq. (28) reads

$$\hat{H}_c(t) = \mathcal{K}\begin{pmatrix} 0 & -\mathrm{e}^{-i\omega_1\tau}\mathrm{e}^{i\omega_{10}t} \\ \mathrm{e}^{i\omega_1\tau}\mathrm{e}^{-i\omega_{10}t} & 0 \end{pmatrix}, \tag{31}$$

and, rearranging terms and comparing, we can find the expression that follows

$$\frac{\mathrm{Re}(V_{01})}{\sqrt{k/2}}\cos(\omega t+\phi) = \left(\cos\left(\omega_1\frac{\pi}{\sqrt{2k}}\right)\sin(\omega_{10}t) - \sin\left(\omega_1\frac{\pi}{\sqrt{2k}}\right)\cos(\omega_{10}t)\right), \tag{32}$$

with the same precise value of τ in Eq. (27). It is well know that the sum of two sinusoidal waves of the same frequency (right hand side of the above equation) gives another wave of the same frequency. Thus, our first conclusion is that the Zermelo control Hamiltonian predicts an electric field of frequency $\omega = \omega_{10}$. After some cumbersome manipulation of this expression, we arrive at the second conclusion, that the modulus of the electric field must be

$$E_0 = \frac{\sqrt{k/2}}{q\,\mathrm{Re}(\langle 0|\hat{z}|1\rangle)}\,. \tag{33}$$

To summarize, for the present case, in order to excite the two-level atom in the least time, the control Hamiltonian conveys that we must apply an electric field of magnitude given by (33) in resonance with the two-level transition. As expected, the intensity of the field depends upon the value of k (the energy invested in the control of the system); the larger it is, the shorter the time to reach the final state of the transition.

For general initial and final states, we expect the raise of diagonal elements on the control Hamiltonian in Eq. (28) to imply some restrictions on the values of k that yield a physical control Hamiltonian.

3.2 Spin 1/2 in a magnetic field

Another two-level system of interest is that of a spin 1/2. The spin down state $|0\rangle$ and the spin up state $|1\rangle$ form an orthonormal set and we can expand our initial and final states in this basis (as we did before).

Let us remind the reader that $\{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\}$, where σ_i are the Pauli matrices, spans the space of 2×2 complex matrices $M_2(\mathbb{C})$. Thus, we are allowed to write the control Hamiltonian in (28) at $t=0$ as $\hat{H}_c(0) = \alpha_0\mathbb{1} + \sum_i \alpha_i\sigma_i$ with α_0 and α_i real constants. After some manipulation, we arrive at

$$\alpha_0 = 0 \quad , \quad \alpha_1 = i\mathcal{K}\Big(\mathrm{Im}(a_0^* b_1 \mathrm{e}^{i\omega_1\tau}) + \mathrm{Im}(a_1^* b_0 \mathrm{e}^{i\omega_0\tau})\Big) \tag{34}$$

$$\alpha_2 = -i\mathcal{K}\Big(\mathrm{Re}(a_0^* b_1 \mathrm{e}^{i\omega_1\tau}) - \mathrm{Re}(a_1^* b_0 \mathrm{e}^{i\omega_0\tau})\Big) \quad \text{and} \quad \alpha_3 = i\mathcal{K}\,\mathrm{Im}(a_0^* b_0 \mathrm{e}^{i\omega_0\tau})\,. \tag{35}$$

In deriving the above relations, we have use the constraint in (26). Therefore, the time evolved control Hamiltonian in this basis is

$$\begin{aligned}\hat{H}_c(t) = {} & (\alpha_1\cos(\omega_{10}t) + \alpha_2\sin(\omega_{10}t))\sigma_1 \\ & + (\alpha_2\cos(\omega_{10}t) - \alpha_1\sin(\omega_{10}t))\sigma_2 + \alpha_3\sigma_3\,,\end{aligned} \tag{36}$$

where the last term is time-invariant because $[\hat{\mathcal{U}}_0(t), \sigma_3] = 0$.

Expression (36) resembles the Hamiltonian of a spin in a magnetic field, namely

$$\hat{H}_{\text{spin}} = -\frac{\gamma}{2}(B_1\sigma_1 + B_2\sigma_2 + B_3\sigma_3)\,, \tag{37}$$

with $\gamma = -g_s\mu_B$ for an electron-like particle. It may also be the spin of an atom. For instance, the silver atom with electronic configuration $[\text{Kr}]4\text{d}^{10}5\text{s}^1$ has an unpaired electron 5s and then the magnetic moment of the silver atom is equal to the magnetic moment of that electron.

In sum, we have demonstrated that the Zermelo control Hamiltonian ensures that we can reach any spin state over the Bloch sphere in the minimum time by just tuning the corresponding magnetic fields in accordance. As a matter of example, imagine our goal is to perform a transition from a spin down to a spin up configuration in the least time. In this case ($a_0 = b_1 = 1$, $a_1 = b_0 = 0$), $\alpha_1 = i\mathcal{K}\sin(\omega_1\tau)$, $\alpha_2 = -i\mathcal{K}\cos(\omega_1\tau)$ and $\alpha_3 = 0$. Thus, the components of the magnetic field we have to apply are

$$B_1(t) = \frac{\sqrt{2k}}{\gamma}\cos(\omega_{10}t + \phi_1) \quad \text{and} \quad B_2(t) = \frac{\sqrt{2k}}{\gamma}\sin(\omega_{10}t + \phi_2)\,, \tag{38}$$

where $B_3 = 0$, and, because of the orthogonality between initial and final states, τ is given by (27). In other words, the radiation needs to be in resonance, and the amplitude of the field is proportional to the constant k, which, as expected, is directly related with the intensity of the radiation fields.

3.3 Implementation of single-qubit quantum gates

Analogous to a classical computer, a quantum computer is buit from a quantum circuit containing quantum gates. These gates, carry around and manipulate the quantum information. Since gates must conserve the norm of the states, they must be unitary [9].

Here, we focus on single-qubit quantum gates, which can be represented by 2×2 unitary matrices. The common single-qubit gates are the Hadamard, the Pauli matrices, the Phase gate and the $\pi/8$ gate. It is worth pointing out that any unitary matrix specifies a valid quantum gate. An arbitrary unitary operator on a single-qubit can be written as a combination of rotations, together with global phase shifts on the qubit. Hence, for real numbers α, β, γ and δ, the unitary gate is $\hat{U} = \mathrm{e}^{i\alpha}\hat{R}_z(\beta)\hat{R}_y(\gamma)\hat{R}_z(\delta)$, where $\hat{R}_{y,z}$ are the rotation operators on the Bloch sphere. In matrix form:

$$\hat{U} = \begin{pmatrix} \mathrm{e}^{i(\alpha-\beta/2-\delta/2)}\cos(\gamma/2) & -\mathrm{e}^{i(\alpha-\beta/2+\delta/2)}\sin(\gamma/2) \\ \mathrm{e}^{i(\alpha+\beta/2-\delta/2)}\sin(\gamma/2) & \mathrm{e}^{i(\alpha+\beta/2+\delta/2)}\cos(\gamma/2) \end{pmatrix}. \tag{39}$$

We claim that the unitary operator in the Zermelo approach $\hat{\mathcal{U}}_z(\tau) = \hat{\mathcal{U}}_0(\tau)\hat{\mathcal{U}}_c(\tau)$ will do the job for any input state in the least time. Finding a method to manipulate qubits rapidly and efficiently is of great significance in quantum computing and therein lies the relevance of our protocol. As an example, in subsection 3.2 we showed that we are able to perform unitary gates on any spin 1/2 system.

4 Three-level systems

In the above section, we dealt with two-level systems. Now, we focus our attention to three-level systems, also called qutrits.

Let us consider a background Hamiltonian $\hat{H}_0 = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$ written in the basis of eigenstates. Any ket can be expanded as a coherent superposition of these eigenkets. The control Hamiltonian (20) can be cast as a three dimensional matrix

$$\hat{H}_c(t) = \begin{pmatrix} h_{00} & h_{01}\mathrm{e}^{i\omega_{10}t} & h_{02}\mathrm{e}^{i\omega_{20}t} \\ h_{10}\mathrm{e}^{-i\omega_{10}t} & h_{11} & h_{12}\mathrm{e}^{i\omega_{21}t} \\ h_{20}\mathrm{e}^{-i\omega_{20}t} & h_{21}\mathrm{e}^{-i\omega_{21}t} & h_{22} \end{pmatrix} ; \tag{40}$$

in obtaining this matrix, we have plugged the initial and final states (written in the eigenbasis of $\hat{H}_0$) into Eq. (19). To avoid unmanageable matrix elements we write them as h_{ij}. The matrix elements depend on the expansion coefficients a_j and b_j for $j = 0, 1, 2$ as

$$h_{jj} = a_j^* b_j \mathrm{e}^{i\omega_j\tau} - \text{c.c.} \quad \text{for} \quad j = 0, 1, 2 \tag{41}$$

$$h_{01} = a_1^* b_0 \mathrm{e}^{i\omega_0\tau} - b_1^* a_0 \mathrm{e}^{-i\omega_1\tau} \quad , \quad h_{10} = -h_{01}^* \tag{42}$$

$$h_{02} = a_2^* b_0 \mathrm{e}^{i\omega_0\tau} - b_2^* a_0 \mathrm{e}^{-i\omega_2\tau} \quad , \quad h_{20} = -h_{02}^* \tag{43}$$

$$h_{12} = a_2^* b_1 \mathrm{e}^{i\omega_1\tau} - b_2^* a_1 \mathrm{e}^{-i\omega_2\tau} \quad , \quad h_{12} = -h_{21}^* \, . \tag{44}$$

The control Hamiltonian needs a physical interpretation in order to be realizable experimentally. The corresponding interpretation of each of the entries in (40) will strongly depend upon the situation at hand. We found that under certain circumstances it can be mapped to the Hamiltonian of a three-level atom interacting with two different laser fields (the probe field and the driving field), or even with the Hamiltonian of a spin 1 system interacting with magnetic fields. But, above all, let us stress carefully, that in order to fully characterize and give a meaningful explanation to the control Hamiltonian we need to have a concrete system at the laboratory, and know its properties properly.

5 Conclusions

We conclude this work with some important remarks and conclusions. The intention of the present manuscript was to solve the quantum counterpart of the Zermelo problem. Stunningly, this goal was achieved by imposing a single condition on the control Hamiltonian, viz., the maximization of its variance. This ensures a time-optimal control of any quantum system.

This being said, we encountered a main drawback, which was to appropriately give the control Hamiltonian a physical meaning. Specifically, we found that not every obtained solution admits a physical structure and thus not all Zermelo Hamiltonians are attainable experimentally. Nonetheless, we provided physical interpretation to various control Hamiltonians and, in particular, we proposed our method as an algorithm to design time-optimal quantum gates.

We do not have room to include the study of a particle in a harmonic potential. We are still working out the interpretation, since in this case, the control Hamiltonian is not local when expressed in the position representation.

Devising good protocols to control quantum systems is at the forefront of scientific research and we pretend to extend our study in more depth to general N dimensional systems in order to find out any constraints the control Hamilton must have to be physically implementable. In addition, it would be interesting to explore whether the field of quantum computation and optical lattices can benefit from our protocol.

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Sadly, Artur Polls Martí, an outstanding professor and great person, passed away few weeks ago. I would like to dedicate this thesis to him.

References

[1] José P Palao and Ronnie Kosloff. Quantum computing by an optimal control algorithm for unitary transformations. *Physical review letters*, 89(18):188301, 2002.

[2] Alberto Carlini, Akio Hosoya, Tatsuhiko Koike, and Yosuke Okudaira. Time-optimal quantum evolution. *Physical review letters*, 96(6):060503, 2006.

[3] Ernst Zermelo. Über das navigationsproblem bei ruhender oder veränderlicher windverteilung. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 11(2):114–124, 1931.

[4] Constantin Carathéodory. Variationsrechnung und partielle differentialgleichungen erster ordnung. *Leipzig und Berlin*, page 31, 1935.

[5] Dorje C Brody and David M Meier. Solution to the quantum zermelo navigation problem. *Physical review letters*, 114(10):100502, 2015.

[6] J Anandan and Yakir Aharonov. Geometry of quantum evolution. *Physical review letters*, 65(14):1697, 1990.

[7] Dorje C Brody, Gary W Gibbons, and David M Meier. Time-optimal navigation through quantum wind. *New Journal of Physics*, 17(3):033048, 2015.

[8] C. C. Gerry and Peter Knight. *Introductory quantum optics*. Cambridge University Press, Cambridge, UK New York, 2005.

[9] J. A. Jones and Dieter Jaksch. *Quantum information, computation and communication*. Cambridge University Press, Cambridge, UK New York, 2012.