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Minimum Time in Quantum State Transitions: Dynamical Foundations and Applications

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Additional information is available at the end of the chapter

Abstract

This chapter is about the minimum time evolution between two quantum states considering the dynamics obeying either time-invariant Hamiltonians or time-varying ones. Merit figures are defined to help quantum control designers to define optimization parameters. The expressions are derived from the time-energy uncertainty relations and a practical case is studied as an example.

Keywords: merit figures, minimum time, quantum control, quantum evolution, uncertainty relations

1. Introduction

One of the most important problems in quantum control [1, 2], as well in quantum information processing and quantum computing [3, 4], is the transition from an initial state to a target state in minimum time. In fact, the existence of the *Decoherence* phenomenon in quantum systems, characterized by extremely short coherence times, presents serious difficulties on implementing quantum information devices [3, 5].

Indeed, one of the difficulties of the operational nature in quantum systems lies in the fact that they are very sensitive to the presence of the external environment, which often destroys its main quantum characteristics, which are essential, for example, for the implementation of systems processing quantum information, as well as for the viability of quantum computing. This is the problem of quantum decoherence. Thus, it is widely desirable for expedients and

methods of optimal control of time minimization, applied to quantum systems, be the most efficient possible accordingly, whether of analytical nature, or of algorithmic and computational nature. However, there are physical limitations inherent by quantum dynamics, which relate to the minimum time, physically possible, so that a transition from quantum states occurs.

Therefore, it is natural to ask, what is the shortest physically possible time for a quantum state to evolve to another? The answer is provided by *time-energy uncertainty relations*. Opposing the famous quantum uncertainty relations regarding non-commuting operators, for example, position and momentum, time-energy uncertainty relations have a different mathematical and physical nature; they are deeply rooted in quantum dynamics.

The Soviet physicists Leonid I Mandelstam and Igor E. Tamm carried out the first successful theoretical approach addressing this issue, in the 1940s [6]. Under the hypothesis of time-independent Hamiltonian, Mandelstam and Tamm deduced a quantum dynamical inequality for time-energy, which sets up the temporal lower bound for a quantum state transition.

It is our goal, in the first section of this Chapter, to follow the theoretical steps of [6], translating the deductions to the modern quantum mechanical formalism, and to perform detailed analyses of the dynamical issues. Thereafter, we wish to apply the Mandelstam-Tamm time-energy inequality to a quantum system of interest, for example, the Fahri-Gutmann model of digital quantum computation [7], in order to obtain an analytical expression for the minimal time required for a state transition in such a quantum system. These analyses allow us to ultimately introduce a quantitative measure for the performance of time-optimal quantum controls [8].

In a subsequent section, we shall drop the time-independent Hamiltonian hypothesis of the original time-energy uncertainty relation and generalize it in the case of a time-dependent Hamiltonian $\hat{H} = \hat{H}(t)$. This is a type of Hamiltonian operators one finds in quantum control systems. In fact, appropriately shaped time-dependent electromagnetic fields or laser beams act as control efforts $u(t)$ [1]. The theoretical starting point for such generalization is to take into account the time evolution operator $\hat{U}(t, t_0)$ for the time-dependent Hamiltonian operator $\hat{H} = \hat{H}(t)$. Other approach to minimal time in quantum dynamical evolution is when one considers time-dependent Hamiltonians to employ the time-energy uncertainty relation obtained by Pfeifer [9].

2. Minimum time for quantum state transitions

Before tackling the control problem in quantum systems with respect to minimum time, that is, to make a given state transfer from a prescribed initial state to a desired target state as quickly as possible, one must take into account a fundamental issue of physical nature, which can be stated as follows. Given an initial state $|\psi_I\rangle$, which evolves over time according to the Schrödinger picture of quantum dynamics, that is, by means of the action of the time-evolution operator, dependent on the Hamiltonian of the system, how fast is the transition to a final state

$- | \psi_F \rangle$? In other words, what is the shortest possible time so that a transition of quantum states can occur?
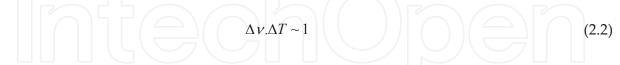
This problem of a theoretical nature has been widely studied and it is closely linked to dynamical characterizations derived from time-energy uncertainty relations. Such relationships differ fundamentally from the Heisenberg's uncertainty principle (e.g., the simultaneous measurement uncertainty of the position and the linear momentum of a quantum particle), which comes from the *incompatibility* between the quantum observables, a physical fact that arises, within the mathematical and theoretical framework of quantum mechanics, from the *non-commutability* of the quantum observables involved in the measurement process. The time-energy uncertainty, on the other hand, finds its roots in quantum dynamics, as we are about to see.

From a historical point of view, since the so-called "old quantum theory," pioneered by Max Planck, Albert Einstein, Niels Bohr, among others, comprising the first two decades of the last century and firmly established, was the Planck-Einstein equation, which relates the energy and frequency of a photon through the Planck's fundamental constant h:

$$E = h\nu \tag{2.1}$$

As we know, such relationship is fundamental not only for the pioneering and groundbreaking Planck's hypothesis of quantization of radiation emission by an ideal black body, written in 1900 but also for the explanation given by Einstein for the photoelectric effect in 1905. Moreover, the atomic model introduced by Bohr in 1913, which explained the stability of the hydrogen atom by means of quantized energy levels corresponding to the stable possible orbits for the electron; postulated in addition that, when jumping to an energy level (or orbit) more or less energetic, the electron absorbed or emitted a quantum of energy, respectively, following the relationship (**2.1**), corresponding to a photon with frequency ν.

So, given a trivial variation in frequency at a given time interval, such as

$$\Delta \nu . \Delta T \sim 1 \tag{2.2}$$

providing the same account of an "uncertainty" $\Delta \nu$ for the frequency measurement of a monochromatic radiation at the ΔT time interval, by making use of the expression (**2.1**), we are led to the following:

$$\Delta E . \Delta T \sim h \tag{2.3}$$

This "uncertainty relation" deduction is eminently heuristic, although expression (**2.3**) still has experimental support within the physical conditions one has evoked to get it. Nevertheless, if one tries to generalize it as something of the form:

$$\Delta H.\Delta T \sim h \tag{2.4}$$

because the Hamiltonian corresponds to the energy of a mechanical system (classical or quantum), one will run into serious difficulties. If H represents a quantum observable in the current quantum mechanical sense, in the same way Paul Dirac had formally stated in the very first edition of his famous treatise [10], dating back to 1930, we can no longer identify the energy with the frequency of the monochromatic radiation times the Planck's constant. Moreover, expression (**2.4**) becomes inherently invalid and devoid of meaning for any quantum system when properly mathematically treated.

The Soviet physicists Leonid I. Mandelstam and Igor E. Tamm in the 1940s carried out the first successful theoretical approach addressing this quantum dynamical issue, the statement of a meaningful time-energy uncertainty relation [6].

So, let us try to present their theoretical starting point drawing on modern quantum mechanical formalism and its current notation, and finally arrive at the desired time-energy uncertainty relation through rigorous deductions combined with detailed analyses. The goal is also to modify it, in order to obtain variants of it and alternative expressions suitable for some purposes, which will become clear in the sections ahead.

Let $\widehat{R}$ and $\widehat{S}$ be two generic Hermitian operators (quantum observables). The following relationships hold [6]:

$$\Delta \widehat{S}.\Delta \widehat{R} \geq \frac{1}{2}\left|\left\langle \widehat{R}\widehat{S} - \widehat{S}\widehat{R} \right\rangle\right| \tag{2.5}$$

$$\frac{d\left\langle \hat{R} \right\rangle}{dt} = \frac{1}{i\hbar}\left\langle \left[\hat{R}, \hat{H} \right] \right\rangle \tag{2.6}$$

where $\Delta \widehat{S}$ and $\Delta \hat{R}$ are the square root of the mean square deviations (or variances) of operators $\widehat{S}$ and $\widehat{S}$, respectively, also known as "dispersion operator," or simply "standard deviation" in statistics terminology. Expression (**2.6**) is nothing but the dynamical evolution equation in the Heisenberg picture for the expectation value of observable $\widehat{R}$. If we impose $\hat{S} \equiv \hat{H}$ on (**2.5**) and apply the result of (**2.6**), the following inequality is obtained:

$$\Delta \hat{H}.\Delta \hat{R} \geq \frac{\hbar}{2}\left|\frac{d\left\langle \hat{R} \right\rangle}{dt}\right| \tag{2.7}$$

This expression provides, therefore, the connection between the standard deviation $\Delta \hat{H}$ of the total energy and the uncertainty in determining the energy of an isolated system, the standard deviation $\Delta \hat{R}$ (uncertainty) of some other dynamical quantity, relating them to the rate of change of the expectation value of the same physical amount.

Relationship (**2.7**) may be expressed otherwise. Since the modulus of an integral is less than or equal to the integral of the integrand modulus [11], upon performing an integration of (**2.7**) from t to $t + \Delta t$, and taking into account that $\Delta \hat{H}$ is constant, one derives inequality:

$$\Delta \hat{H}.\Delta t \geq \frac{\hbar}{2} \frac{\left| \left\langle \hat{R}_{t+\Delta t} \right\rangle - \left\langle \hat{R}_t \right\rangle \right|}{\left\langle \Delta \hat{R} \right\rangle} \tag{2.8}$$

in which the denominator of the right side of the inequality denotes the average value of $\Delta \hat{R}$ during the amount of time Δt.

It is appropriate to introduce, at this point, a special notation, ΔT, for the shortest time, during which the average value of a certain physical quantity is changed by an amount equal to the standard deviation thereof. Thus, ΔT can be called standard deviation (uncertainty) of time; making use of this notation, (**2.8**) can be rewritten as follows:

$$\Delta \hat{H}.\Delta T \geq \frac{\hbar}{2} \tag{2.9}$$

Now, let us consider a projection operator of form $\hat{\Lambda} \equiv | \psi_0 \rangle\langle \psi_0 |$. One can immediately notice that only one of its eigenvalues is unitary (when the projection operator is applied to the eigenstate $| \psi_0 \rangle$) and all the others are zero. Thus, we have:

$$\hat{\Lambda}^2 = \hat{\Lambda}\hat{\Lambda} = \hat{\Lambda} \tag{2.10}$$

Indeed, $\hat{\Lambda}$ is an idempotent operator, as one can easily verify.

Furthermore, the expectation value $\langle \hat{\Lambda} \rangle$ may be interpreted as the probability of finding the quantum system in a specific quantum state $| \psi \rangle$, considering the initial state $| \psi_0 \rangle$, since from the average value (or expectation value) definition, we have $\langle \hat{\Lambda} \rangle_\psi \equiv \langle \psi | \hat{\Lambda} | \psi \rangle = \langle \psi | \psi_0 \rangle\langle \psi_0 | \psi \rangle = | \langle \psi | \psi_0 \rangle |^2 = P_\psi$. Of course, $\langle \hat{\Lambda} \rangle$ has its values within the interval $0 \leq \langle \hat{\Lambda} \rangle \leq 1$. According to (**2.10**), it follows that

$$\Delta \hat{\Lambda} = \sqrt{\left\langle \hat{\Lambda}^2 \right\rangle - \left\langle \hat{\Lambda} \right\rangle^2} = \sqrt{\left\langle \hat{\Lambda} \right\rangle - \left\langle \hat{\Lambda} \right\rangle^2} \tag{2.11}$$

Therefore, making use of the expressions (**2.7**) and (**2.11**); then, applying operator $\overset{\wedge}{\Lambda}$ in the place of $\hat{R}$, we obtain

$$\Delta\hat{H}.\sqrt{\left\langle\hat{\Lambda}\right\rangle-\left\langle\hat{\Lambda}\right\rangle^2} \geq \frac{\hbar}{2}\left|\frac{\mathrm{d}\left\langle\hat{\Lambda}\right\rangle}{\mathrm{d}t}\right| \tag{2.12}$$

This inequality contains only one-time variable quantity, $\overset{\wedge}{\Lambda}=\overset{\wedge}{\Lambda}(t)$, and its time derivative, so that it can be integrated with respect to time. If, for example, $\overset{\wedge}{\Lambda}(t)=\overset{\wedge}{\Lambda}(0)=1$, that is, at the instant of time $t=0$, we were certain that the system was in the initial state $|\psi_0\rangle$, then it follows from (**2.12**) that, for $t\geq0$,

$$\frac{\pi}{2}-\arcsin\sqrt{\left\langle\hat{\Lambda}(t)\right\rangle} \leq \frac{\Delta\hat{H}.t}{\hbar} \tag{2.13}$$

From (**2.13**), by using basic trigonometric properties and simple algebraic manipulations, it leads to the following expression:

$$\left\langle\hat{\Lambda}(t)\right\rangle \geq \cos^2\left(\frac{\Delta\hat{H}.t}{\hbar}\right) \tag{2.14}$$

for $t\geq0$.

Here, an important fact should be noted. Although the projection operator $\overset{\wedge}{\Lambda}$ as $\overset{\wedge}{\Lambda}\equiv|\psi_0\rangle\langle\psi_0|$ has been defined with the outer product given by the *ket* and the *bra* corresponding to a state ψ_0, we could have also defined it, in a more general manner, such as $\overset{\wedge}{\Lambda}\equiv|\psi_t\rangle\langle\psi_t|$; that is, for a generic quantum state ψ_t evolved in time, for any instant of time t, so that the idempotency property of $\overset{\wedge}{\Lambda}$, as well as all the expressions, arguments, and previous deductions are analogous, remaining valid, thus, enjoying full generality.

From (**2.14**), two expressions relevant to our purposes shall be deduced. Since the average value of the projection operator $\overset{\wedge}{\Lambda}$ corresponds to the probability of observing the system at a given quantum state $|\psi\rangle$, more generally, at a certain state $|\psi_t\rangle$ evolving over time, having been (or been prepared) at an initial state $|\psi_0\rangle$ of the system, then inequality (**2.14**) shall be rewritten as

$$P_t \geq \cos^2\left(\frac{\Delta\hat{H}.t}{\hbar}\right) \tag{2.15}$$

where $P_t = |\langle \psi_t | \psi_0 \rangle|^2$ is the probability of finding the system in $|\psi_t\rangle$ from $|\psi_0\rangle$; indeed, $\langle \hat{\Lambda}(t) \rangle = \langle \psi_0 | \hat{\Lambda}(t) | \psi_0 \rangle = \langle \psi_0 | \psi_t \rangle \langle \psi_t | \psi_0 \rangle = |\langle \psi_t | \psi_0 \rangle|^2 = P_t$.

Finally, from (**2.15**), it can be deduced that the lowest physically possible time, or more generally, the inferior time limit,[1] physically needed to perform a transition between quantum states, under the assumption of a time-independent Hamiltonian, is given by the following inequality, which takes into account the uncertainty in determining the energy (dispersion or standard deviation of $\hat{H}$):
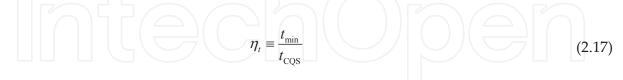
$$t \geq \frac{\hbar}{\Delta \hat{H}} \arccos \sqrt{P_t} \tag{2.16}$$

in which t is the necessary time for a quantum transition of states that its associated probability is $P_t = |\langle \psi_t | \psi_0 \rangle|^2$.

From (**2.16**), it is immediately noticed that the time t is always a real number, despite the internal product ("bracket") of states being, in general, a complex number. Likewise, as any quantum observable, $\Delta \hat{H}$ always results in a real number. Moreover, since $P_t = |\langle \psi_t | \psi_0 \rangle|^2$ is defined in [0,1], when the state normalization conditions are taken for granted, ensuring that the obtained probabilities vary always in the real interval [0,1]; it follows that the range of *arccos* function for this specific domain and, therefore, the values of t, will always be positive.

Some remarks about technological issues and its terminology are in order here. In quantum control literature, inequality (**2.16**) is also known as the "Bhattacharyya limit," after a paper by the Indian physicist Kamal Bhattacharyya, in which the author revisits the Mandelstam-Tamm's time-energy uncertainty relations, in order to apply them in decay or non-decay problems in quantum systems [12].

Inequality (**2.16**) gives a strong motivation to introduce a quantitative measure for the evaluation of the quantum control systems performance, with special interest on the time-optimal quantum control, for example, [1] and [13]. Lets then define the following *figure of merit*,

$$\eta_t \equiv \frac{t_{\min}}{t_{\mathrm{CQS}}} \tag{2.17}$$

where $t_{\min}$ is the shortest physically possible time to obtain a desired transition of quantum states, and t_{CQS} is the time by which such transition can be effectively accomplished in the *controlled quantum system*, hence, the notation chosen is [8].

In general, analytical solutions to problems of optimal quantum control are rare, and in most cases, control algorithms and numerical simulations are employed to obtain the desired results

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[1] Mathematically speaking, one can say it is the *inf* or greatest lower bound (GLB) of the subset *S* of the physically possible times for quantum states transitions.

[1]. Indeed, in an article by Caneva and other authors [13], the Krotov algorithm is employed, for example, [14] and [15], and applied on the Landau-Zener system, as well as on a theoretical scheme of quantum information transfer in a spin chain ("One dimensional Heisenberg spin chain of length N"). The authors obtained state transition times close to the "Bhattacharyya limit," which is equivalent to inequality (2.16) for both systems studied [13].

Regarding the figure of merit η_t, it is easy to notice that η_t is a real number and a dimensionless quantity, defined on the interval $[0,1]$: $\eta_t \in \mathsf{R} : 0 \leq \eta_t \leq 1$, such that the extremal values correspond, respectively, to the cases in which the transition of quantum states has not been accomplished; in other words, the employed control algorithm did not converge to the desired target state (or mathematically speaking, it took an "infinite time"); on the other hand, there has been an ideal temporal state transfer: the control algorithm has achieved maximum efficiency in terms of the demanded time to perform the desired quantum state transition.

Combining the expressions (2.16) and (2.17), η_t can be more explicitly expressed as

$$\eta_t = \frac{\hbar.\arccos\sqrt{P_t}}{\Delta\hat{H}.t_{\mathrm{CQS}}}$$

(2.18)

or, alternatively as

$$\eta_T = \frac{\hbar\arccos\left|\langle\psi_{\mathrm{F}}|\psi_{\mathrm{I}}\rangle\right|}{\Delta\hat{H}.t_{\mathrm{CQS}}}$$

(2.19)

where $|\psi_{\mathrm{I}}\rangle$ and $|\psi_{\mathrm{F}}\rangle$ correspond, respectively, to some initial state and a certain desired final state (or target state, in control terminology).

From the dimensional analysis point of view, it is straightforward to verify that η_t, as expressed by (2.18) and (2.19), is consistent with the adimensionality requirement, since the constant $\hbar$ has dimension of action (energy × time), and the dispersion operator (or standard deviation) of the system's Hamiltonian $\Delta\hat{H}$ has natural dimension of energy.

Frequently, in practical applications, it is not always possible to obtain the "exact transition" of quantum states by the use of control algorithms and numerical simulations per se, from an initial state to the desired goal state, such as $|\psi_{\mathrm{G}}\rangle$. Instead, one looks for optimal control actions that maximizes the measure of *quantum fidelity*:

$$F = \left|\langle\psi_{\mathrm{G}}|\psi_T\rangle\right|^2$$

(2.20)

or, in dual form, which minimize the amount of *quantum infidelity*:

$$I = 1 - \left| \langle \psi_G | \psi_T \rangle \right|^2 \tag{2.21}$$

that is, control actions such that, once elapsed control time T, the probability for the evolved state in time $| \psi(T) \rangle$ to be found at the target state $| \psi_G \rangle$ gets arbitrarily close to unity. Therefore, one can analyze the performance of the iterative process as a function of T and show that the algorithmic method in question is capable of producing infidelities arbitrarily close to zero [13].

3. Application to a particular quantum state transition

Now, consider the application of the time-energy uncertainty relations (**2.15**) and (**2.16**) to a specific and very important quantum state transition, namely the transition between two orthogonal states.[2] By rewriting inequality (**2.15**), in order to make explicit the probability associated to the transition from an initial state to a time-evolving state, on the left side of the expression, we have

$$\left| \langle \psi_t | \psi_0 \rangle \right|^2 \geq \cos^2 \left(\frac{\Delta \hat{H}.t}{\hbar} \right) \tag{3.1}$$

where $\Delta \hat{H} = \sqrt{\langle \hat{H}^2 \rangle_\psi - \langle \hat{H} \rangle_\psi^2}$ is the dispersion of $\hat{H}$ or the uncertainty for determining the energy.

Let us consider a quantum dynamical evolution, starting from a generic state $| \psi \rangle$, which the system dynamics leads it to the orthogonal state $| \psi^\perp \rangle$, by means of the actuation of the time-evolution operator $\hat{U}(t, t_0)$. Schematically, we have

$$| \psi \rangle \rightarrow \hat{U}(t, t_0) \rightarrow | \psi^\perp \rangle$$

with $\hat{U}(t, t_0) = e^{\frac{-i \hat{H}(t - t_0)}{\hbar}}$ — the time-evolution operator for a time-independent Hamiltonian $\hat{H}$, upon which $t_0 = 0$ can be imposed without loss of generality.

Adapting the expression (**3.1**) for such a case, results in

$$\left| \langle \psi | \hat{U}(t, t_0) | \psi \rangle \right|^2 \geq \cos^2 \left(\frac{\Delta \hat{H}.t}{\hbar} \right) \tag{3.2}$$

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[2] Or orthonormal states, once the normalization condition is taken for granted.

which its associated probability amplitude, $\langle\psi\,|\,\hat{U}(t,\,t_0)\,|\,\psi\rangle$, can be regarded as a survival amplitude of the state $|\,\psi\rangle$, evolving in time according to $\hat{U}(t,\,t_0)$ and $\Delta\hat{H}$, the energy uncertainty is given by

$$\Delta_\psi\hat{H} = \sqrt{\langle\psi|\hat{H}^2|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle^2} \tag{3.3}$$

If a state transition from $|\,\psi\rangle$ to $|\,\psi^\perp\rangle$ occurs, the probability amplitude of (**3.2**) becomes zero, being able to define formally the first instant of time t, for which such transition takes place as follows:

$$\tau_{\psi\to\psi\perp} \equiv \inf\{t\geq 0 : \langle\psi|\hat{U}(t,t_0)|\psi\rangle = 0\} \tag{3.4}$$

Therefore, it is straightforward to conclude from (**3.2**) that $\tau_{\psi\to\psi\perp}$ is inferiorly bounded by the inequality:

$$\tau_{\psi\to\psi\perp} \geq \frac{\pi\hbar}{2\Delta\hat{H}} \tag{3.5}$$

Furthermore, the quantitative measure of temporal transfer efficiency can be defined for this specific case, figure of merit $\eta_{\psi\to\psi\perp}$ for such quantum state transfer, as

$$\eta_{\psi\to\psi\perp} \equiv \frac{\tau_{\psi\to\psi\perp}}{\tau_{\mathrm{CQS}}} \tag{3.6}$$

or, more explicitly, taking into account (**3.5**),

$$\eta_{\psi\to\psi\perp} = \frac{\pi\hbar}{2\Delta\hat{H}\tau_{\mathrm{CQS}}} \tag{3.7}$$

where $\tau_{\psi\to\psi\perp}$ is the shortest physically possible time, such that the first transition to the orthogonal state occurs, and τ_{CQS} can be stated as the time effectively spent by the controlled system or control algorithm, in order to perform such state transfer.

Finally, it is worthwhile mentioning the transitions or transfers between orthogonal (orthonormal) quantum states are of paramount importance to any schemes or devices, whether theoretical, experimental, or of technological nature, aimed at implementing quantum information processing, or quantum computing. The interested reader is referred to standard and authoritative sources like [3,4].

4. An analytical case study: The Fahri-Gutmann system

In this section, an application example is presented for illustrating the ideas and theoretical concepts developed so far. The Fahri-Gutmann system is a digital quantum computing model, which in its turn can be interpreted as a variation of the quantum search algorithm, similar to the well-known Grover's algorithm [16]. Here, we follow the steps of [17].

Let $|a\rangle$ and $|b\rangle$ be the initial and the target state, respectively, and the system's Hamiltonian defined as:

$$\hat{H} = E_a |a\rangle\langle a| + E_b |b\rangle\langle b| \tag{4.1}$$

where E_a and E_b are positive constants.

As already stressed, there can be computational difficulties to achieve the exact desired transfer of states, that is, from the initial state to the target one over the time evolution. Nevertheless, one can think of formulating the quantum control problem in a less restrictive manner, namely in terms of a state transition, as fast as possible, such that one can ensure maximum fidelity. Translating it into quantum mechanical language, we want to maximize the quantity:

$$F \equiv P_t = \left| \langle b | \hat{U}(t, t_0) | a \rangle \right|^2 \tag{4.2}$$
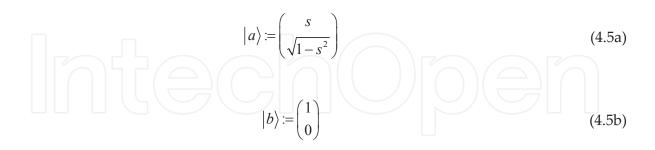
Firstly, let us impose $\langle a | b \rangle = s$. Without loss of generality, is assumed that s is a real number, since a phase factor can be associated to $|a\rangle$ or $|b\rangle$. Given the Fahri-Gutmann Hamiltonian expression (**4.1**), it is evident that it acts non-trivially only on the subspace spanned by the eigenstates $|a\rangle$ and $|b\rangle$, so it suffices to consider only this two-dimensional subspace. The computational basis of this quantum model is as follows:

$$\{|b\rangle, |b'\rangle\}, \text{such that} |b'\rangle = \frac{1}{\sqrt{1 - s^2}} \left(|a\rangle - s|b\rangle \right) \tag{4.3}$$

which, in fact, consists of an orthonormal basis for the subspace spanned by $|a\rangle$ and $|b\rangle$.

Considering $E = E_a + E_b$, $x = E_a - E_b$, and defining the quantity:

$$\mu \equiv \sqrt{s^2 + \left(\frac{x}{E}\right)^2 (1 - s^2)} \tag{4.4}$$

We shall assume that $E_a > 0$ and $E_b > 0$. It is evident that $s \leq \mu \leq 1$ and $s = \mu$ if, and only if, $E_a = E_b$. In the computational basis $\{|b\rangle, |b'\rangle\}$, states $|a\rangle$ and $|b\rangle$ are represented, respectively, by the vectors:

$$|a\rangle := \begin{pmatrix} s \\ \sqrt{1-s^2} \end{pmatrix} \tag{4.5a}$$

$$|b\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{4.5b}$$

By defining the auxiliary constant λ as follows:

$$\lambda = s^2 - \frac{x}{E}(1 - s^2) \tag{4.6}$$

the Hamiltonian $\hat{H} = E_a |a\rangle\langle a| + E_b |b\rangle\langle b|$, considering the basis given by (**4.6**), has its matricial representation, with E being an arbitrary constant:

$$\hat{H} := \begin{pmatrix} 1 + s^2 - \dfrac{x}{E}(1 - s^2) & \left(1 + \dfrac{x}{E}\right)s\sqrt{1-s^2} \\ \left(1 + \dfrac{x}{E}\right)s\sqrt{1-s^2} & 1 - s^2 + \dfrac{x}{E}(1 - s^2) \end{pmatrix} = \frac{E}{2}\begin{pmatrix} 1 + \lambda & \sqrt{\mu^2 - \lambda^2} \\ \sqrt{\mu^2 - \lambda^2} & 1 - \lambda \end{pmatrix} \tag{4.7}$$

so that this matrix can be diagonalized as follows:

$$\hat{H} = U\begin{pmatrix} \dfrac{E}{2}(1 + \mu) & 0 \\ 0 & \dfrac{E}{2}(1 - \mu) \end{pmatrix}U^{-1} \tag{4.8}$$

with the U matrix given by

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1 + \dfrac{\lambda}{\mu}} & \sqrt{1 - \dfrac{\lambda}{\mu}} \\ \sqrt{1 - \dfrac{\lambda}{\mu}} & -\sqrt{1 + \dfrac{\lambda}{\mu}} \end{pmatrix} \tag{4.9}$$

corresponding to the diagonalization unitary operator built up with the eigenvectors of $\hat{H}$ as given by its matrix representation (**4.7**).

After performing some cumbersome, but straightforward calculations, to diagonalize $\hat{H}$, given by (**4.7**), making use of (**4.8**) and (**4.9**), one finally obtains from (4.5a) and (4.5b) the time transition probability P_t, which can be regarded as a fidelity measure between the "search state" $e^{\frac{-i\hat{H}(t-t_0)}{\hbar}} |a\rangle$ and the target state $|b\rangle$:

$$P_t = \left| \langle b | \exp(\frac{-i\hat{H}t}{\hbar}) | a \rangle \right|^2 = s^2 \left(\left(\frac{1}{\mu^2} - 1 \right) \sin^2 \left(\frac{\mu E t}{2\hbar} \right) + 1 \right) \tag{4.10}$$

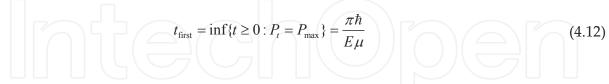where we have imposed $t_0 = 0$ on the time-evolution operator $\hat{U}(t, t_0) = e^{\frac{-i\hat{H}(t-t_0)}{\hbar}}$.

Noting that $s \leq \mu \leq 1$, it is easy to see that the maximum value of the probability P_t is

$$P_{\max} = \max_{t \geq 0} P_t = \left(\frac{s}{\mu} \right)^2 \tag{4.11}$$

indeed, it suffices to impose that the value of the function $\sin^2\left(\frac{\mu E t}{2\hbar}\right)$ must be 1 in the expression (**4.10**) to obtain (**4.11**).

In the same way, once achieving $\sin^2\left(\frac{\mu E t}{2\hbar}\right) = 1$ in (**4.10**), it can be conclude that the first instant of time t, for which maximum probability (or maximum fidelity), is given by

$$t_{\text{first}} = \inf\{t \geq 0 : P_t = P_{\max}\} = \frac{\pi\hbar}{E\mu} \tag{4.12}$$

Thus, for the Fahri-Gutmann's quantum computing model, the particular figure of merit that quantifies the time transition efficiency can be stated as

$$\eta_{\text{FG}} = \frac{\pi\hbar}{E\mu\tau_{\text{CQS}}} \tag{4.13}$$

where τ_{CQS} is the time effectively spent to drive the search state $\hat{U}(t, t_0) |a\rangle$ to the target state $|b\rangle$.

5. Quantum systems with time-dependent Hamiltonians: Two theoretical approaches to minimum time in quantum state transitions

Let us consider, a time-evolution operator $\hat{U}(t, t_0)$ characterized by a time-dependent Hamiltonian $\hat{H} = \hat{H}(t)$, such that $[\hat{H}(t_1), \hat{H}(t_2)] = 0$, $\forall\, t_1, t_2 \in I \subset \mathbb{R}^+$, $t_1 \neq t_2$; that is, the Hamiltonian operator of the quantum system of interest varies with time; however, it always commutes for any distinct instants of time t_1 and t_2, $t_1 \neq t_2$.

In quantum control, this is by far the most commonly found and studied case regarding the attempts to find control laws $u(t)$ to achieve a certain control goal of interest, which involves, for example, the minimization or maximization of dynamical variables to perform desired state transitions. Here, we are interested in minimizing transfer times between quantum states. Physically speaking, for example, a spin ½ system (e.g., an electron) subjected to a magnetic field which magnitude varies in time, but not in direction.

The time-evolution operator $\hat{U}(t, t_0)$ associated with such a time-dependent Hamiltonian is given by [18]

$$\hat{U}(t, t_0) = \exp\left[-\left(\frac{i}{\hbar}\right)\int_{t_0}^{t} dt'\, \hat{H}(t')\right] \tag{5.1}$$

Therefore, given an initial state $|\psi_I\rangle$ and a final state $|\psi_F\rangle$ (or "target state"), the shortest physically possible time (or minimum time) can be formally defined such that this transition of states occurs as follows:

$$t_{\min} \equiv \inf\{t \geq 0 : \left|\langle\psi_F|\hat{U}(t, t_0)|\psi_I\rangle\right|^2 = 1\} \tag{5.2}$$

where $\hat{U}(t, t_0)$ is given by the expression (**5.1**).

In an applied point of view, given the vector representations of $|\psi_I\rangle$ and $|\psi_F\rangle$ expressed in terms of a suitable basis (built up of linearly independent and orthonormal vectors), as well a matrix representation of $\hat{H} = \hat{H}(t)$, by calculating the integral of (**5.1**), expression (**5.2**) will provide the necessary formula to obtain the minimum time value.[3]

Now, the focus is on another possible formulation addressing this quantum dynamical issue. The goal is to directly employ a time-dependent energy uncertainty (or standard deviation) $\Delta(\hat{H}(t))$ to formally obtain an expression for the minimum time associated with transitions of states in quantum systems with dynamics governed by a time-dependent Hamiltonian $\hat{H} = \hat{H}(t)$. The Schrödinger equation taking into account such a Hamiltonian is written as

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[3] In [8], we present an analytical case study of a time-dependent Hamiltonian, namely the Landau-Zener system.

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H}(t)|\psi(t)\rangle \tag{5.3}$$

with a time-evolving state $|\psi(t)\rangle$, from an initial state $|\psi_0\rangle$.

From this particular Schrödinger equation, Pfeifer proposed the following expression for a time-dependent energy uncertainty [9]:

$$\Delta(\hat{H}(t),|\psi(t)\rangle,|\dot{\psi}(t)\rangle) = \hbar \left\| \left(\hat{1} - |\psi(t)\rangle\langle\psi(t)|\right) \frac{\partial |\psi(t)\rangle}{\partial t} \right\| \tag{5.4}$$

in which we can immediately notice the dependency on the time-evolved state $|\psi(t)\rangle$, as well on its time derivative. From the original expression (**5.4**), some manipulations are carried out to deduce an alternative expression for the time-dependent energy uncertainty $\Delta(\hat{H}(t), |\psi(t)\rangle, |\dot{\psi}(t)\rangle)$, such that it may be more useful for our purposes:

$$\Delta(\hat{H}(t),|\psi(t)\rangle) = \hbar \left\| \left(\hat{1} - |\psi(t)\rangle\langle\psi(t)|\right)\left(\frac{1}{i\hbar}\hat{H}(t)|\psi(t)\rangle\right) \right\| =$$

$$\Delta(\hat{H}(t),|\psi(t)\rangle) = \hbar \left\| \left(\frac{1}{i\hbar}\hat{H}(t)|\psi(t)\rangle - \frac{1}{i\hbar}\langle\psi(t)|\hat{H}(t)|\psi(t)\rangle|\psi(t)\rangle\right) \right\| =$$

$$\Delta(\hat{H}(t),|\psi(t)\rangle) = \hbar \left| \frac{1}{i\hbar} \right| \left\| \left(\hat{H}(t)|\psi(t)\rangle - \langle\psi(t)|\hat{H}(t)|\psi(t)\rangle|\psi(t)\rangle\right) \right\| =$$

$$\Delta(\hat{H}(t),|\psi(t)\rangle) = \left\| \hat{H}(t)|\psi(t)\rangle - \left\langle \hat{H}(t) \right\rangle_{\psi(t)} |\psi(t)\rangle \right\| \tag{5.5}$$

wherein, at the first step, we replaced the time derivative of $|\psi(t)\rangle$ making use of (**5.3**), so that we could eliminate the dependency on $|\psi(t)\rangle$, the outer product $|\psi(t)\rangle\langle\psi(t)|$, and the constant $\hbar$, as well (second and third steps, respectively). As a result, we were able to express $\Delta(\hat{H}(t), |\psi(t)\rangle)$ as a functional of vector $\hat{H}(t)|\psi(t)\rangle$ and of the time-evolving state $|\psi(t)\rangle$, multiplied by the scalar quantity correspondent to the expectation value of the Hamiltonian $\hat{H}(t)$.

Now, let us consider a time-energy uncertainty relation of the form $\Delta E.\Delta t \approx \hbar$, similar to those one can find in the time-independent Hamiltonian case, in terms of stationary states of energy [18]. Afterwards, through methods and concepts from the time-dependent perturbative theory, Sakurai shows that such relation remains valid for the time-dependent case [18]. So, it

becomes natural to evoke one of the Mandelstam-Tamm's time-energy uncertainty relations, namely

$$\Delta \hat{H}.\Delta T \geq \frac{\hbar}{2} \tag{5.6}$$

Furthermore, to achieve the perspective of our chain of theoretical reasoning so far, we restate it in the following way:

$$\Delta(\hat{H}(t),|\psi(t)\rangle).t \geq \frac{\hbar}{2} \tag{5.7}$$

in which the energy uncertainty is now considered as depending on a time-dependent Hamiltonian $\hat{H}(t)$, and, without loss of generality, $t_0 = 0$ in ΔT is imposed.

Finally, the minimum time for a generic quantum state transition, between an initial state $|\psi_0\rangle$, which begins to evolve over time, and a final state $|\psi_F\rangle = |\psi(T)\rangle$, can be formally defined in such a way that it can also be defined in function of an instant of time T. Its final state is achieved or characterized by

$$t_{\min} \equiv \inf\{t \geq 0 : P(t) = |\langle\psi_F|\psi(t,t_0)\rangle|^2 = 1\} = T \tag{5.8}$$

or, in terms of the maximum possible quantum fidelity, also by

$$t_{\min} \equiv \inf\{t \geq 0 : F \equiv |\langle\psi_F|\psi(t,t_0)\rangle|^2 \to 1\} = T \tag{5.9}$$

Finally, taking into account expressions (**5.7**) and (**5.5**), we have

$$t_{\min} \geq \frac{\hbar/2}{\Delta(\hat{H}(t),|\psi(t)\rangle)} \tag{5.10}$$

$$t_{\min} \geq \frac{\hbar/2}{\left\|\hat{H}(T)|\psi(T)\rangle - \langle\hat{H}(T)\rangle_{\psi(T)}|\psi(T)\rangle\right\|} \tag{5.11}$$

obtaining an alternative expression for the greatest temporal lower bound for a generic transition of states, that occurs in a quantum system with dynamics governed by a time-

dependent Hamiltonian $\hat{H}(t)$, thus, without relying on the approximative hypothesis of time independency in the characteristic Hamiltonian of the system.

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