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Elementary derivation for passage times

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Abstract
When a quantum system undergoes unitary evolution in accordance with a
prescribed Hamiltonian, there is a class of states $|\psi\rangle$ such that, after the passage
of a certain time, $|\psi\rangle$ is transformed into a state orthogonal to itself. The shortest
time for which this can occur, for a given system, is called the passage time.
We provide an elementary derivation of the passage time, and demonstrate that
the known lower bound, due to Fleming, is typically attained, except for special
cases in which the energy spectra have particularly simple structures. It is also
shown, using a geodesic argument, that the passage times for these exceptional
cases are necessarily larger than the Fleming bound. The analysis is extended
to passage times for initially mixed states.

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1. Introduction

The notion of a characteristic time arises in a variety of situations in quantum mechanics. For
example, concerning the decay of an atom, one is interested in the characteristic decay time,
or lifetime. Typically, one would conduct measurements on an ensemble of independently
and identically prepared systems, whereby the lifetime is estimated as an ensemble mean. For
a particle trapped in a potential, one would be interested in the tunnelling time, the time in
which the particle escapes from the trap.

There are many other circumstances in which one is interested in the time required for an
initial state of the system to evolve into another state under the action of a given Hamiltonian,
or more generally, under some given setup. See, for example, [1] (and references cited therein)
for a discussion on various characteristic times in quantum theory. It is curious that, despite
its experimental importance, precise statistical bounds on the estimation accuracy of time in
quantum mechanics have only been obtained fairly recently [2, 3].

One of such characteristic times, namely, the time required for a given initial state $|\psi\rangle$
to evolve into another state orthogonal to $|\psi\rangle$, has attracted some attention because of its
relevance to quantum computation and computational capacity (see, for example, [4–6]), and
also to fidelity between a pair of quantum states [7, 8]. Of course, given a generic state $|\psi\rangle$
and a Hamiltonian, it is more likely that $|\psi\rangle$ will never evolve into a state orthogonal to $|\psi\rangle$.

Nevertheless, for some special cases this can occur, which is the situation we study here. In particular, we call the minimum time required for a state to be transformed into an orthogonal state a passage time. The lower bound for the passage time is known as the Fleming bound [9]. Our main objective here is to give an elementary derivation of the passage time, and illustrate the result for some simple systems. Let us first state more explicitly the problem at hand.

Consider an n-dimensional Hilbert space $\mathcal{H}$, and a Hamiltonian $\hat{H}$ with eigenvalues $\{E_l\}$ ($l = 1, 2, \ldots, n$). For definiteness, we suppose that the energy eigenvalues are all distinct, although this is not essential in the ensuing argument. The time evolution of the wavefunction is thus effected by a one-parameter family of unitary operators

$$\hat{U}(t) = \exp(-\mathrm{i}\hat{H}t/\hbar). \tag{1}$$

Now, the Hilbert space $\mathcal{H}$ carries an essentially redundant complex degree of freedom, i.e. the overall complex phase associated with the wavefunction. Thus, we consider equivalence classes of wavefunctions, obtained by the identification

$$|\psi\rangle \sim \lambda|\psi\rangle \tag{2}$$

where $\lambda \in \mathbb{C} - \{0\}$. In other words, we consider the space of rays through the origin of $\mathcal{H}$. This is just the projective Hilbert space $\mathcal{P}$, endowed with the usual Fubini–Study metric defined by the transition probability [10]. By abuse of notation, we use the symbol $|\psi\rangle$ to denote both a point of $\mathcal{P}$, *and* its representative elements in $\mathcal{H}$. This should not cause confusion.

Given a Hilbert space and a Hamiltonian $\hat{H}$, we seek to determine the time required for a state $|\psi\rangle$ to be transformed, under unitary evolution, into another state $|\eta\rangle$ orthogonal to $|\psi\rangle$. More precisely, the problem addressed here can be stated as follows:

(a) Does there exist a time τ such that the state defined by

$$|\eta\rangle = \hat{U}(\tau)|\psi\rangle \tag{3}$$

is orthogonal to $|\psi\rangle$, that is, $\langle\psi|\eta\rangle = 0$, and,

(b) If so, what is the minimum value of τ?

Such a minimum time τ, if it exists, will be called the *passage time*, and denoted by τ_{P}. We shall show that, in fact, there exist infinitely many, although rather special, states $|\psi\rangle$ such that $\langle\psi|\eta\rangle = 0$ for a suitable choice of passage time τ_{P}, and that the value of τ_{P} for these states is typically given *exactly* by the expressions

$$\tau_{\mathrm{P}} = \frac{\pi\hbar}{\Delta E} = \frac{\pi\hbar}{2\Delta H} \tag{4}$$

where ΔE and ΔH are as defined below (note that the passage time in [1] is defined to be given by $\pi\hbar/2\Delta H$ for an arbitrary state, whereas our definition here is more refined because we impose orthogonality condition). There are also cases for which passage times exist but are larger than τ_{P} of (4). Explicit examples will be given. We also show, using the Anandan–Aharonov relation, that (4) actually provides the *sharpest obtainable bound* for the passage time.

2. Derivation of passage times

In order to verify (4), we first take note of the Hermitian correspondence between points and hyperplanes of codimension one in a projective Hilbert space $\mathcal{P}$ [11]. Specifically, given a point $|\psi\rangle \in \mathcal{P}$, the corresponding projective hyperplane consists of those points $|\xi\rangle$ satisfying the algebraic relation
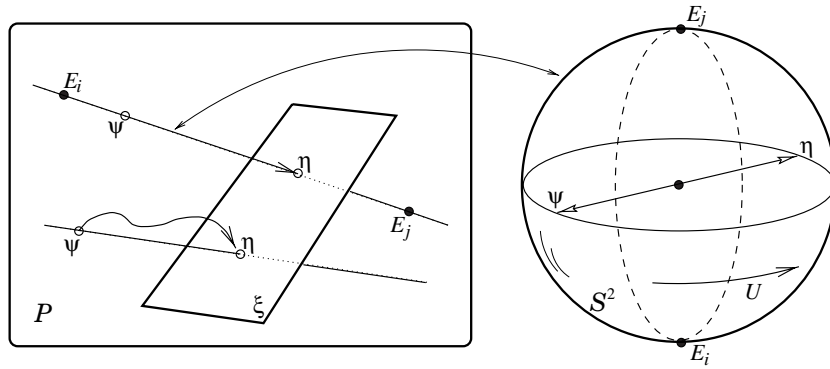
$$\langle\psi|\xi\rangle = 0. \tag{5}$$

Figure 1. Hermitian correspondence and projective line. The orthogonal complement of a state $|\psi\rangle \in \mathcal{P}$ is a hyperplane of codimension one such that for any element $|\xi\rangle$ on this plane we have $\langle\psi|\xi\rangle = 0$. If a state $|\psi\rangle$ is transformed into an orthogonal state $|\eta\rangle$, then $|\eta\rangle$ must lie on this plane. The join of $|\psi\rangle$ and $|\eta\rangle$ is a projective line, which in real terms is just a two-sphere S^2. If the transformation $|\psi\rangle \to |\eta\rangle$ along a geodesic curve on the projective line is obtained by the action of the unitary operators $\hat{U}(t)$, then there must be a pair of energy eigenstates $|E_i\rangle$ and $|E_j\rangle$ at the poles of the sphere, such that $|\psi\rangle$ and $|\eta\rangle$ lie on the equator, and the action of $\hat{U}(t)$ is merely a rigid rotation of the sphere with respect to these poles. Conversely, if the transformations $\hat{U}(t)$ carrying $|\psi\rangle$ into $|\eta\rangle$ do not describe a geodesic curve, then there does not exist any pair of energy eigenstates on the projective line joining $|\psi\rangle$ and $|\eta\rangle$.

Thus, if $|\psi\rangle$ is transformed by $\hat{U}(t)$ into a point $|\eta\rangle$ orthogonal to $|\psi\rangle$, then $|\eta\rangle$ must lie on this hyperplane, i.e. $\langle\psi|\eta\rangle = 0$. Assuming that such a pair $(|\psi\rangle, |\eta\rangle)$ of points exists, we can join the two points by a projective line $\mathcal{P}^1$; the points on this line represent the totality of normalized superpositions of the states $|\psi\rangle$ and $|\eta\rangle$. Since a complex projective line in real terms is just a two-sphere S^2, we can visualize this configuration as illustrated in figure 1. Note that the orthogonality of $|\psi\rangle$ and $|\eta\rangle$ implies that they are *antipodal* on S^2. Furthermore, the geodesics of the Fubini–Study metric that join the two points $|\psi\rangle$ and $|\eta\rangle$ are just the great circle arcs of the sphere S^2 that contain these points.

   Next, we observe that, *if there exists a unitary evolution transforming $|\psi\rangle$ into $|\eta\rangle$ along a geodesic curve, then there must be a pair of energy eigenstates, $|E_i\rangle$ and $|E_j\rangle$, say, at the poles of S^2, such that $|\psi\rangle$ and $|\eta\rangle$ lie on the equator*. This is because the dynamics induced by unitary evolution on any projective line joining a pair of energy eigenstates corresponds to a rigid rotation of the two-sphere S^2 in $\mathcal{P}$, with the said energy eigenstates as fixed points. Therefore, if we regard, conversely, the states $|\psi\rangle$ and $|\eta\rangle$ as forming a pair of poles on S^2, then the two energy eigenstates $|E_i\rangle$ and $|E_j\rangle$ will lie on the corresponding equator. In other words, we have, for some $\phi \in [0, 2\pi)$, the relations

$$\frac{1}{\sqrt{2}}(|\psi\rangle + \mathrm{e}^{\mathrm{i}\phi}|\eta\rangle) = |E_i\rangle \tag{6}$$

and

$$\frac{1}{\sqrt{2}}(|\psi\rangle - \mathrm{e}^{\mathrm{i}\phi}|\eta\rangle) = |E_j\rangle \tag{7}$$

since $|E_i\rangle$ and $|E_j\rangle$ are antipodal points of S^2. Applying the unitary operator $\hat{U}(\tau)$ to both sides of (6) and (7), we obtain

$$\frac{1}{\sqrt{2}}(\mathrm{e}^{\mathrm{i}\phi}|\psi\rangle + |\eta\rangle) = \mathrm{e}^{-\mathrm{i}E_i\tau/\hbar}|E_i\rangle \tag{8}$$

and

$$\frac{1}{\sqrt{2}}(-\mathrm{e}^{\mathrm{i}\phi}|\psi\rangle + |\eta\rangle) = \mathrm{e}^{-\mathrm{i}E_j\tau/\hbar}|E_j\rangle. \tag{9}$$

This follows from the fact that, by assumption, the unitary operator $\hat{U}(\tau)$ for a particular value of τ interchanges two states $|\psi\rangle$ and $|\eta\rangle$. Thus, forming the inner products of the respective right-hand and left-hand sides of (6) and (8), we find that

$$\tfrac{1}{2}(e^{i\phi} + e^{-i\phi}) = e^{-iE_i\tau/\hbar}. \tag{10}$$

Similarly, from (7) and (9) we obtain

$$-\tfrac{1}{2}(e^{i\phi} + e^{-i\phi}) = e^{-iE_j\tau/\hbar}. \tag{11}$$

Then, addition of equations (10) and (11) yields the condition

$$e^{-i(E_j-E_i)\tau/\hbar} = -1 \tag{12}$$

which is satisfied if we set

$$\tau = \frac{\pi\hbar k}{E_j - E_i} \qquad (k = 1, 3, 5, \ldots), \tag{13}$$

where we assume $E_j > E_i$. Choosing the smallest value for k and writing $\Delta E = E_j - E_i$ we thus obtain the minimum value τ_P of the passage time, given by

$$\tau_P = \frac{\pi\hbar}{\Delta E}. \tag{14}$$

To summarize, when $|\psi\rangle$ is transformed into an orthogonal state $|\eta\rangle$ by a one-parameter family of unitary transformations *along a geodesic curve*, then the time required is given *exactly* by (14). We have not yet considered the possibility that $|\psi\rangle$ unitarily evolves into $|\eta\rangle$ along another curve. If an alternative path exists, then the length of the trajectory is necessarily longer, since any such path will not be a geodesic. If $|\psi\rangle$ is expressible as a superposition of $|E_i\rangle$ and $|E_j\rangle$, then the trajectory of $\hat{U}(t)|\psi\rangle$ never leaves the projective line that joins these two states, and hence there does not exist any alternative path. The case in which $|\psi\rangle$ is expressed as a superposition of more than two energy eigenstates will be discussed below.

We note, incidentally, that an alternative bound on passage time was proposed by Margolus and Levitin [4], who *argued* that a sharper bound for τ_P exists and is given by the expression

$$\tau_{\text{ML}} \geqslant \frac{\pi\hbar}{2E} \tag{15}$$

where $E = \langle \hat{H} \rangle$ is the expectation value of the Hamiltonian in the state $|\psi\rangle$. However, this inequality is in general not physically viable, and it is in fact never sharper than the right-hand side of (14). This is because the physical characteristics of quantum systems are invariant under an overall shift of the energy spectrum, and hence without loss of generality we may set, for example, $E = 0$ or $E < 0$, and (15) becomes meaningless. To avoid this problem, Margolus and Levitin fix the energy scale so that $E_l \geqslant 0$ for all $l = 1, 2, \ldots, n$. Only then does the inequality (15) become technically valid. However, this bound, when $2E \geqslant \Delta E$, is never attained except in one special case where $E_i = 0$, so that $\Delta E = E_j$ and $2E = E_j$.

3. Fleming's bound

We now consider how the passage time τ_P obtained in (14) is related to the dispersion $\Delta H^2 = \langle (\hat{H} - \langle \hat{H} \rangle)^2 \rangle$ of the energy. This is of interest, because a previously derived bound on the passage time is expressed in terms of the energy dispersion [9]. In the present situation, we can compute ΔH explicitly, because the state is expressible in the form

$$|\psi\rangle = \tfrac{1}{\sqrt{2}}(|E_i\rangle + e^{i\varphi}|E_j\rangle) \tag{16}$$

for some $\varphi \in [0, 2\pi)$. By a direct calculation, the energy dispersion in the state (16) is

$$\Delta H^2 = \tfrac{1}{4}(E_j - E_i)^2 \tag{17}$$

from which we obtain Fleming's bound

$$\tau_{\mathrm{P}} = \frac{\pi\hbar}{2\Delta H} \tag{18}$$

as indicated in [1].

This relation is indeed natural if we recall the Anandan–Aharonov relation [12] which states that the 'speed' of the evolution of a given quantum state is given by $2\hbar^{-1}\Delta H$. The Fubini–Study distance between a pair of orthogonal states is given by π, and this distance divided by the velocity determines the required time. Since the velocity $2\hbar^{-1}\Delta H$ of the quantum state is a constant under the action of the unitary group, while the minimum distance of the trajectory joining a pair of orthogonal states is always π, it follows that the Fleming bound can be derived directly from the Anandan–Aharonov relation. We note that a similar line of idea has been applied in search of optimal quantum algorithms [5].

We have considered thus so far the case in which the state $|\psi\rangle$ is expressible as a superposition of two energy eigenstates. Next, suppose that $|\psi\rangle$ is expressed as a superposition of more than two energy eigenstates. It is not difficult to see that, in this case, if $|\psi\rangle$ can be transformed into an orthogonal state by a unitary operator $\hat{U}(t)$, then the energy spectrum $\{E_l\}$ must fulfil rather stringent constraints. Thus, such a transformation can occur only for rather special states, in systems such that the energy spectrum $\{E_j\}$ has a particularly simple structure. In other words, a generic state in this case will not evolve into an orthogonal state under the action of $\hat{U}(t)$. It is, nevertheless, of some interest to analyse such examples in order to gain further insight into the phenomena involved.

Let us consider, for simplicity, a state $|\psi\rangle$ that is expressed as a superposition of three energy eigenstates. The most general form of such a state can be expressed as

$$|\psi\rangle = \cos\alpha|E_i\rangle + \sin\alpha\cos\beta\,\mathrm{e}^{\mathrm{i}\phi}|E_j\rangle + \sin\alpha\sin\beta\,\mathrm{e}^{\mathrm{i}\varphi}|E_k\rangle \tag{19}$$

where α, β are angular coordinates, ϕ, φ are phase variables, and we assume that $E_i < E_j < E_k$. If $\hat{U}(T)$ transforms this state into an orthogonal state, then the condition

$$\cos^2\alpha + \sin^2\alpha\cos^2\beta\,\mathrm{e}^{-\mathrm{i}\omega_{ji}T/\hbar} + \sin^2\alpha\sin^2\beta\,\mathrm{e}^{-\mathrm{i}\omega_{ki}T/\hbar} = 0 \tag{20}$$

must be satisfied, where $\omega_{ji} = E_j - E_i$ and so on. To render the analysis more tractible, we further simplify this constraint by assuming that $\alpha = \beta = \pi/4$. Then, (20) implies that a necessary condition for the state $|\psi\rangle$ to evolve into an orthogonal state is given by the relation

$$\frac{\omega_{ki}}{\omega_{ji}} = \frac{2m-1}{2n-1} \tag{21}$$

where m, n are natural numbers such that $m \neq n$. Because the spectrum of a generic Hamiltonian $\hat{H}$ will not satisfy (21), a state $|\psi\rangle$ will never evolve into a state orthogonal to $|\psi\rangle$. The constraint becomes even more severe if $|\psi\rangle$ is expressed as a superposition of more than three eigenstates. The precise form of the constraint in such cases is just a straightforward generalization of (20).

Notwithstanding these conditions, let us suppose that the constraint (21) is indeed satisfied for some given Hamiltonian. Then, the state indeed evolves into an orthogonal state. The first time that $|\psi\rangle$ becomes orthogonal to $|\psi\rangle$, in particular, is given by

$$T = \frac{\pi\hbar}{\omega_{ji}} = \frac{3\pi\hbar}{\omega_{ki}}. \tag{22}$$

However, *since in this case $\hat{U}(t)|\psi\rangle$ does not describe a geodesic path, T will be larger than Fleming's passage time τ_P given in* (18). Indeed, without loss of generality, we may set $E_i = 0$. Then, it is straightforward to verify that $T = \sqrt{6}\tau_P$. This follows from the fact that, under the constraint $\omega_{ki} = 3\omega_{ji}$ that follows from (21), the squared energy dispersion in the state (19) is given by $\Delta H^2 = \frac{3}{2}\omega_{ji}^2$.

Another simple example is the cyclic evolution of a spin-1 system, with energy eigenvalues -1, 0 and +1. Consider a state

$$|\psi\rangle = \tfrac{1}{2}|-\rangle + \tfrac{1}{\sqrt{2}}|0\rangle + \tfrac{1}{2}|+\rangle. \tag{23}$$

The application of $\hat{U}(\pi\hbar)$ yields

$$|\eta\rangle = -\tfrac{1}{2}|-\rangle + \tfrac{1}{\sqrt{2}}|0\rangle - \tfrac{1}{2}|+\rangle \tag{24}$$

and we have $\langle\psi|\eta\rangle = 0$. Likewise, the action of $\hat{U}(\pi\hbar)$ on $|\eta\rangle$ yields $|\psi\rangle$, hence, we have a cyclic evolution that interchanges a pair of orthogonal states $|\psi\rangle$ and $|\eta\rangle$. However, because the trajectory $\hat{U}(t)|\psi\rangle$ in $\mathcal{P}$ does not correspond to a geodesic curve, the time required to interchange these states, given by $T = \pi\hbar$, is longer than the Fleming bound. Indeed, we have $T = \sqrt{2}\tau_P$ in this example, because in the state (23) we have $\langle H^2 \rangle = \frac{1}{2}$ and $\langle H \rangle = 0$ so that $\Delta H^2 = \frac{1}{2}$. In general, if a quantum state expressible in the form other than (16) does evolve into an orthogonal state, then the passage time is necessarily longer than Fleming's bound (18).

4. Mixed initial states

The foregoing analysis can be extended in a natural way to the case in which the initial state of the system is impure. The situation considered here can be described as follows. Suppose that we have an initial state, known to be either $|\psi_1\rangle$, with probability p, or $|\psi_2\rangle$, with probability $1 - p$, where both of these pure states are of the form (16). In other words, the initial state is a mixed-state density matrix

$$\hat{\rho} = p|\psi_1\rangle\langle\psi_1| + (1 - p)|\psi_2\rangle\langle\psi_2|. \tag{25}$$

This density matrix evolves in accordance with the Heisenberg law

$$\hat{\rho}(t) = \hat{U}^{\dagger}(t)\hat{\rho}\hat{U}(t). \tag{26}$$

Our objective in the present context is to examine the possibility that, after some lapse of time τ_P, the initial pure state $|\psi_i\rangle$ evolves *with certainty* into a state orthogonal to $|\psi_i\rangle$, irrespective of whether $i = 1$ or $i = 2$.

If the state $|\psi_1\rangle$ is a superposition of energy eigenstates $|E_i\rangle$ and $|E_j\rangle$, and if $|\psi_2\rangle$ is a superposition of $|E_k\rangle$ and $|E_l\rangle$, then the passage time for $|\psi_1\rangle$ is just $\pi\hbar/\omega_{ji}$, and similarly, for $|\psi_2\rangle$, is just $\pi\hbar/\omega_{lk}$. Therefore, if the initial state evolves with certainty into an orthogonal state, then the required passage time is given by

$$\tau_P = \pi\hbar \times \mathrm{LCM}\!\left(\omega_{ji}^{-1}, \omega_{lk}^{-1}\right) \tag{27}$$

where $\mathrm{LCM}(x, y)$ denotes the least common multiple of x and y. In other words, since we are uncertain about the initial state, we must, in general, wait considerably longer before we can be sure that the state is in another state orthogonal to the initial state, even though in the meantime the state may evolve into an orthogonal state and then return to itself many times. It is straightforward to generalize this argument to the case where the initial state is one of many states of the form (16). In this case, the passage time is simply given by $\pi\hbar$ times the least common multiple of the inverses of the energy differences.

Note that, even though each possible pure state will be transformed into an orthogonal state after the system has evolved for the time τ_P given in (27), one cannot clearly argue that the density matrix $\hat{\rho}(\tau_P)$ has evolved into another mixed state orthogonal to $\hat{\rho}(0)$. Indeed, the diagonal elements of $\hat{\rho}(0)$ and $\hat{\rho}(\tau_P)$, when expressed in the energy basis, are identical, and therefore the expectation values of any observable commuting with the Hamiltonian will also be identical. This observation leads to an interesting open problem, namely, can the orthogonality of impure density matrices be defined in a meaningful fashion, and if so, does a passage time exist for mixed-state density matrices with respect to this definition.

Acknowledgments

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