Fundamental Limit on the Rate of Quantum Dynamics: The Unified Bound Is Tight

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How fast a quantum state can evolve has attracted considerable attention in connection with quantum measurement and information processing. A lower bound on the orthogonalization time, based on the energy spread ΔE, was found by Mandelstam and Tamm. Another bound, based on the average energy E, was established by Margolus and Levitin. The bounds coincide and can be attained by certain initial states if $\Delta E = E$. Yet, the problem remained open when $\Delta E \neq E$. We consider the unified bound that involves both ΔE and E. We prove that there exist no initial states that saturate the bound if $\Delta E \neq E$. However, the bound remains tight: for any values of ΔE and E, there exists a one-parameter family of initial states that can approach the bound arbitrarily close when the parameter approaches its limit. These results establish the fundamental limit of the operation rate of any information processing system.

After the classical result of Mandelstam and Tamm [1], it was shown by Fleming [2], Anandan and Aharonov [3], and Vaidman [4] that the minimum time τ required for arriving to an orthogonal state is bounded by

$$\tau \geq h/4\Delta E, \qquad (1)$$

where $(\Delta E)^2 = \langle \psi | H^2 | \psi \rangle - (\langle \psi | H | \psi \rangle)^2$, H is the Hamiltonian, and $|\psi\rangle$ the wave function of the system. A different bound was obtained in [5], namely,

$$\tau \geq h/4E. \qquad (2)$$

Here, $E = \langle \psi | H | \psi \rangle$ is the quantum-mechanical average energy of the system (the energy of the ground state is taken to be zero). Both bounds (1) and (2) are tight, and achieved for a quantum state such that $\Delta E = E$.

Since then, a vast literature has been devoted to various aspects of this problem. In particular, inequality (2) has been proved for mixed states and for composite systems both in separable and in entangled states (e.g., Giovannetti *et al.* [6,7], Zander *et al.* [8]). Bound (2) obtained for an isolated system has been generalized to a system driven by an external Hamiltonian (a "quantum gate") in [9,10]. Various derivations of (1) and (2) (e.g., [11–13]), bounds based on energy-distribution moments [14], more general problems of time-optimal quantum evolution [12,15–23], and the ultimate limits of computation [24,25] have been considered.

However, what remained unnoticed is the paradoxical situation of the existence of two bounds based on two different characteristics of the quantum state, seemingly independent of one another. Since the average energy E and the energy uncertainty ΔE play the most determinative role in quantum evolution, it is important to have a unified bound that would take into account both of these characteristics.

In all known cases where bounds (1) and (2) can be exactly attained, the ratio $\alpha = \frac{\Delta E}{E}$ equals 1. A question arises: what happens if $\alpha \neq 1$? Some authors just assumed

without justification that the minimum orthogonalization time is

$$\tau_{\min} = \max\left(\frac{h}{4E}, \frac{h}{4\Delta E}\right) = \frac{h}{2(E + \Delta E - |E - \Delta E|)}. \qquad (3)$$

In fact, the situation is not so simple. Bound (3), indeed, can only be achieved for $\alpha = 1$. However, this bound remains tight when $\alpha \neq 1$ as well, though in this case it is only asymptotically attainable.

Theorem 1.—Under the assumption that the smallest (ground) energy of a quantum system is zero,

(i) Bound (1) is attained only by the two-level state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\psi_0\rangle + |\psi_1\rangle), \qquad (4)$$

where $H|\psi_k\rangle = kE_1|\psi_k\rangle$ and $k = 0, 1$.

(ii) The only state that attains bound (2) is likewise (4).

State (4) is unique up to degeneracy of the energy level E_1 and arbitrary phase factors for $|\psi_0\rangle$ and $|\psi_1\rangle$.

To prove statement (i) we shall use the trigonometric inequality

$$\cos x \geq 1 - \frac{4}{\pi^2} x \sin x - \frac{2}{\pi^2} x^2, \qquad (5)$$

which is valid for any real x. Note that (5) turns into an equality iff $x = 0$ or $x = \pm\pi$. Let the initial state be $|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n |E_n\rangle$, where the $|E_n\rangle$ are energy eigenstates of the system and $\sum_{n=0}^{\infty} |c_n|^2 = 1$. Then

$$|S(t)|^2 = |\langle \psi(0) | \psi(t)\rangle|^2$$

$$= \sum_{n,n'=0}^{\infty} |c_n|^2 |c_{n'}|^2 e^{-i(E_n - E_{n'})t/\hbar}$$

$$= \sum_{n,n'=0}^{\infty} |c_n|^2 |c_{n'}|^2 \cos\frac{E_n - E_{n'}}{\hbar/t}. \qquad (6)$$

Using inequality (5), we obtain

$$|S(t)|^2 \geq 1 - \frac{4}{\pi^2} \sum_{n,n'=0}^{\infty} |c_n|^2 |c_{n'}|^2 \frac{E_n - E_{n'}}{\hbar/t} \sin\frac{E_n - E_{n'}}{\hbar/t}$$

$$- \frac{2}{\pi^2} \sum_{n,n'=0}^{\infty} |c_n|^2 |c_{n'}|^2 \left(\frac{E_n - E_{n'}}{\hbar/t}\right)^2$$

$$= 1 + \frac{4t}{\pi^2} \frac{d|S(t)|^2}{dt} - \frac{1}{\pi^2}\left(\frac{\Delta E}{\hbar/2t}\right)^2. \tag{7}$$

Since $|S(t)|^2 \geq 0$, it follows that $\frac{d|S(t)|^2}{dt} = 0$ whenever $S(t) = 0$. Thus, at a time τ such that $S(\tau) = 0$, the second term in (7) vanishes, and we obtain

$$0 \geq 1 - \frac{4\tau^2}{\pi^2 \hbar^2}(\Delta E)^2, \tag{8}$$

which yields inequality (1); this is just another way to derive that bound. Yet, for (8) to turn into an equality it is necessary that inequality (5) turn into an equality for every term of the double summation (6). Hence, either $x_{nn'} = \frac{E_n - E_{n'}}{\hbar/\tau} = 0$ or $x_{nn'} = \frac{E_n - E_{n'}}{\hbar/\tau} = \pm\pi$ for all n, n' such that $c_n \neq 0$, $c_{n'} \neq 0$. It follows that, to attain bound (1), $|\psi(0)\rangle$ must be a superposition of only two energy eigenstates with energies $E_0 = 0$ and E_1.

To prove statement (ii), we repeat briefly the derivation given in [5]. This time we use the trigonometric inequality

$$\cos x \geq 1 - \frac{2}{\pi}(x + \sin x), \tag{9}$$

valid for all $x \geq 0$. Again, (9) turns into an inequality only for $x = 0$ or $x = \pi$. Then

$$\mathrm{Re}\, S(t) = \sum_{n=0}^{\infty} |c_n|^2 \cos\frac{E_n t}{\hbar}$$

$$\geq \sum_{n=0}^{\infty} |c_n|^2 \left[1 - \frac{2}{\pi}\left(\frac{E_n t}{\hbar} + \sin\frac{E_n t}{\hbar}\right)\right]$$

$$= 1 - \frac{2Et}{\pi\hbar} + \frac{2}{\pi} \mathrm{Im}\, S(t). \tag{10}$$

At time τ, $\mathrm{Re}\, S(\tau) = \mathrm{Im}\, S(\tau) = 0$. Hence $0 \geq 1 - \frac{2Et}{\pi\hbar}$, which results in bound (2). However, to actually attain this bound, inequality (9) must become an equality for every term of the sum (10); that is, for any n, either $x_n = \frac{E_n t}{\hbar} = 0$ or $x_n = \frac{E_n t}{\hbar} = \pi$. This is possible iff $|\psi(0)\rangle$ has the form (4).

Let us show now that no mixed state can attain bound (3). Consider an initial mixed state density matrix $\rho(0)$ with spectral decomposition

$$\rho(0) = \sum_i \lambda_i |\psi^{(i)}(0)\rangle\langle\psi^{(i)}(0)|, \tag{11}$$

where $\lambda_i > 0$, $\sum_i \lambda_i = 1$, and $\langle\psi^{(i)}(0)|\psi^{(j)}(0)\rangle = \delta_{ij}$. At time t, the density matrix becomes

$$\rho(t) = \sum_i \lambda_i |\psi^{(i)}(t)\rangle\langle\psi^{(i)}(t)|.$$

Hence, if τ is the orthogonalization time, then

$$\mathrm{Tr}[\rho(0)\rho(\tau)] = \sum_i \sum_j \lambda_i \lambda_j |\langle\psi^{(i)}(0)|\psi^{(j)}(\tau)\rangle|^2 = 0. \tag{12}$$

Note that all terms in the above sum are non-negative, and therefore all of them must be zero to satisfy (12). As shown above, terms $\langle\psi^{(i)}(0)|\psi^{(i)}(\tau)\rangle = 0$, for τ given by (3), iff each $|\psi^{(i)}(0)\rangle$ has the form (4). Consider two functions from spectral decomposition (11),

$$|\psi^{(i)}(0)\rangle = \frac{1}{\sqrt{2}}(|\psi_0\rangle + |\psi_1^{(i)}(0)\rangle) \quad \text{and}$$

$$|\psi^{(j)}(0)\rangle = \frac{1}{\sqrt{2}}(|\psi_0\rangle + a|\psi_1^{(i)}(0)\rangle + b|\psi_1^{(j)}(0)\rangle), \tag{13}$$

where $\langle\psi^{(i)}(0)|\psi^{(j)}(0)\rangle = 0$ and $|a|^2 + |b|^2 = 1$ (the zero-energy state is nondegenerate). Since $\langle\psi^{(i)}(0)|\psi^{(j)}(0)\rangle = \frac{1}{2}(\langle\psi_0|\psi_0\rangle + a\langle\psi_1^{(i)}(0)|\psi_1^{(i)}(0)\rangle) = 0$, it follows that $a = -1$ and $|\psi^{(j)}(0)\rangle = \frac{1}{\sqrt{2}}(|\psi(0)\rangle - |\psi_1^{(i)}(0)\rangle)$. But then $\langle\psi^{(i)}(0)|\psi^{(j)}(\tau)\rangle = \frac{1}{2}(\langle\psi_0|\psi_0\rangle - \langle\psi_1^{(i)}(0)|\psi_1^{(i)}(\tau)\rangle) = \frac{1}{2} \neq 0$. Hence, equality (12) is not satisfied for τ given by (3). Thus, this bound is not attainable by a mixed state.

For pure states, results of theorem 1 also follow from the analyses presented in [11,14].

Theorem 1 shows that bounds (1) and (2) can only be attained by a state for which $\alpha = \frac{\Delta E}{E} = 1$. It follows from that theorem that there exists no initial state $|\psi(0)\rangle$ with $\alpha \neq 1$ that would attain bound (3); i.e., no state can evolve into an orthogonal state in the minimum time given by (1) or (2). The question to be answered is how close it is possible to approach the unified bound (3). Let us rewrite (3) in a different form,

$$\tau_{\min} = \max\left(\frac{h}{4E}, \frac{h}{4\Delta E}\right) = \frac{h(1 + e^{|\ln\alpha|})}{4E(1 + \alpha)}. \tag{14}$$

Theorem 2.—For any $\alpha \neq 1$ and any $\varepsilon > 0$, there exists a state $|\psi(0)\rangle$ such that $\langle\psi(0)|\psi(\tau)\rangle = 0$ at time

$$\tau \leq \frac{h(1 + e^{|\ln\alpha|})}{4E(1 + \alpha)}(1 + \varepsilon). \tag{15}$$

We will show that in both cases, $\alpha < 1$ and $\alpha > 1$, there exist families of initial states that approach limit (14) arbitrarily close.

(1) Let $\alpha < 1$. Consider a family of states

$$|\psi(0)\rangle = c_0|0\rangle + c_1|E_1\rangle + c_2|E_2\rangle. \tag{16}$$

Denote $|c_i|^2 = p_i$, and introduce dimensionless variables

$$x_i(t) = 2\pi E_i \frac{t}{h}, \qquad i = 0, 1, 2 \tag{17}$$

(the rotation angles of the state vectors $|E_i\rangle$). Then $S(\tau) = \langle\psi(0)|\psi(\tau)\rangle = 0$ iff $x_i(\tau) = x_i$ such that

$$p_1 \sin x_1 + p_2 \sin x_2 = 0, \qquad p_0 + p_1 \cos x_1 + p_2 \cos x_2 = 0,$$

$$\text{where} \quad p_0 + p_1 + p_2 = 1. \tag{18}$$

Let $0 < p_0 \ll 1$ be a parameter of the family of states (16) (one cannot set $p_0 = 0$, since that would change the

ground energy level). When p_0 is small, the values of x_1 and x_2 differ almost exactly by π. Let $x_2 = \pi + x_1 - \delta \sin x_1$, with $\delta \ll 1$. Then, from (18),

$$p_1 = \frac{1}{2} - \frac{\delta}{4}(1 + \cos x_1) + O(\delta^2),$$

$$p_2 = \frac{1}{2} - \frac{\delta}{4}(1 - \cos x_1) + O(\delta^2), \qquad p_0 = \frac{\delta}{2} + O(\delta^2). \tag{19}$$

Using (19), we can calculate the average value $\langle x \rangle = \frac{2\pi\tau}{h}E$, namely,

$$\langle x \rangle = p_1 x_1 + p_2 x_2$$
$$= \frac{\pi}{2} + x_1 - \frac{\delta}{4}[2x_1 - 2\sin x_1 + \pi(1 - \cos x_1)]$$
$$+ O(\delta^2). \tag{20}$$

The standard deviation $\Delta x = \frac{2\pi\tau}{h}\Delta E$ is obtained as

$$\Delta x = \sqrt{p_1 x_1^2 + p_2 x_2^2 - (p_1 x_1 + p_2 x_2)^2}$$
$$= \frac{\pi}{2} + \frac{\delta}{2\pi}[x_1(\pi + x_1) - \pi\sin x_1] + O(\delta^2). \tag{21}$$

On the other hand, $\alpha = \frac{\Delta E}{E} = \frac{\Delta x}{\langle x \rangle} = \frac{\pi}{\pi + 2x_1} + O(\delta)$; hence

$$x_1 = \frac{\pi}{2}\left(\frac{1}{\alpha} - 1\right) + O(\delta). \tag{22}$$

Substituting (22) into (21) and taking into account the last expression from (19) yields

$$\Delta x = \frac{\pi}{2} + p_0\left[\frac{\pi}{4}\left(\frac{1}{\alpha^2} - 1\right) - \sin\frac{\pi}{2}\left(\frac{1}{\alpha} - 1\right)\right] + O(p_0^2), \tag{23}$$

which results in

$$\tau = \frac{h\Delta x}{2\pi\Delta E}$$
$$= \frac{h}{4\Delta E}\left[1 + \frac{p_0}{2}\left(\frac{1}{\alpha^2} - 1 - \frac{4}{\pi}\sin 2\pi\left(\frac{1}{\alpha} - 1\right)\right) + O(p_0^2)\right]. \tag{24}$$

Finally, choosing

$$p_0 < 2\varepsilon\left[\frac{1}{\alpha^2} - 1 - \frac{2}{\pi}\sin\frac{\pi}{2}\left(\frac{1}{\alpha} - 1\right)\right]^{-1},$$

we obtain

$$h/4\Delta E < \tau \le h(1 + \varepsilon)/4\Delta E. \tag{25}$$

(2) Let $\alpha > 1$. Consider a family of states

$$|\psi(0)\rangle = c_0|0\rangle + c_1|E_1\rangle + c_{2k+1}|E_{2k+1}\rangle, \tag{26}$$

where

$$k = 1, 2, \ldots; \qquad E_{2k+1} = (2k + 1)E_1;$$

$$|c_0|^2 = p_0 = \frac{1}{2}; \qquad |c_1|^2 = p_1 = \frac{1}{2}\left(1 - \frac{\beta}{k^2}\right); \tag{27}$$

$$|c_{2k+1}|^2 = p_{2k+1} = \frac{\beta}{2k^2}.$$

Using the dimensionless variables (17), it is readily seen from (26) and (27) that $S(\tau) = 0$ at the least time τ for which $x_1(\tau) = x_1 = \frac{2\pi\tau}{h}E_1 = \pi$ and $x_{2k+1} = \frac{2\pi\tau}{h} \times (2k + 1)E_1 = \pi(2k + 1)$.

Then $\langle x \rangle = p_1 x_1 + p_{2k+1}x_{2k+1} = \frac{\pi}{2}(1 + \frac{2\beta}{k})$ and

$$\Delta x = \sqrt{p_1 x_1^2 + p_{2k+1}x_{2k+1}^2 - (p_1 x_1 + p_{2k+1}x_{2k+1})^2}$$
$$= \frac{\pi}{2}\left(1 + 4\beta + \frac{2\beta}{k}\right) + O\left(\frac{1}{k^2}\right). \tag{28}$$

Hence, $\alpha = \frac{\Delta x}{\langle x \rangle} = 1 + 4\beta + O(\frac{1}{k})$ and

$$\beta = \frac{\alpha - 1}{4} + O\left(\frac{1}{k}\right). \tag{29}$$

Since $\langle x \rangle = \frac{2\pi\tau}{h}E$, it follows from (28) and (29) that

$$\tau = \frac{h}{4E}\left[1 + \frac{\alpha - 1}{2k} + O\left(\frac{1}{k^2}\right)\right]. \tag{30}$$

Thus, choosing $k > \frac{\alpha-1}{2\varepsilon}$ guarantees that

$$\frac{h}{4E} < \tau \le \frac{h}{4E}(1 + \varepsilon). \tag{31}$$

∎

As graphically illustrated in Fig. 1, Theorem 2 means that there are families of states that approach equality in (3) for a given value of α, in the limit as a certain parameter approaches zero (for $\alpha < 1$) or infinity (for $\alpha > 1$), but no state yields a strict equality in (3) for $\alpha \ne 1$. It turns out that bound (1) is tight whenever $\alpha = \frac{\Delta E}{E} \le 1$, while (2) is tight whenever $\alpha \ge 1$.

Another interesting question is the relationship between the maximum energy eigenvalue E_{max} that contributes to $|\psi(0)\rangle$, the orthogonalization time, τ, and the average energy E. Note that determining the minimum τ for a given E is equivalent to determining the minimum E for a given τ. The next theorem provides simple but useful results.

Theorem 3.—Let τ be the minimum time such that $S(\tau) = \langle\psi(0)|\psi(\tau)\rangle = 0$. Then there exist a state $|\psi(0)\rangle$ and a set of energy eigenvalues $\{E_n\}$ of all energy eigenfunctions that contribute to $|\psi_0\rangle$ such that
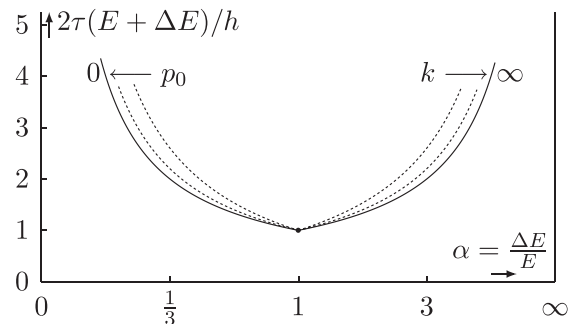

FIG. 1. The solid line shows bound (14); the dotted lines—parametrized, respectively, by $p_0 \to 0$ and $k \to \infty$—show successive approximations to this bound, corresponding to initial states from families (16) and (26).

$$E_{max} < h/\tau \qquad (32)$$

and

$$E_{max}/4 \leq E \leq E_{max}/2. \qquad (33)$$

$$\text{Let} \quad S(\tau) = \sum_{n=0}^{\infty} |c_n|^2 e^{-2\pi i E_n \tau/h} = 0. \qquad (34)$$

Suppose $E_k \geq \frac{h}{\tau}$. Then $E'_k = E_k - \frac{h}{\tau} \geq 0$ and $e^{-2\pi i E_k \tau/h} = e^{-2\pi i E'_k \tau/h}$. Hence, replacing E_k by E'_k in (34) will not affect the equality. Thus, the same orthogonalization time τ can be achieved with smaller average energy $E' = E - |c_k|^2 h/\tau$. This proves inequality (32).

Now, let E_{max} be the largest energy of the energy eigenfunctions that contribute to $|\psi(0)\rangle$, and let the average energy be $E^{(1)}$. Obviously, the validity of (34) will not be affected if we replace all energy levels E_n by $E_{max} - E_n$. Then the average energy will become $E^{(2)} = E_{max} - E^{(1)}$. Since E can be chosen as $\min(E^{(1)}, E^{(2)})$, this proves that $E \leq E_{max}/2$. Also, substituting (2) into (32) yields $E_{max}/4 \leq E$. Thus, (33) is proved. ∎

Theorem 3 allows us to restrict our attention to states that satisfy (32) and (33) for further analysis of the orthogonalization time τ.

Theorem 4.—Let E_{max} be the maximum energy of all energy eigenfunctions that contribute to $|\psi(0)\rangle$. Then the minimum orthogonalization time τ obeys the inequality

$$\tau \geq h/2E_{max}, \qquad (35)$$

and equality is attained iff $|\psi(0)\rangle$ has the form (4) with $E_1 = E_{max}$.

$$\text{Let} \quad S(\tau) = \langle \psi(0)|\psi(\tau)\rangle = \sum_{n=0}^{m} |c_n|^2 e^{-2\pi i E_n/h} = 0,$$
$$\qquad (36)$$

where $E_m = E_{max}$. Then, if $\tau < \frac{h}{2E_{max}}$, all terms in the above sum except the zeroth have strictly positive imaginary parts—which violates equality (36). Similarly, if $\tau = \frac{h}{2E_{max}}$, then (36) is satisfied iff $|\psi(0)\rangle$ is of form (4) with $E_1 = E_{max}$. ∎

The equality case in (35) had been considered in [13].

Some authors (e.g., [13]) prefer to write expressions (2) and (35) as $\tau \geq h/4(E - E_0)$ and $\tau \geq h/2(E_{max} - E_0)$, arguing that a constant shift of the energy spectrum affects only the overall time-dependent phase of the wave function. In our opinion, however, it is just this "freedom of shift" that allows one to set to zero the energy of the ground state even if the smallest eigenvalue of the Hamiltonian is not zero (just as in the hydrogen atom).

Let us summarize the Letter's main results. The unified bound (14) can be saturated exactly only if $\alpha = \Delta E/E = 1$. However, the bound remains tight for all values of ΔE

and E. Namely, if for any $\varepsilon > 0$ there exist a state $|\psi(0)\rangle$ such that $\frac{h}{4\Delta E} < \tau \leq \frac{h}{4\Delta E}(1 + \varepsilon)$; if $\alpha > 1$, there exists a $|\psi(0)\rangle$ such that $\frac{h}{4E} < \tau \leq \frac{h}{4E}(1 + \varepsilon)$. A transition from a state to an orthogonal one can be taken as the elementary step of a computational process [26]. Therefore, the number of orthogonal states visited by the system per unit time can be viewed as the maximum rate of operation. Thus our results establish the fundamental quantum limit of the operation rate of any information processing system.

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