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A unifying quantum speed limit for time-independent Hamiltonian evolution

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Abstract

Quantum speed limit (QSL) is the study of fundamental limits on the evolution time of quantum systems. For instance, under the action of a time-independent Hamiltonian, the evolution time between an initial and a final quantum state obeys various mutually complementary lower bounds. They include the Mandelstam–Tamm (MT) bound, the Margolus–Levitin (ML) bound, the Luo–Zhang bound, the Lee–Chau (LC) bound together with the dual ML bound introduced by Ness and coworkers. Here we show that the MT bound can be obtained by optimizing the LC bound over a certain parameter. More importantly, we report a QSL that includes all the above bounds as special cases before optimizing over the physically meaningless reference energy level of a quantum system. This unifying bound depends on a certain parameter p. For any fixed p, we find all pairs of time-independent Hamiltonian and initial pure quantum state that saturate this unifying bound. More importantly, these pairs allow us to compute this bound accurately and efficiently using an oracle that returns certain pth moments related to the absolute value of energy of the quantum state. Moreover, this oracle can be simulated by a computationally efficient and accurate algorithm for finite-dimensional quantum systems as well as for certain infinite-dimensional quantum states with bounded and continuous energy spectra. This makes our computational method feasible in a lot of practical situations. We further compare the performance of this bound for the case of a fixed p as well as the case of optimizing over p with existing QSLs. We find that if the dimension of the underlying Hilbert space is $\lesssim$2000, our unifying bound optimized over p can be computed accurately in a few minutes

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using Mathematica code with just-in-time compilation in a typical desktop. Besides, this optimized unifying QSL is at least as good as all the existing ones combined and can occasionally be a few percent to a few times better.

Keywords: quantum speed limit, numerical stability, time-independent Hamiltonian evolution, efficient algorithm

1. Introduction

Quantum speed limit (QSL) is the study of fundamental limits in quantum information processing speed [1]. The first and probably the most well-known QSL is the Mandelstam–Tamm (MT) bound. It says that the evolution time τ under the action of a time-independent Hamiltonian obeys the inequality

$$\frac{\tau}{\hbar} \geqslant \frac{\cos^{-1}\left(\sqrt{\epsilon}\right)}{\Delta E}, \tag{1}$$

where ϵ is the fidelity between the initial and final quantum state and ΔE is the energy standard deviation of the quantum state [2]. Actually, the MT bound was discovered well before the quantum information era and the coinage of the term QSL. Moreover, it can be extended to cover the cases of evolution under a time-dependent Hamiltonian or open system dynamics [3].

A lot of QSL bounds have been discovered. A few are applicable to time-dependent Hamiltonians as well as open systems. Relations with quantum control, entanglement, resource theory as well as the so-called time-fractional Schrödinger equation have also been explored [4–12]. Recently, a collection of articles on QSL and its applications was published in a special section of a journal [13]. In there, Takahashi considered not just lower bound but also upper bound on evolution time of quantum system [14]; also Aifer and Deffner relates QSL to energy efficient implementation of quantum gates [15]. Along a different line, Shanahan *et al* [16] as well as Okuyama and Ohzeki [17] found that there is a classical correspondence to certain QSL and concluded that QSL is a universal dynamical property of Hilbert space rather than a pure quantum phenomenon. In this paper, we go back to the basics by studying QSLs of time-independent Hamiltonians for closed systems. We make the following four major contributions in this study.

First, we report a QSL that we called the CZ bound for easy reference. This bound generalizes a number of existing QSLs for time-independent Hamiltonian evolution. They include the MT bound [2], the Margolus–Levitin (ML) bound [18–20], the Luo–Zhang (LZ) bound [21], the Lee–Chau (LC) bound [22] as well as the dual ML bound introduced by Ness *et al* [23]. Actually, the LZ, LC and CZ bounds are families of bounds each depending on a parameter p [21, 22]. In addition, for a given p, the LC bound is optimized over the physically meaningless reference energy level E_r of the quantum state [22]. And for the CZ bound, we will see that it is optimized over both E_r and another variable named θ. In this Paper, we prove that the CZ bound generalizes the MT, ML, dual ML, LZ and LC bounds in two steps. Because all but the MT bound have similar forms, our first step is to show that the CZ bound can be reduced to all but the MT bound above by fixing one or more of these three parameters to certain specific values instead of optimizing over them. Surprisingly, even though the forms of the ML, dual ML, LZ, LC and CZ bounds are very different from that of the MT bound, in our second step, we prove that the MT bound is in fact a result of the LC bound by optimizing over the parameter p.

Our second major contribution is to study the necessary and sufficient conditions for a pair of time-independent Hamiltonian and initial pure quantum state to saturate the CZ bound, and as a result explicitly write them down in a computationally usable form. This analysis can be extended to give the set of all time-independent Hamiltonian and initial pure state pairs that saturate the LC bound as well.

Our third contribution is a numerically efficient (that is, polynomial-time computable) and accurate (that is, numerically stable and rounding error is not serious) method to compute the CZ bound (and hence also the LC bound) under the assumption that there is an efficient and accurate method to evaluate the minimum pth moment of the absolute value of energy of the quantum state and the corresponding pth signed moment of the absolute value of energy of the state. This assumption is true for finite-dimensional quantum systems as well as certain infinite-dimensional systems with bounded and continuous energy spectra. Hence, the CZ bound is computationally feasible in almost all realistic situations. Interestingly, this method is closely related to the Hamiltonian and quantum state pairs that saturate the CZ bound.

Our last contribution is an extensive comparison of the evolution time lower bound and actual runtime between the CZ bound that is further optimized over the parameter p and other existing bounds. We discover that even when the dimension of the underlying Hilbert space is as large as 2048, this optimized CZ bound can be computed in a few minutes using Mathematica with just-in-time compilation installed in a typical desktop computer. Furthermore, the bound obtained can be a few percent to a few times better than the best existing one. In this regard, the CZ bound is the best choice in practice.

In what follows, we first state various QSLs that we are going to extend in section 2. We then report several auxiliary results in section 3. These results allow us to prove the CZ bound and to study the necessary and sufficient conditions for its saturation in section 4. In doing so, we find the set of all time-independent Hamiltonian and initial pure state pairs that saturate the CZ and the LC bounds, respectively. Also in section 4, we show that by optimizing over the parameter p, the LC bound is reduced to the MT bound. Besides, the CZ bound extends the ML, dual ML, LZ and LC bounds. Hence, the CZ bound unifies the MT, ML, dual ML, LC and LC bounds. Next, we report an accurate and efficient method to numerically compute the CZ as well as the LC bounds given an oracle returning the minimum pth moment of the absolute value of energy of the quantum state and the corresponding pth signed moment of the absolute value of energy of the state in section 5. We also show that this efficient oracle exists in the sense that it can be replaced by an efficient and accurate algorithm for finite-dimensional as well as certain infinite-dimensional systems. As a byproduct, we report there a simple expression for the CZ bound for two-dimensional quantum systems. Using the numerical method developed in section 5, we compare the performance of the CZ bound optimized over the parameter p with existing ones in practice in section 6. Finally, we summarize our findings in section 7.

2. Prior art

Here we list some of the most important QSL bounds for quantum state evolution under time-independent Hamiltonian discovered so far. Collectively, they are the most powerful QSLs for time-independent Hamiltonian evolution among those based on a single parameter describing the energy of the initial quantum state.

- The MT bound [2] is given by Inequality (1).
- Several equivalent forms of the ML bound have been reported [18–20, 24, 25]. The one we use here is [25]

$$\frac{\tau}{\hbar} \geqslant \max_{\theta\in\left[-\cos^{-1}\left(\sqrt{\epsilon}\right),0\right]} \frac{\cos\theta-\sqrt{\epsilon}}{\langle E-E_0\rangle\sin\varphi\left(\theta\right)}, \tag{2}$$

where $\langle E - E_0 \rangle$ is the expected energy of the state relative to the ground state energy of the Hamiltonian, and $\varphi(\theta)$ is the unique root of the equation

$$\cos\varphi(\theta) - \cos\theta + [\varphi(\theta) - \theta]\sin\varphi(\theta) = 0 \tag{3}$$

in the interval $[\max(\pi/2, |\theta|), \pi]$.

- The dual ML bound is the ML-like bound reported by Ness *et al* [23]. Using the notation in equation (2), it says that for states with bounded energy spectrum,

$$\frac{\tau}{\hbar} \geqslant \max_{\theta\in[-\cos^{-1}(\sqrt{\epsilon}),0]} \frac{\cos\theta - \sqrt{\epsilon}}{\langle E_{\max} - E\rangle \sin\varphi(\theta)} \tag{4}$$

where $\langle E - E_{\max}\rangle = -\langle E_{\max} - E\rangle$ is the expectation energy of the state relative to the maximum eigenenergy of the system. Actually, the dual ML bound can be derived from the ML bound through the following duality. Any initial state $|\Psi(0)\rangle$ can be written in the form $\sum_j a_j |E_j\rangle$ with $|E_j\rangle$ being an energy eigenstate with energy E_j. Denote its 'energy-reversed' state $\sum_j a_j |-E_j\rangle$ by $|\tilde{\Psi}(0)\rangle$. Clearly, the time-evolved state $|\Psi(t)\rangle$ equals the reversed-time evolved state $|\tilde{\Psi}(-t)\rangle$. More importantly, the fidelity between $|\Psi(0)\rangle$ and $|\Psi(t)\rangle$ equals the fidelity between $|\tilde{\Psi}(0)\rangle$ and $|\tilde{\Psi}(-t)\rangle$, which in turn equals the fidelity between $|\tilde{\Psi}(0)\rangle$ and $|\tilde{\Psi}(t)\rangle$. Consequently, the ML bound for $|\Psi(0)\rangle$ induces a bound for $|\tilde{\Psi}(0)\rangle$. And this induced bound is the dual ML bound. Thus, the dual ML bound holds for a slightly more general case when the energy spectrum is bounded from above. Surely, the arguments reported here is general and can be used to obtain the corresponding dual QSL from any given QSL involving fidelity between the initial and final states.
- The LZ bound [21] refers to the family of QSLs in the form

$$\frac{\tau}{\hbar} \geqslant \pi \left[\frac{1 - \sqrt{\epsilon(1 + 4p^2/\pi^2)}}{2\langle (E - E_0)^p\rangle}\right]^{\frac{1}{p}} \tag{5}$$

for $0 \leqslant p \leqslant 2$ and $0 \leqslant \epsilon \leqslant \pi^2/(\pi^2 + 4p^2)$. Surely, one may consider optimizing LZ bound by taking supremum of the RHS of Inequality (5) over p. We call this the optimized LZ bound.
- The LC bound [22] is the family of inequalities

$$\frac{\tau}{\hbar} \geqslant \max_{E_r} \left(\frac{1 - \sqrt{\epsilon}}{A_p \langle |E - E_r|^p\rangle}\right)^{\frac{1}{p}}, \tag{6}$$

for $0 < p \leqslant 2$, where $A_p = \sup\{(1 - \cos x)/x^p : x > 0\}$. Just like the optimized LZ bound, we refer to the LC bound optimized over all possible p as the optimized LC bound. Note that the special case of $p = 1$ is also known as the Chau bound [26]. Moreover, by adapting from [25], we know that

$$A_1 = \sin\varphi(0). \tag{7}$$

Actually, all but the LC bound above can be saturated in the sense that for each $p \in (0, 2]$ and for any $\epsilon \in [0, 1]$, there exists a pair of time-independent Hamiltonian and initial pure quantum state that attains the bound. Whereas for the LC bound, it can be saturated for all $\epsilon \in [0, 1]$ when $p \leqslant \pi/2$. However, it is not clear if it can be saturated for $p \in (\pi/2, \pi]$ [22]. We give a negative answer to this question in section 4 by showing that the LC bound may not be tight when $p \in (\pi/2, \pi]$ for a general ϵ. Lastly, we remark that all these bounds are complementary in the sense that each of the bounds cannot be reduced to another if we are not allowed to optimize the LZ and LC bounds over the parameter p.

Observe that all the above QSLs are in the form of a product of two terms. One is a function of a certain energy moment of the quantum state only. The other one is a function of the fidelity and perhaps also the parameter p only. We will contrast this feature when we discuss an efficient algorithm in computing the CZ bound in section 5 below.

Last but not least, there is a different type of QSL reported in the literature known as the exact QSLs. In particular, Pati *et al* proved an exact evolution time expression for finite-dimensional quantum systems as well as systems evolving under an Hamiltonian H with $H^2 = I$. These expressions are valid for time-dependent as well as time-independent Hamiltonians under a technical condition to be discussed below. Moreover, such an exact relation becomes an inequality for infinite-dimensional systems [10]. So why extending and strengthening other more 'conventional' QSLs if the actual evolution time is know? Here we answer this question by discussing the case of a two-dimensional quantum state as the starting point.

For a two-dimensional initial state $|\Psi(0)\rangle$ evolving under a time-independent Hamiltonian, Pati *et al* proved that evolution time τ satisfies [10]

$$\frac{\tau}{\hbar} = \frac{\cos^{-1}\left(\sqrt{\epsilon}\right)}{\langle\langle \Delta H^{\mathrm{nc}} \rangle\rangle_\tau} \tag{8}$$

where

$$\langle\langle \Delta H^{\mathrm{nc}} \rangle\rangle_\tau = -\frac{\hbar}{2\tau} \int_0^\tau \frac{\mathrm{d}p_t/\mathrm{d}t}{\sqrt{p_t(1-p_t)}}\,\mathrm{d}t \tag{9}$$

provided that $p_t \equiv |\langle \Psi(0)|\Psi(t)\rangle|^2$ is monotonic decreasing for $t \in [0, \tau]$. Note that even though the Hamiltonian is time-independent, computing $\langle\langle \Delta H^{\mathrm{nc}} \rangle\rangle$ requires integration over time. More importantly, since p_t is the fidelity square between $|\Psi(0)\rangle$ and $|\Psi(t)\rangle$, knowing p_t at all times is equivalent to knowing $|\Psi(0)\rangle$ and the Hamiltonian. That is to say, the information needed to determine the evolution time is encoded in p_t. Therefore, the τ in equation (8) is an equality because it comes from tracing the time evolution of $|\Psi(0)\rangle$. Actually, explicitly integrating the RHS of equation (9), Pati *et al* obtains [10]

$$\langle\langle \Delta H^{\mathrm{nc}} \rangle\rangle_\tau = \frac{\hbar \cos^{-1}\left(\sqrt{p_\tau}\right)}{2}. \tag{10}$$

Thus, $2\langle\langle \Delta H^{\mathrm{nc}} \rangle\rangle_\tau/\hbar$ is the Bures angle between $|\Psi(0)\rangle$ and $|\Psi(\tau)\rangle$ in disguise. This explains why a monotonically decreasing p_t is needed to arrive at equation (8). In this regard, it is more efficient and accurate as well as conceptually simpler to compute the evolution time τ by finding the smallest non-negative root of the equation $p_t = \epsilon^2$. By the same token, an exact QSL is simply an alternative, possibly mathematically pleasing and inspiring, form of expressing the evolution time given a complete description of the initial state and evolution Hamiltonian. This argument holds for all exact QSLs.

To conclude, the exact QSL is equivalent to computing the actual evolution time given complete information on the Hamiltonian and the initial state. Obviously, its calculation is difficult in general. In contrast, this type of bounds are markedly different from the conventional QSLs that give lower time bounds that are relatively easy to calculate based on partial information on the system (such as $\langle E-E_0\rangle$ or ΔE). Since the study of exact QSL is conceptually different from those of conventional QSLs, we do not consider this type of exact QSLs in this paper.

3. Auxiliary results

We need the following auxiliary results whose proofs can be found in the Appendix. Lemma 1 below generalizes lemma 1 in [26] as well as lemma 1 and corollary 1 in [25]. Its proof is based partly on those of lemma 1 and corollary 1 in [25]. Lemma 3 was first reported in one of the authors' capstone project report [27]. In addition, corollary 2 extends corollary 1 in [25].

Lemma 1. *Suppose* $(p,\theta)\in\mathcal{R}\equiv(0,1]\times(-\pi,\pi/2]\cup(1,2]\times(-\pi,0]$, *then*

$$\cos x \geqslant \cos\theta - A_{p,\theta}\,(x-\theta)^p \tag{11}$$

for all $x>\theta$, *where*

$$A_{p,\theta} = \max_{x\in[|\theta|,\pi)} \frac{\cos\theta-\cos x}{(x-\theta)^p} > 0. \tag{12}$$

(Note that for the case of $x=\theta$*, the RHS of equation (12) is regarded as the limit* $x\to\theta^+$*. It exists for* $(p,\theta)\in\mathcal{R}$*). Moreover, the* x *that maximizes the RHS of equation (12) is unique. By writing this unique* x *as* $\varphi_p\equiv\varphi_p(\theta)$*, then* $A_{p,\theta}$ *can be expressed as*

$$A_{p,\theta} = \frac{\sin\varphi_p(\theta)}{p\,[\varphi_p(\theta)-\theta]^{p-1}}. \tag{13}$$

In fact, φ_p *is also the unique solution of the equation*

$$f_{p,\theta}(\varphi_p) \equiv p\,(\cos\varphi_p-\cos\theta) + (\varphi_p-\theta)\sin\varphi_p = 0 \tag{14}$$

in the interval $(|\theta|,\pi)$ *if* $(p,\theta)\neq(2,0)$*. Whereas if* $(p,\theta)=(2,0)$*, then* $\varphi_2(0)=0$*, which is the unique solution of equation (14) in the interval* $[|\theta|,\pi)$*. Furthermore, for* $p\in(0,1]$*, the maximum in the RHS of equation (12) can be taken over* $x\in[\max(|\theta|,\pi/2),\pi)$*. Moreover, in the domain* $x\in[\theta,+\infty)$*, Inequality (11) becomes an equality if and only if* $x=\theta$ *or* $\varphi_p(\theta)$*. Lastly,* $\varphi_p(\theta)$ *is a simple root of equation (14) if* $(p,\theta)\neq(2,0)$*; and it is a root of order 4 otherwise.*

The following corollary follows directly from applying lemma 1 to $x\geqslant\theta$ and to $y=-x\geqslant\theta$ separately.

Corollary 1. *For* $p\in(0,1]$ *and* $\theta\in[-\pi/2,\pi/2]$*, we have*

$$\begin{aligned}\cos x &\geqslant \cos\theta - 1_{x\geqslant\theta}A^+_{p,\theta}|x-\theta|^p - 1_{x<\theta}A^-_{p,\theta}|\theta-x|^p\\ &\equiv \cos\theta - 1_{x\geqslant\theta}A_{p,\theta}|x-\theta|^p - 1_{x<\theta}A_{p,-\theta}|\theta-x|^p\\ &= \cos\theta - \frac{1_{x\geqslant\theta}|x-\theta|^p\sin\varphi^+_p(\theta)}{p\left[\varphi^+_p(\theta)-\theta\right]^{p-1}} + \frac{1_{x<\theta}|\theta-x|^p\sin\varphi^-_p(\theta)}{p\left[\theta-\varphi^-_p(\theta)\right]^{p-1}}\end{aligned} \tag{15}$$

for all $x\in\mathbb{R}$*, with equality holds if and only if* $x=\theta$*,* $x=\varphi^+_p(\theta)\equiv\varphi_p(\theta)$ *or* $x=\varphi^-_p(\theta)\equiv-\varphi_p(-\theta)$*. Here* $\varphi_p(\pm\theta)$ *are (unique) solutions of equation (14) in the interval* $(|\theta|,\pi)$*,*

$$1_{x\geqslant\theta} = \begin{cases}1 & \text{if } x\geqslant\theta,\\ 0 & \text{otherwise}.\end{cases} \tag{16}$$

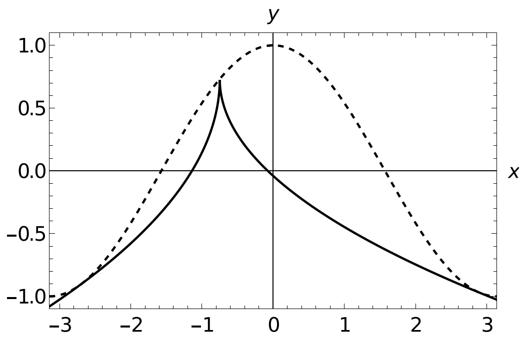

Figure 1. The dashed curve is $y = \cos x$. The solid curve corresponds to the RHS of Inequality (15) for $\theta = -0.75$ and $p = 0.5$. Clearly, the two curves meets at three distinct points with two of them being points of tangency.

and $1_{x<\theta}$ *is similarly defined. Moreover, for the special case of* $\theta = 0$*, Inequality* (15) *holds also for* $p \in (1,2]$. *That is to say, for* $p \in (0,2]$,

$$\cos x \geqslant 1 - \frac{|x|^p \sin \varphi_p^+(0)}{p \varphi_p^+(0)^{p-1}} \tag{17}$$

with equality holds if and only if $x = 0, \varphi_p^{\pm}(0)$.

Remark 1. Figure 1 plots the LHS and RHS of Inequality (15) and highlights its geometric meaning. Clearly, $x = \varphi_p^+(\theta) = \varphi_p(\theta)$ is the (unique) point in $[|\theta|, \pi)$ where the curves $\cos x$ and $\cos\theta - A_{p,\theta}(x-\theta)^p$ meet tangentially. Similarly, we may also interpret $x = -\varphi_p(-\theta)$ as the (unique) point in $(-\pi, -|\theta|]$ where the curves $\cos x$ and $\cos\theta - A_{p,-\theta}(\theta - x)^p$ meets tangentially. Consequently, $\varphi_p^-(\theta) = -\varphi_p(-\theta)$ must be the unique solution of equation (14) in the interval $(-\pi, -|\theta|]$ if $(p,\theta) \neq (2,0)$.

Since Inequality (15) plays a key role in this study, we use the notations $\varphi_p^{\pm}(\theta)$ and $A_{p,\theta}^{\pm}$ instead of, $\varphi_p(\theta)$, $A_{p,\theta}$ and $A_{p,-\theta}$ from now on except possibly for the case when $\theta = 0$.

Corollary 2. *Suppose* $0 < p \leqslant 1$ *and* $\theta \in [-\pi/2, \pi/2]$. *Then,* $\varphi_p^+(\theta) \pm \theta \in [0, 3\pi/2)$ *and* $\varphi_p^-(\theta) \pm \theta \in (-3\pi/2, 0]$. *Besides,* $\varphi_p^{\pm}(\theta) - \theta$ *are strictly decreasing functions of* θ *and* $\varphi_p^{\pm}(\theta) + \theta$ *are strictly increasing functions of* θ.

Remark 2. Chau [25] further showed that for $p = 1$, $\varphi_p^+(\theta)$ is an increasing function of θ in the domain $[-\pi/2, \pi/2]$. Nevertheless, this is not true for $0 < p < 1$.

Lemma 2. *Let*

$$h(x) = \begin{cases} x\cot(x/2) & \text{for } x \in (0,\pi), \\ \lim_{x\to 0^+} h(x) = 2 & \text{for } x = 0. \end{cases} \tag{18}$$

Then, h *is a strictly decreasing function in* $[0,\pi]$. *Moreover,* $h\colon [0,\pi] \mapsto [0,2]$ *is a homeomorphism.*

Lemma 3. *Let* $\epsilon \in [0,1]$. *Then*

$$\sup_{x\in(0,\pi)} \left[x \left(\frac{1-\sqrt{\epsilon}}{2\sin^2 \frac{x}{2}} \right)^{\frac{1}{x\cot(x/2)}} \right] = \cos^{-1}\left(\sqrt{\epsilon}\right). \tag{19}$$

In fact, this supremum is attained at $x = \cos^{-1}(\sqrt{\epsilon})$. *In other words, this is actually a maximum.*

Lemma 4. *Let* $w\colon [a,b] \to \mathbb{R}$ *be a doubly differentiable function, w is continuous on* $[a,b]$, w'' *is continuous on (a, b). Suppose further that* $w(a) \geqslant 0$, $w(b) \leqslant 0$, $w'(b) < 0$ *and* $w''(x) \leqslant 0$ *for all* $x \in [a,b]$. *Then by choosing b as the initial guess, Newton's method of finding a root of* $w(x) = 0$ *in* $[a,b]$ *always converges. Surely, the convergence is quadratic if this root is simple.*

4. The CZ bound

In what follows, we adopt the following notations. We write a time-independent Hamiltonian as a formal sum of its energy eigenvectors, namely, $\sum_j E_j |E_j\rangle\langle E_j|$ with $|E_j\rangle$'s being the energy eigenstate of the Hamiltonian. In addition, we write a normalized initial pure state $|\Psi(0)\rangle$ as $\sum_j a_j |E_j\rangle$ with $\sum_j |a_j|^2 = 1$. From now on, unless otherwise stated, a Hamiltonian and a quantum state in this paper are time-independent and pure, respectively.

Theorem 1 (CZ bound). *The evolution time* τ *needed for any quantum state to evolve to another state whose fidelity between them is* ϵ *under a (time-independent) Hamiltonian satisfies the inequality*

$$\frac{\tau}{\hbar} \geqslant \frac{T_p(\epsilon)}{\hbar} \equiv \max_{\substack{|\theta| \leqslant \cos^{-1}(\sqrt{\epsilon}),\\ E_r\in\mathbb{R}}} \left[\frac{\cos\theta - \sqrt{\epsilon}}{A^{+}_{p,\theta} \left\langle \left[(E-E_r)^{+} \right]^{p} \right\rangle + A^{-}_{p,\theta} \left\langle \left[(E_r-E)^{+} \right]^{p} \right\rangle} \right]^{\frac{1}{p}} \tag{20a}$$

for $p \in (0,1]$ *and*

$$\frac{\tau}{\hbar} \geqslant \frac{T_p(\epsilon)}{\hbar} \equiv \max_{E_r\in\mathbb{R}} \left[\frac{1-\sqrt{\epsilon}}{A_{p,0}\langle |E-E_r|^p \rangle} \right]^{\frac{1}{p}} \tag{20b}$$

for $p \in (1,2]$ *provided that*

$$\left\langle \left[(E-E_r)^{+} \right]^{p} \right\rangle = \sum_{j\colon E_j > E_r} |a_j|^2 |E_j - E_r|^p \tag{21}$$

and the similarly defined $\langle [(E_r-E)^{+}]^p \rangle$ *exist. (Note that* $\langle [(E-E_r)^{+}]^p \rangle$ *and* $\langle [(E_r-E)^{+}]^p \rangle$ *are the expected measurement results of valid observables. Physically, they relate to the pth moment of the absolute value of energy and the pth signed moment of the absolute value of energy of the initial state* $|\Psi(0)\rangle$ *via the relations*

$$\langle |E-E_r|^p \rangle = \left\langle \left[(E-E_r)^{+} \right]^{p} \right\rangle + \left\langle \left[(E_r-E)^{+} \right]^{p} \right\rangle \tag{22a}$$

and

$$\langle \operatorname{sgn}(E-E_r)\, |E-E_r|^p \rangle = \left\langle \left[(E-E_r)^{+} \right]^{p} \right\rangle - \left\langle \left[(E_r-E)^{+} \right]^{p} \right\rangle. \tag{22b}$$

Note further that the denominator of the RHS of Inequality (20) vanishes if the initial state is an energy eigenstate of the Hamiltonian. In this case, Inequality (20) still holds if one interprets its RHS as 0 if $\epsilon = 1$ and $+\infty$ otherwise.) The necessary and sufficient conditions for the Inequality (20) to be saturated by a pair of Hamiltonian and initial quantum state are as follows. Let $(\theta_{\text{opt}}, E_{r,\text{opt}})$ be one of the possible pairs of values of (θ, E_r) that maximize the RHS of Inequality (20). (We shall show in section 5.1 that $E_{r,\text{opt}}$ is unique if $1 < p \leqslant 2$. For the other cases, $E_{r,\text{opt}}$ may not be unique. Also, we shall show in theorem 4 of section 5.2 that θ_{opt} is unique for any given $E_{r,\text{opt}}$.) Let us denote $\varphi_p^{\pm}(\theta_{\text{opt}})$ by $\varphi_{p,\text{opt}}^{\pm}$. Then, we have the followings.

- *For $p \in (0, 2]$ and $\epsilon = 1$ (and hence $\theta_{\text{opt}} = 0$), Inequality (20) can be saturated by any Hamiltonian and initial quantum state pair.*
- *For $p = 2$ and $\epsilon < 1$, Inequality (20) cannot be saturated.*
- *For $p \in (0, 1]$ and $\theta_{\text{opt}} \in [-\cos^{-1}(\sqrt{\epsilon}), \cos^{-1}(\sqrt{\epsilon})]$, Inequality (20) is saturated if and only if the (normalized) initial pure quantum state, when expressed in terms of energy eigenvectors of the corresponding Hamiltonian, equals*

$$|\Psi(0)\rangle = a_+|E_+\rangle + a_r|E_{r,opt}\rangle + a_-|E_-\rangle. \tag{23}$$

Here $E_- < E_{r,\text{opt}} < E_+$, $(E_+ - E_{r,\text{opt}}) : (E_- - E_{r,\text{opt}}) = (\varphi_{p,\text{opt}}^{+} - \theta_{\text{opt}}) : (\varphi_{p,\text{opt}}^{-} - \theta_{\text{opt}})$ and

$$\begin{bmatrix} |a_+|^2 \\ |a_r|^2 \\ |a_-|^2 \end{bmatrix} = \frac{1}{2\sin\frac{\varphi_{p,opt}^{+}-\varphi_{p,opt}^{-}}{2}\sin\frac{\varphi_{p,opt}^{+}-\theta_{opt}}{2}\sin\frac{\theta_{opt}-\varphi_{p,opt}^{-}}{2}} \times \begin{bmatrix} \sin\frac{\theta_{opt}-\varphi_{p,opt}^{-}}{2}\left(\cos\frac{\theta_{opt}-\varphi_{p,opt}^{-}}{2} - \sqrt{\epsilon}\cos\frac{\theta_{opt}+\varphi_{p,opt}^{-}}{2}\right) \\ -\sin\frac{\varphi_{p,opt}^{+}-\varphi_{p,opt}^{-}}{2}\left(\cos\frac{\varphi_{p,opt}^{+}-\varphi_{p,opt}^{-}}{2} - \sqrt{\epsilon}\cos\frac{\varphi_{p,opt}^{+}+\varphi_{p,opt}^{-}}{2}\right) \\ \sin\frac{\varphi_{p,opt}^{+}-\theta_{opt}}{2}\left(\cos\frac{\varphi_{p,opt}^{+}-\theta_{opt}}{2} - \sqrt{\epsilon}\cos\frac{\varphi_{p,opt}^{+}+\theta_{opt}}{2}\right) \end{bmatrix}. \tag{24}$$

(To be more explicit, the corresponding optimizing Hamiltonian is in the form $H = E_+|E_+\rangle\langle E_+| + E_r|E_r\rangle\langle E_r| + E_-|E_-\rangle\langle E_-| + H^{\perp}$ where $H^{\perp}$ is a Hamiltonian whose support is orthogonal to $|E_+\rangle$, $|E_r\rangle$ and $|E_-\rangle$.)
- *For $p \in (1, 2)$ (and hence $\theta_{\text{opt}} = 0$), Inequality (20) is saturated if and only if Equations (23) and (24) hold. Furthermore,*

$$\sqrt{\epsilon} \geqslant \cos\varphi_{p,opt}^{+}. \tag{25}$$

Proof. This proof follows the basic ideas used in [26] as well as the proof of theorem 1 in [25]. The part on the saturation of Inequality (20) extends the proof of theorem 2 in [25].

Since the fidelity between two pure states does not decrease under partial trace and the RHS of Inequality (20) is a decreasing function of fidelity, we only need to consider pure state evolution in the extended Hilbert space in our proof [20].

To save space, we only prove the case of $p \in (0, 1]$ here. The case of $p \in (1, 2]$ can be proven in the same way. Details are left to interested readers. Using the notations stated at the beginning of this section and by corollary 1, we get

$$\sqrt{\epsilon} = |\langle \Psi(0)|\Psi(\tau)\rangle| \geqslant \Re\left(\langle \Psi(0)|\Psi(\tau)\rangle e^{iE_r\tau/\hbar}e^{-i\theta}\right) = \sum_j |a_j|^2 \cos\left[\frac{(E_j - E_r)\tau}{\hbar} + \theta\right]$$
$$\geqslant \sum_j |a_j|^2 \left[\cos\theta - \left(1_{E_j \geqslant E_r} A^+_{p,\theta} + 1_{E_j < E_r} A^-_{p,\theta}\right) \left|\frac{(E_j - E_r)\tau}{\hbar}\right|^p\right]$$
$$= \cos\theta - \left\{A^+_{p,\theta}\left\langle \left[(E - E_r)^+\right]^p\right\rangle + A^-_{p,\theta}\left\langle \left[(E_r - E)^+\right]^p\right\rangle\right\} \left(\frac{\tau}{\hbar}\right)^p \quad (26)$$

for any $|\theta| \leqslant \pi/2$ and for any reference energy level E_r. Here $\Re(\cdot)$ denotes the real part of its argument.

We assume that the coefficient of the $(\tau/\hbar)^p$ term is positive. (If not, $|\Psi(0)\rangle = |E_r\rangle$ up to an irrelevant phase and hence equation (20) is trivially true according to the convention stated in this theorem.) Then, Inequality (26) can be rewritten as

$$\left(\frac{\tau}{\hbar}\right)^p \geqslant \frac{\cos\theta - \sqrt{\epsilon}}{A^+_{p,\theta}\left\langle \left[(E - E_r)^+\right]^p\right\rangle + A^-_{p,\theta}\left\langle \left[(E_r - E)^+\right]^p\right\rangle}. \quad (27)$$

Clearly, Inequality (27) gives meaningful constraint on the evolution time τ if $\cos\theta \geqslant \sqrt{\epsilon}$. Furthermore, the denominator of the RHS of Inequality (27) is a continuous non-negative function of θ. Besides, it is unbounded if $E_r \to \pm\infty$. So, for fixed values of p, ϵ and θ, there is an E_r that minimizes the denominator of the RHS of Inequality (27) even though such an E_r need not be unique in general. Hence, we can maximize the RHS of Inequality (27) by minimizing its denominator over E_r as well as maximizing over $\theta \in [-\cos^{-1}(\sqrt{\epsilon}), \cos^{-1}(\sqrt{\epsilon})]$. (Obviously, the order of minimization and maximization does not affect the final outcome.) This gives Inequality (20*a*).

We now find the set of all (time-independent) Hamiltonian and initial (pure) quantum state pairs that saturate Inequality (20). The necessary and sufficient conditions for the case of $\epsilon = 1$ are obvious as $\tau = 0$. So, we assume that $\epsilon \in [0, 1)$ from now on. The necessary and sufficient conditions for the first line of Inequality (26) to be an equality are that $\Re(\langle\Psi(0)|\Psi(\tau)\rangle e^{iE_r\tau/\hbar}e^{-i\theta}) = \sqrt{\epsilon} \geqslant 0$ and $\Im(\langle\Psi(0)|\Psi(\tau)\rangle e^{iE_r\tau/\hbar}e^{-i\theta}) = 0$, where $\Im(\cdot)$ denotes the imaginary part of the argument. In addition, from corollary 1, the second line of Inequality (26) is an equality if and only if $\langle E_j|\Psi(0)\rangle = 0$ for all $(E_j - E_r)\tau/\hbar \notin \{0, \varphi^\pm_p - \theta\}$. As a result, the normalized initial state $|\Psi(0)\rangle$ must be in the form of equation (23) (with all the 'opt' subscripts removed).

Now we have enough information to discuss the necessary and sufficient conditions for saturation of Inequality (20) for the case of $p = 2$ and $\epsilon < 1$. According to lemma 1, $\varphi^\pm_2(0) = 0$. Thus, the saturating state $|\Psi(0)\rangle$ in equation (23) is simply $|E_r\rangle$ up to a global phase. Being an energy eigenstate, $|\Psi(0)\rangle$ does not evolve with time. That is why Inequality (20) cannot be saturated in this situation.

Let us continue our saturation condition analysis for the remaining cases. From our discussions so far, the normalization of $|\Psi(0)\rangle$ together with the requirements on the real and imaginary parts of $\langle\Psi(0)|\Psi(\tau)\rangle e^{iE_r\tau/\hbar}e^{-i\theta}$, we have

$$\begin{bmatrix} 1 & 1 & 1 \\ \cos\varphi^+_p & \cos\theta & \cos\varphi^-_p \\ \sin\varphi^+_p & \sin\theta & \sin\varphi^-_p \end{bmatrix} \begin{bmatrix} |a_+|^2 \\ |a_r|^2 \\ |a_-|^2 \end{bmatrix} = \begin{bmatrix} 1 \\ \sqrt{\epsilon} \\ 0 \end{bmatrix}. \quad (28)$$

Recall from lemma 1 that $-\pi < \varphi^-_p < \theta < \varphi^+_p < \pi$ for $(p, \theta) \in \mathcal{R} \setminus (2, 0)$. Hence, equation (28) has a unique solution. By solving equation (28) and then substituting

$\theta \in [-\cos^{-1}(\sqrt{\epsilon}), \cos^{-1}(\sqrt{\epsilon})]$ by its optimal value θ_{opt} obtained in the RHS of Inequality (20), we conclude that a_+, a_r and a_- must obey equation (24).

Finally, a valid $|\Psi(0)\rangle$ requires $|a_+|^2, |a_r|^2$ and $|a_-|^2$ to be non-negative. In the case of $p \in (0,1]$ and $\theta_{\text{opt}} \geqslant 0$, lemma 1 and corollary 2 imply that $\varphi^+_{p,\text{opt}} - \varphi^-_{p,\text{opt}} \in [\pi, 2\pi)$, $\varphi^+_{p,\text{opt}} + \varphi^-_{p,\text{opt}} \in (-\pi/2, \pi/2)$, $\varphi^+_{p,\text{opt}} - \theta_{\text{opt}} \in [0,\pi)$, $\varphi^+_{p,\text{opt}} + \theta_{\text{opt}} \in [\pi/2, 3\pi/2)$, $\theta_{\text{opt}} - \varphi^-_{p,\text{opt}} \in [\pi/2, 3\pi/2)$ and $\theta_{\text{opt}} + \varphi^-_{p,\text{opt}} \in (-\pi, 0]$. So, from equation (24), $|a_r|^2 \geqslant 0$. As $(\varphi^+_{p,\text{opt}} + \theta_{\text{opt}})/2 = (\varphi^+_{p,\text{opt}} - \theta_{\text{opt}})/2 + \theta_{\text{opt}}$, we conclude from the ranges of the arguments of the cosine function that $\cos[(\varphi^+_{p,\text{opt}} - \theta_{\text{opt}})/2] \geqslant \cos[(\varphi^+_{p,\text{opt}} + \theta_{\text{opt}})/2]$. Hence, from equation (24), $|a_-|^2 \geqslant 0$. Recall from corollary 2, $\varphi^\pm_{p,\text{opt}} - \theta_{\text{opt}}$ are strictly decreasing functions of $\theta_{\text{opt}} \in (-\cos^{-1}[\sqrt{\epsilon}], \cos^{-1}[\sqrt{\epsilon}]) \subset (-\pi/2, \pi/2)$. Thus,

$$\frac{\mathrm{d}}{\mathrm{d}\theta_{opt}} \left(\cos \frac{\theta_{opt} - \varphi^-_{p,opt}}{2} - \sqrt{\epsilon} \cos \frac{\theta_{opt} + \varphi^-_{p,opt}}{2} \right) < 0. \tag{29}$$

By writing $\theta_{\text{crit}} \equiv \cos^{-1}(\sqrt{\epsilon}) \in [0, \pi/2]$ and $\varphi^-_{p,\text{crit}} \equiv \varphi^-_p(\theta_{\text{crit}})$, we know that

$$\begin{aligned}
\cos \frac{\theta_{opt} - \varphi^-_{p,opt}}{2} - \sqrt{\epsilon} \cos \frac{\theta_{opt} + \varphi^-_{p,opt}}{2} &\geqslant \cos \frac{\theta_{crit} - \varphi^-_{p,crit}}{2} - \cos\theta_{crit} \cos \frac{\theta_{crit} + \varphi^-_{p,crit}}{2} \\
&= \cos \frac{\theta_{crit} - \varphi^-_{p,crit}}{2} \\
&\quad - \frac{1}{2} \left(\cos \frac{3\theta_{crit} + \varphi^-_{p,crit}}{2} + \cos \frac{\theta_{crit} - \varphi^-_{p,crit}}{2} \right) \\
&= \sin\theta_{crit} \sin \frac{\theta_{crit} + \varphi^-_{p,crit}}{2} \geqslant 0.
\end{aligned} \tag{30}$$

From equation (24), we find that $|a_+|^2 \geqslant 0$. Thus, $|\Psi(0)\rangle$ is a valid quantum state because $|a_\pm|^2, |a_r|^2 \geqslant 0$.

The case of $(p,\theta) \in (0,1] \times [0, \pi/2]$ can be proven in a similar way. Actually, showing $|a_+|^2, |a_r|^2 \geqslant 0$ is straightforward. Proving $|a_-|^2 \geqslant 0$ is more involved. Its validity is due to

$$\begin{aligned}
\cos \frac{\varphi^+_{p,opt} - \theta_{opt}}{2} - \sqrt{\epsilon} \cos \frac{\varphi^+_{p,opt} + \theta_{opt}}{2} &\geqslant \cos \frac{\varphi^+_{p,crit} + \theta_{crit}}{2} + \cos\theta_{crit} \cos \frac{\varphi^+_{p,crit} - \theta_{crit}}{2} \\
&= \frac{3}{2} \cos \frac{\varphi^+_{p,crit} + \theta_{crit}}{2} + \frac{1}{2} \cos \frac{\varphi^+_{p,crit} - 3\theta_{crit}}{2} \geqslant 0,
\end{aligned} \tag{31}$$

where $\varphi^+_{p,\text{crit}} \equiv \varphi^+_p(\theta_{\text{crit}})$. Here we have used $\varphi^+_p - 3\theta_{\text{crit}} \in [-\pi, \pi)$ to arrive at the last inequality.

The proof for the case of $p \in (1,2)$ follows similar logic though it is simpler as $\theta_{\text{opt}} = 0$. In fact, $|a_\pm|^2 \geqslant 0$ is trivially true in this case. And the condition in Inequality (25) is due to the requirement that $|a_r|^2 \geqslant 0$. Details are left to interested readers. □

Remark 3. From the above proof, it is clear that by replacing θ_{opt} with any $\theta \in [-\cos^{-1}(\sqrt{\epsilon}), \cos^{-1}(\sqrt{\epsilon})]$ as well as by replacing $E_{r,\text{opt}}$ with any E_r, we obtain all Hamiltonian and initial quantum state pairs that saturate Inequality (20) with the optimization over θ and E_r removed.

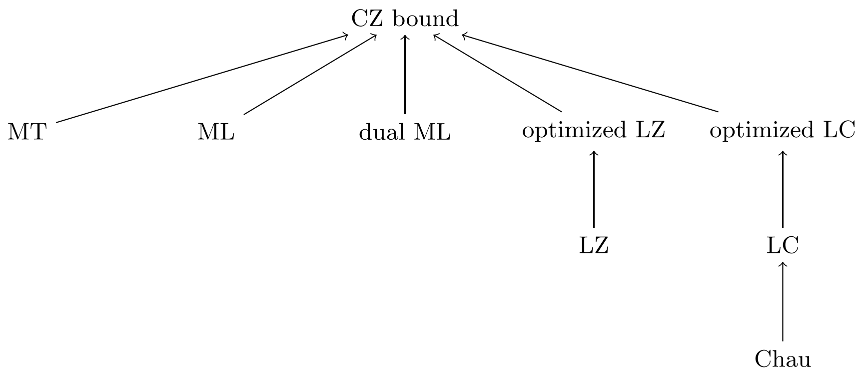

Figure 2. Relations between various QSLs. Here A $\to$ B means that A is a special case of B.

Remark 4. By comparing lemma 1, theorem 1 and their proofs with the prior works summarized in section 2, we observe that

- By putting $p=1$ together with $E_r=E_0$ and optimizing Inequality (27) over θ alone, we obtain the ML bound.
- By putting $p=1$, $E_r=E_{\max}$ and optimizing Inequality (27) over θ alone, we arrive at the dual ML bound.
- When $\theta=\tan^{-1}(2p/\pi)$, Inequality (15) becomes the key lemma in [21]. Hence, Inequality (27) reduces to the LZ bound for this θ when $E_r=E_0$.
- By setting $(p,\theta)=(1,0)$ and by optimizing Inequality (27) over E_r only, we get back the Chau bound.
- By putting $\theta=0$ and by optimizing over E_r alone, the CZ bound reduces to the LC bound. In this regard, theorem 1 gives the necessary and sufficient conditions for saturating the LC bound. This fills the gap in [22]. Specifically, by going through the proof of theorem 1, we find that the LC bound can be saturated if and only if Inequality (25) holds with $\varphi^+_{p,\text{opt}}=\varphi^+_p(0)$. In particular, the LC bound can be saturated for all $\epsilon\in[0,1]$ if and only if $\varphi^+_p(0)\geqslant\pi/2$. According to equation (14), $p=\varphi^+_p(0)\cot[\varphi^+_p(0)/2]$. As $p=\pi/2$ if $\varphi^+_p(0)=\pi/2$, lemma 2 implies that the LC bound can be saturated for all ϵ if and only if $p\leqslant\pi/2$. More importantly, if $p\geqslant\pi/2$, the LC bound can be saturated if and only if $\epsilon\geqslant\epsilon_c\equiv\cos^2[h^{-1}(p)]$. Clearly, ϵ_c is a strictly increasing function of p in $[\pi/2,2]$.
- For $p=2$, Inequality (20*b*) agrees with the MT bound up to $O([1-\epsilon]^2)$ in the limit $\epsilon\to 1^-$. Moreover, for $\epsilon<1$, Inequality (20*b*) alone is not as powerful as the MT bound. Nevertheless, theorem 2 below means that by optimizing over p with $\theta=0$, we recover the MT bound.

These relations can be schematically represented in figure 2.

A closely related result is the following theorem. Its special case for $p=2$ was originally proven in the capstone project report of one of the authors [27].

Theorem 2. *The MT bound can be deduced by optimizing the LC bound over* $p\in(0,2)$. *In fact,*

$$\frac{\tau}{\hbar}\geqslant\max_{E_r}\frac{\cos^{-1}(\sqrt{\epsilon})}{\langle|E-E_r|^p\rangle^{\frac{1}{p}}} \tag{32}$$

for any $p\in(0,2]$ *provided that* $\varphi_p(0)\leqslant\cos^{-1}(\sqrt{\epsilon})$.

Proof. Note that x^λ is a concave function for $0 < \lambda \leqslant 1$ in the domain $x \geqslant 0$. So, Jensen's inequality implies that $\langle |E - E_r|^{q\lambda} \rangle \geqslant \langle |E - E_r|^q \rangle^\lambda$ for any reference energy level E_r provided that $\lambda \in (0,1]$. Applying this inequality to Inequality (26) with $\theta = 0$ (which is nothing but the LC bound) and using equation (22*a*), we get

$$\frac{\tau}{\hbar} \geqslant \left(\frac{1-\sqrt{\epsilon}}{A_{p,0}} \right)^{\frac{1}{q}} \frac{1}{\langle |E - E_r|^{q\lambda} \rangle^{\frac{1}{q\lambda}}}. \tag{33}$$

for all $q \in (0,2)$.

From equation (14),

$$q = \varphi_q \cot \frac{\varphi_q}{2} \equiv \varphi_q(0) \cot \frac{\varphi_q(0)}{2}. \tag{34}$$

(Note that for this range of q, $\cot \varphi_q \neq 0$. So equation (34) is well-defined.) By lemma 2, equation (34) is a homeomorphism from $\varphi_q \in (0,\pi)$ to $q \in (0,2)$.

By fixing $q\lambda$ to a certain $p \in (0,2]$ as well as by using equations (13) and (34), we obtain

$$\frac{\tau}{\hbar} \geqslant \sup_{q \in (0,p)} \left(\frac{1-\sqrt{\epsilon}}{A_{q,0}} \right)^{\frac{1}{q}} \frac{1}{\langle |E - E_r|^p \rangle^{\frac{1}{p}}} = \sup_{q \in (0,p)} \left[\frac{(1-\sqrt{\epsilon})\,\varphi_q^q}{2\sin^2 \frac{\varphi_q}{2}} \right]^{\frac{1}{\varphi_q \cot(\varphi_q/2)}} \frac{1}{\langle |E - E_r|^p \rangle^{\frac{1}{p}}}. \tag{35}$$

From the discussion in the last paragraph, we can replace $q \in (0,p)$ in the supremum in the last line of Inequality (35) by $\varphi_q \in (\varphi_p, \pi) \equiv (\varphi_p(0), \pi)$. And from lemma 3, we conclude that the supremum of the RHS of Inequality (35) is attained at $\varphi_q = \cos^{-1}(\sqrt{\epsilon})$ provided that $\varphi_p \leqslant \cos^{-1}(\sqrt{\epsilon})$. In this case, the first factor in the RHS of Inequality (35) equals $\cos^{-1}(\sqrt{\epsilon})$. By maximizing the resultant inequality over E_r, we prove Inequality (32). We also mention on passing that in case $\varphi_p > \cos^{-1}(\sqrt{\epsilon})$, then from the proof of lemma 3, the supremum of Inequality (35) is attained at $\varphi_q = \varphi_p$. In other words, we simply get back the LC bound. □

Remark 5. Recall from lemma 3 that the optimized evolution time τ in theorem 2 is attained when $\varphi_p = \cos^{-1}(\sqrt{\epsilon})$. By compound angle formula, the corresponding p equals

$$p_{opt} = \sqrt{\frac{1+\sqrt{\epsilon}}{1-\sqrt{\epsilon}}} \cos^{-1}\left(\sqrt{\epsilon}\right). \tag{36}$$

An important consequence of remark 4 is that we can further strengthen the QSL reported in theorem 1 as

$$\tau \geqslant \max_{p \in (0,2]} T_p(\epsilon). \tag{37}$$

By theorem 2, this is stronger than the combined MT, ML and dual ML bounds studied in [23, 28]. From remark 4, the optimized CZ bound generalizes the MT, ML, dual ML, LZ and LC bounds. Nevertheless, the comparison between the combined MT, ML and dual ML bounds in [23, 28] with the optimized CZ bound is not entirely fair. This is because the combined bound in [23, 28] makes use of three numbers describing the initial quantum state, namely, $\langle E - E_0 \rangle$, $\langle E_{\max} - E \rangle$ and ΔE. In contrast, Inequality (37) uses an infinite number of descriptions of the quantum state, each in the form $\langle [(E - E_r)^+]^p \rangle$ or $\langle [(E_r - E)^+]^p \rangle$.

Along another line, one can generalize corollary 1 by using two different values of p — one for $E > E_r$ and the other for $E < E_r$. By the same argument as in the proof of theorem 1, we have the following QSL.

Theorem 3. *Let* $(p,q,\theta) \in (0,1] \times (0,1] \times [-\pi/2,\pi/2] \cup (0,1] \times (1,2] \times [0,\pi/2] \cup (1,2] \times (0,1] \times [-\pi/2,0] \cup (1,2] \times (1,2] \times \{0\}$, *we have*

$$\sqrt{\epsilon} \geqslant \cos\theta - \left\{ A^+_{p,\theta} \langle \left[(E-E_r)^+\right]^p \rangle \left(\frac{\tau}{\hbar}\right)^p + A^-_{q,\theta} \langle \left[(E_r-E)^+\right]^q \rangle \left(\frac{\tau}{\hbar}\right)^q \right\} \quad (38)$$

for all reference energy level E_r. *In particular, by putting* $p = 2q$, *we arrive at*

$$\frac{\tau}{\hbar} \geqslant \max_{E_r \in \mathbb{R}} \left(\frac{\left\{ 4A^+_{2q,\theta} \langle \left[(E-E_r)^+\right]^{2q} \rangle (\cos\theta - \sqrt{\epsilon}) + \left(A^-_{q,\theta}\right)^2 \langle \left[(E_r-E)^+\right]^q \rangle^2 \right\}^{1/2} - A^-_{q,\theta} \langle \left[(E_r-E)^+\right]^q \rangle}{2A^+_{2q,\theta} \langle \left[(E-E_r)^+\right]^{2q} \rangle} \right)^{\frac{1}{q}} \quad (39a)$$

for $(q,\theta) \in R \equiv (0,1/2] \times [-\pi/2,\pi/2] \cup (1/2,1] \times [0,\pi/2]$. *Similarly, the QSL corresponding to the case of* $q = 2p$ *is*

$$\frac{\tau}{\hbar} \geqslant \max_{E_r \in \mathbb{R}} \left(\frac{\left\{ 4A^-_{2p,\theta} \langle \left[(E_r-E)^+\right]^{2p} \rangle (\cos\theta - \sqrt{\epsilon}) + \left(A^+_{p,\theta}\right)^2 \langle \left[(E-E_r)^+\right]^p \rangle^2 \right\}^{1/2} - A^+_{p,\theta} \langle \left[(E-E_r)^+\right]^p \rangle}{2A^-_{2p,\theta} \langle \left[(E_r-E)^+\right]^{2p} \rangle} \right)^{\frac{1}{p}}. \quad (39b)$$

Remark 6. In the proof of the saturation conditions for the CZ bound in theorem 1, we do not use the property that the same p is used for $\varphi^+_{p,\mathrm{opt}}$ and $\varphi^-_{p,\mathrm{opt}}$. Therefore, simply by changing $\varphi^-_{p,\mathrm{opt}}$ to $\varphi^-_{q,\mathrm{opt}}$ in the saturation description part of theorem 1, we obtain the necessary and sufficient conditions for the QSL expressed in Inequality (38).

Although the QSL reported in Inequality (38) of theorem 3 is stronger than the QSL in theorem 1, it has a few drawbacks. First, an additional optimization over q together with a numerical solution of the least positive root of Inequality (38) with the inequality replaced by equality is required. Second, the absence of a closed form for τ makes finding τ more troublesome and the QSL conceptually less appealing. These two facts make the evaluation of the optimized version of this QSL very time consuming. One may consider the special cases such as Inequalities (39*a*) and (39*b*) in which the p and q are constrained. Even though they are better than Inequality (38) both in terms of the simplicity of the expression and computational tractability, they still lack the appeal of simplicity compared to the CZ bound. Moreover, as compared to the computational methods for the CZ bound to be reported in section 5, it is not likely to obtain a similarly efficient method for the QSLs stated in theorem 3. This is because these methods all start from an explicit expression of τ. Last but not least, we know from remark 6 that Inequalities (39*a*) and (39*b*) are complementary to the CZ bound. This is because by writing in energy eigenbasis, those initial states saturating, say, Inequality (39*a*) must be in the form $a_+|E_+\rangle + a_r|E_{r,\mathrm{opt}}\rangle + a_-|E_-\rangle$ with $(E_+ - E_{r,\mathrm{opt}}) : (E_{r,\mathrm{opt}} - E_-) = (\varphi^+_{2q,\mathrm{opt}} - \theta_{\mathrm{opt}}) : (\varphi^-_{q,\mathrm{opt}} - \theta_{\mathrm{opt}})$. They are clearly different from those in equation (23).

5. Accurate and efficient computation of the CZ bound

Although the optimized CZ bound in the form of Inequality (20) in theorem 1 is conceptually appealing, using it to calculate the optimized CZ bound, namely, the CZ bound optimized over p, θ and E_r, seems to be inefficient for the case of $p \in (0,1]$. This is because one has to optimize over both θ and E_r for any given ϵ (together with $\langle [(E-E_r)^+]^p \rangle$ and $\langle [(E_r-E)^+]^p \rangle$). Furthermore, we have to further optimize over p to obtain Inequality (37).

Here we report an accurate and efficient way to compute Inequalities (20) given an oracle that accurately computes the minimized pth moment of the absolute value of energy of a quantum state and its corresponding pth signed moment of the absolute value of energy, or more precisely, $\langle |E-E_{r,\text{opt}}|^p \rangle \equiv \min_{E_r \in \mathbb{R}} \langle |E-E_r|^p \rangle$ and $\langle \text{sgn}(E-E_{r,\text{opt}})|E-E_{r,\text{opt}}|^p \rangle$. And from equation (22), this is equivalent to having an oracle that accurately computes $\langle [(E-E_{r,\text{opt}})^+]^p \rangle$ and $\langle [(E_{r,\text{opt}}-E)^+]^p \rangle$. The key observation is that $E_{r,\text{opt}}$, the optimized value of E_r, is θ independent. So, we may first compute $E_{r,\text{opt}}$. Then, we evaluate $\langle [(E-E_{r,\text{opt}})^+]^p \rangle$ and $\langle [(E_{r,\text{opt}}-E^+]^p \rangle$ together with the optimized values of θ given $E_{r,\text{opt}}$. More explicitly, Inequality (20*a*) can be rewritten as

$$\begin{aligned}\left(\frac{\tau}{\hbar}\right)^p &\geqslant \max_{|\theta| \leqslant \cos^{-1}(\sqrt{\epsilon})} \left\{ \frac{\cos\theta - \sqrt{\epsilon}}{\left[\mu^+(E_{r,opt}) A^+_{p,\theta} + \mu^-(E_{r,opt}) A^-_{p,\theta}\right] \min_{E_r \in \mathbb{R}} \langle |E-E_r|^p \rangle} \right\} \\ &= \max_{|\theta| \leqslant \cos^{-1}(\sqrt{\epsilon})} \left\{ \frac{\cos\theta - \sqrt{\epsilon}}{\left[\mu^+(E_{r,opt}) A^+_{p,\theta} + \mu^-(E_{r,opt}) A^-_{p,\theta}\right] \langle |E-E_{r,opt}|^p \rangle} \right\}, \end{aligned} \tag{40}$$

where

$$\left\langle \left[(E-E_{r,opt})^+\right]^p \right\rangle : \left\langle \left[(E_{r,opt}-E)^+\right]^p \right\rangle = \mu^+(E_{r,opt}) : \mu^-(E_{r,opt}) \tag{41}$$

with $\mu^+(E_{r,\text{opt}}) + \mu^-(E_{r,\text{opt}}) = 1$.

Here we remark that Inequality (40) is in almost the same form as all the QSLs mentioned in section 2. More precisely, it is a product of a term depending only on the pth moment of the absolute value of energy of the quantum state optimized over the reference energy level with a term depending on ϵ and $\mu^\pm(E_{r,\text{opt}})$. In other words, the second term can be pre-computed and reused if $\mu^\pm(E_{r,\text{opt}})$ are known in advance.

5.1. On the computation of $\langle |E-E_r|^p \rangle$ *and* $E_{r,\text{opt}}$

Here we justify our assumption on the existence of an oracle to evaluate $\langle [(E-E_{r,\text{opt}})^+]^p \rangle$ and $\langle [(E_{r,\text{opt}}-E)^+]^p \rangle$ by showing that it can be replaced by computationally efficient and accurate algorithms in a number of useful situations. In all cases, the idea is to first find $E_{r,\text{opt}}$ and use it to obtain $\langle [(E-E_{r,\text{opt}})^+]^p \rangle$ and $\langle [(E_{r,\text{opt}}-E)^+]^p \rangle$ (or equivalently $\langle |E-E_{r,\text{opt}}|^p \rangle$ and $\mu^\pm(E_{r,\text{opt}})$). The first case is when the normalized initial quantum state can be expressed in the form

$$|\Psi(0)\rangle = \sum_{j=1}^{n} a_j |E_j\rangle \tag{42}$$

where $\{E_j\}$ is a strictly increasing sequence of real numbers and $|a_j| \neq 0$ for all j. We assume that all a_j's and E_j's are known. (Note that this assumption is not as restrictive as it appears. For Hamiltonian H and initial quantum state $|\Psi(0)\rangle$ express in another basis, E_j's can be found, say, by Householder transformation and QR algorithm—both are fast and numerically stable [29]. As for a_j's, they are the projection of $|\Psi(0)\rangle$ on invariant subspaces of H. Since

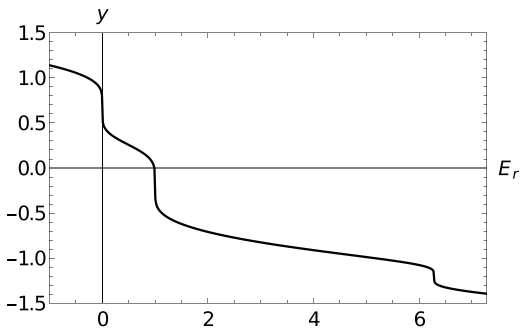

Figure 3. The LHS of equation (43) as a function of E_r for $p=1.2$ and $|\Psi(0)\rangle = \sqrt{0.4}|0\rangle + \sqrt{0.45}|1\rangle + \sqrt{0.15}|2\pi\rangle$, namely, one of the initial states used in section 6 to study the performance of various QSLs. The shape of this curve is typical among finite-dimensional $|\Psi(0)\rangle$'s. Notice that the curve makes sharp turns with infinite slope at each E_j.

finding invariant subspaces of a Hermitian matrix is efficient and numerically stable [30, 31], so is computing a_j's.)

Note that x^p is a strictly convex (concave) function of $x \geqslant 0$ if $1 < p \leqslant 2$ $(0 < p < 1)$. And when $p = 1$, this function is both convex and concave. Since the sum of convex (concave) functions is convex (concave), $\langle |E - E_r|^p \rangle$ is a piecewise convex (concave) function of E_r for $1 \leqslant p \leqslant 2$ $(0 < p \leqslant 1)$. Consequently, for $p > 1$, $\langle |E - E_r|^p \rangle$ attains its minimum at a certain $E_{r,\mathrm{opt}} \in (E_j, E_{j+1})$ for some $j = 1, 2, \ldots, n-1$ where $E_{r,\mathrm{opt}}$ is the solution of the equation

$$\left\langle \left[(E - E_r)^+ \right]^{p-1} \right\rangle - \left\langle \left[(E_r - E)^+ \right]^{p-1} \right\rangle = 0 \tag{43}$$

for $p \geqslant 1$. It is easy to see that the LHS of equation (43) is strictly decreasing and continuous for $p > 1$. Besides, $\langle [(E_1 - E)^+]^{p-1} \rangle = 0 = \langle [(E - E_n)^+]^{p-1} \rangle$. So, $E_{r,\mathrm{opt}}$ exists and is unique. Furthermore, it can be evaluated accurately and efficiently via bisection method. Nevertheless, as depicted in figure 3, the LHS of equation (43) makes sharp turns around and has infinite slopes at E_j's. (The latter can be proven by differentiating the LHS of equation (43) with respect to E_r.) This greatly lowers the efficiency of bisection method if $E_{r,\mathrm{opt}}$ is near one of the E_j's. Here we recommend first using binary search to efficiently limit $E_{r,\mathrm{opt}}$ to one of the intervals (E_j, E_{j+1}). Then, since the second derivative of the LHS of equation (43) with respect to E_r changes sign exactly once in this interval, lemma 4 implies that using either $E_j + \delta$ or $E_{j+1} - \delta$ for a sufficiently small $\delta > 0$ as initial guess, Newton's method is guaranteed to converge to $E_{r,\mathrm{opt}}$. Indeed, this is what we have observed in our numerical experiments.

As for the case of $p = 1$, the LHS and RHS of equation (43) are only piecewise continuous in general. Thus, standard calculus technique does not work. Fortunately, equation (43) means that $E_{r,\mathrm{opt}}$ can be chosen to be the median energy of the state [26]. That is to say, $E_{r,\mathrm{opt}}$ obeys $\sum_{j\,:\,E_j \geqslant E_{r,\mathrm{opt}}} |a_j|^2 \geqslant 1/2$ and $\sum_{j\,:\,E_j \leqslant E_{r,\mathrm{opt}}} |a_j|^2 \geqslant 1/2$. Note that in this case, the values of $\mu^\pm$ are unique even though $E_{r,\mathrm{opt}}$ need not be unique.

The case of $0 < p < 1$ is computationally more involved. Since $\langle |E - E_r|^p \rangle$ is a piecewise concave function, its minimum is attained at $E_r = E_j$ for some $j = 1, 2, \ldots, n$. That is,

$$E_{r,opt} \in \{E_j \colon \langle |E - E_j|^p \rangle \leqslant \langle |E - E_\ell|^p \rangle \quad \forall \ell = 1, 2, \ldots, n\}. \tag{44}$$

Finding $E_{r,\text{opt}}$ is accurate whose time complexity scales as $O(n^2)$. Unfortunately, there is no way to further reduce the computing time using a deterministic algorithm for $\langle |E-E_j|^p\rangle$ shows no trend in general.

Another case of importance is when H has a bounded and continuous energy spectrum, $\langle[(E-E_r)^+]^p\rangle$ and $\langle[(E_r-E)^+]^p\rangle$ are differentiable functions of E_r with $p\in(0,2]$. Moreover, $\langle[(E-E_r)^+]^{p-1}\rangle$ and $\langle[(E_r-E)^+]^{p-1}\rangle$ are continuous functions of E_r. So the above four functions can be accurately and efficiently computed via any standard numerical integrator of choice. Using the same argument in this Subsection plus differentiation under the integral sign, equation (43) holds for any $p\in(0,2]$. The only difference is that the LHS and RHS of equation (43) are strictly decreasing (increasing) and strictly increasing (decreasing) functions of E_r for $p<1$ ($p\geqslant 1$), respectively. In both cases, Newton's method must converge to unique $E_{r,\text{opt}}$ according to lemma 4.

5.2. Computation of φ_p and θ_{opt}

We now study how to efficiently compute θ_{opt} for fixed $\mu^\pm\equiv\mu^\pm(E_{r,\text{opt}})$. To do so, we need a way to calculate the optimal θ that maximizes the RHS of Inequality (40).

Theorem 4. *Let $0<p\leqslant 1$. Suppose $\langle|E-E_r|^p\rangle\neq 0$, and denote $\langle[(E-E_r)^+]^p\rangle:\langle[(E_r-E)^+]^p\rangle=\mu^+:\mu^-$ with $\mu^++\mu^-=1$. Then*

$$\max_{|\theta|\leqslant\cos^{-1}(\sqrt{\epsilon})}\frac{\cos\theta-\sqrt{\epsilon}}{\mu^+A^+_{p,\theta}+\mu^-A^-_{p,\theta}} \tag{45}$$

attains its maximum when θ is the unique solution of

$$s_\epsilon(\theta)\equiv\mu^+s^+_\epsilon(\theta)+\mu^-s^-_\epsilon(\theta)\equiv\frac{\mu^+\sin\frac{\varphi_p^+-\theta}{2}\left(\cos\frac{\varphi_p^+-\theta}{2}-\sqrt{\epsilon}\cos\frac{\varphi_p^++\theta}{2}\right)}{\left(\varphi_p^+-\theta\right)^p}+\frac{\mu^-\sin\frac{\varphi_p^--\theta}{2}\left(\cos\frac{\varphi_p^--\theta}{2}-\sqrt{\epsilon}\cos\frac{\varphi_p^-+\theta}{2}\right)}{\left(\theta-\varphi_p^-\right)^p}=0 \tag{46}$$

in the interval $[-\theta_{\text{crit}},\theta_{\text{crit}}]$. Here, θ_{crit} is the unique solution of

$$r^-_\epsilon(\theta)\equiv\cos\left(\frac{\varphi_p^--\theta}{2}\right)-\sqrt{\epsilon}\cos\left(\frac{\varphi_p^-+\theta}{2}\right)=0 \tag{47}$$

in the interval $[0,\cos^{-1}(\sqrt{\epsilon})]$.

Proof. From equations (13)–(14) and (A.5), we have

$$\begin{aligned}\frac{\mathrm{d}A^+_{p,\theta}}{\mathrm{d}\theta}&=A^+_{p,\theta}\left[\frac{\mathrm{d}\varphi_p^+}{\mathrm{d}\theta}\cot\varphi_p^+-\frac{(p-1)\left(\frac{\mathrm{d}\varphi_p^+}{\mathrm{d}\theta}-1\right)}{\varphi_p^+-\theta}\right]\\&=\frac{pA^+_{p,\theta}}{\varphi_p^+-\theta}\left(1-\frac{\sin\theta}{\sin\varphi_p^+}\right)=\frac{\sin\varphi_p^+-\sin\theta}{\left(\varphi_p^+-\theta\right)^p}.\end{aligned} \tag{48}$$

Hence,

$$A^{+}_{p,\theta}\sin\theta+\left(\cos\theta-\sqrt{\epsilon}\right)\frac{\mathrm{d}A^{+}_{p,\theta}}{\mathrm{d}\theta}=\frac{2\sin\frac{\varphi_p^{+}-\theta}{2}\left(\cos\frac{\varphi_p^{+}-\theta}{2}-\sqrt{\epsilon}\cos\frac{\varphi_p^{+}+\theta}{2}\right)}{\left(\varphi_p^{+}-\theta\right)^{p}}. \tag{49a}$$

Similarly, we have

$$A^{-}_{p,\theta}\sin\theta+\left(\cos\theta-\sqrt{\epsilon}\right)\frac{\mathrm{d}A^{-}_{p,\theta}}{\mathrm{d}\theta}=\frac{2\sin\frac{\varphi_p^{-}-\theta}{2}\left(\cos\frac{\varphi_p^{-}-\theta}{2}-\sqrt{\epsilon}\cos\frac{\varphi_p^{-}+\theta}{2}\right)}{\left(\theta-\varphi_p^{-}\right)^{p}}. \tag{49b}$$

Since the argument in expression (45) is a differentiable function of $\theta\in(-\cos^{-1}[\sqrt{\epsilon}],\cos^{-1}[\sqrt{\epsilon}])$, by differentiating this expression with respect to θ with the help of equations (13) and (49), after some algebraic manipulation, we conclude that the extremum in expression (45) occurs when θ obeys equation (46).

Recall from corollary 1 that $\varphi_p^{-}(\theta)=-\varphi_p^{+}(-\theta)$. So from the proof of theorem 1, we know that $r_\epsilon^{-}(\theta)$ is a strictly decreasing function of $\theta\in[-\cos^{-1}(\sqrt{\epsilon}),\cos^{-1}(\sqrt{\epsilon})]$. Applying compound angle formula twice and from corollary 2, we obtain $r_\epsilon^{-}(\theta)|_{\theta=\cos^{-1}(\sqrt{\epsilon})}=\cos[(\varphi_p^{-}-\theta)/2]-\cos\theta\cos[(\varphi_p^{-}+\theta)/2]=\sin[(\varphi_p^{-}+\theta)/2]\sin\theta\leqslant 0$ and $r_\epsilon^{-}(\theta)|_{\theta=0}=(1-\sqrt{\epsilon})\cos(\varphi_p^{-}/2)\geqslant 0$. Therefore, θ_{crit} is the unique solution of equation (47) in the interval $[0,\cos^{-1}(\sqrt{\epsilon})]$. From corollary 2, $\sin[(\varphi_p^{-}-\theta)/2]\geqslant 0$ for $|\theta|\leqslant\pi/2$. In other words, $s_\epsilon^{-}(\theta)\geqslant 0$ for $\theta\in[-\pi/2,\theta_{\text{crit}}]$ and $s_\epsilon^{-}(\theta)<0$ for $\theta\in(\theta_{\text{crit}},\pi/2]$. As $\varphi_p^{+}(\theta)=-\varphi_p^{-}(-\theta)$, we know that $s_\epsilon^{+}(\theta)=-s_\epsilon^{-}(-\theta)$. So $s_\epsilon^{+}(\theta)\geqslant 0$ for $\theta\in[-\pi/2,-\theta_{\text{crit}}]$ and $s_\epsilon^{+}(\theta)<0$ for $\theta\in[\theta_{\text{crit}},\pi/2]$. Hence, solutions of equation (46), if any, must lie in $[-\theta_{\text{crit}},\theta_{\text{crit}}]$.

Let us rewrite $s_\epsilon^{+}(\theta)$ in equation (46) as $s_{\epsilon,1}^{+}(\theta)-\sqrt{\epsilon}s_{\epsilon,2}^{+}(\theta)$. Note that $s_\epsilon^{-}(\theta)=-s_\epsilon^{+}(-\theta)$. Moreover, from the proof of theorem 4, s_ϵ^{+} is differentiable for $\theta\in[-\cos^{-1}(\sqrt{\epsilon}),\cos^{-1}(\sqrt{\epsilon})]$. Furthermore, $s_\epsilon^{+}(-\theta_{\text{crit}})\leqslant 0$ and $s_\epsilon^{+}(\theta_{\text{crit}})\geqslant 0$. So equation (46) has a unique solution in the domain $[-\theta_{\text{crit}},\theta_{\text{crit}}]\subset[-\cos^{-1}(\sqrt{\epsilon}),\cos^{-1}(\sqrt{\epsilon})]$ if we could show that $\mathrm{d}s_{\epsilon,1}/\mathrm{d}\theta>0$ and $\mathrm{d}s_{\epsilon,2}/\mathrm{d}\theta<0$ for any $|\theta|<\theta_{\text{crit}}$.

Clearly, $\theta=\theta_{\text{crit}}$ is the unique solution of equation (46) in $[-\theta_{\text{crit}},\theta_{\text{crit}}]$ in the case of $\theta_{\text{crit}}=0$. So, we only need to consider the case of $\theta_{\text{crit}}>0$. Since $\mathrm{d}s_{\epsilon,2}/\mathrm{d}\theta<0$ if

$$\begin{aligned}&\frac{\mathrm{d}\left(\varphi_p^{+}-\theta\right)}{\mathrm{d}\theta}\cos\left(\frac{\varphi_p^{+}+\theta}{2}\right)\left[\left(\varphi_p^{+}-\theta\right)\cos\left(\frac{\varphi_p^{+}-\theta}{2}\right)-p\sin\left(\frac{\varphi_p^{+}-\theta}{2}\right)\right]\\&\quad-\frac{\mathrm{d}\left(\varphi_p^{+}+\theta\right)}{\mathrm{d}\theta}\left(\varphi_p^{+}-\theta\right)\sin\left(\frac{\varphi_p^{+}-\theta}{2}\right)\sin\left(\frac{\varphi_p^{+}+\theta}{2}\right)<0.\end{aligned} \tag{50}$$

From corollary 2, we know that the second term in the LHS of Inequality (50) is negative and $\cos[(\varphi_p^{+}+\theta)/2]\mathrm{d}(\varphi_p^{+}-\theta)/\mathrm{d}\theta<0$. Therefore, it remains to show that

$$\frac{\varphi_p^{+}-\theta}{2}\cot\left(\frac{\varphi_p^{+}-\theta}{2}\right)\geqslant\frac{p}{2} \tag{51}$$

for all $|\theta|<\theta_{\text{crit}}$. Note that from corollary 2, $(\varphi_p^{+}-\theta)/2\in[0,3\pi/4)$ is a decreasing function of θ. Therefore, according to lemma 2, Inequality (51) holds if this inequality is true for $\theta=\theta_{\text{crit}}$. From equation (47), corollary 2 and the fact that $\varphi_p^{+}(\theta)=-\varphi_p^{-}(-\theta)$, we see that $\varphi_p^{+}-\theta_{\text{crit}}$ is maximized when $\epsilon=1$. This happens when $\theta_{\text{crit}}=0$. From equation (14), $p(1-\cos\varphi_{p,\text{crit}}^{+})=$

$\varphi^+_{p,\text{crit}} \sin\varphi^+_{p,\text{crit}}$. In other words, $[\varphi^+_{p,\text{crit}} - \theta_{\text{crit}}]\cot[(\varphi^+_{p,\text{crit}} - \theta_{\text{crit}})/2] = p$. Hence, Inequality (51) holds for all $|\theta| < \theta_{\text{crit}}$.

Surely, $\mathrm{d}s_{\epsilon,1}/\mathrm{d}\theta > 0$ provided that $(\varphi^+_p - \theta)\cot(\varphi^+_p - \theta) < p$ for all $|\theta| < \theta_{\text{crit}}$. By the similar argument in the previous paragraph, we know that $\varphi^+_p - \theta$ is minimized if $\theta = -\theta_{\text{crit}}$. This happens when $\epsilon = 1$ and hence $\theta_{\text{crit}} = 0$. Therefore, $p(1 - \cos\varphi^+_{p,-\text{crit}}) = \varphi^+_{p,-\text{crit}} \sin\varphi^+_{p,-\text{crit}}$, where $\varphi^+_{p,-\text{crit}}$ is the shorthand notation for $\varphi^+_p(-\theta_{\text{crit}})$. Hence, $p = [\varphi^+_{p,-\text{crit}} + \theta_{\text{crit}}]\cot[(\varphi^+_{p,-\text{crit}} + \theta_{\text{crit}})/2] > (\varphi^+_{p,-\text{crit}} + \theta_{\text{crit}}]\cot(\varphi^+_{p,-\text{crit}} + \theta_{\text{crit}})$. This completes our proof. □

Remark 7. From equations (24) and (46), the θ maximizing expression (45), which we denote by θ_{opt}, obeys

$$\mu^+ |a_-|^2 \left(\theta_{opt} - \varphi^-_p\right)^p = \mu^- |a_+|^2 \left(\varphi^+_p - \theta_{opt}\right)^p. \tag{52}$$

In particular, for the initial quantum state in equation (23) and (52) becomes $\langle[(E - E_r)^+]^p\rangle : \langle[(E_r - E)^+]^p\rangle = \mu^+ : \mu^-$. In other words, from theorem 1, for any $p \in (0,1]$, $\epsilon \in [0,1]$ and for any ratio $\mu^+ : \mu^-$, the CZ bound can be saturated. As expected, θ_{opt} is also equal to the optimized value of θ in Inequality (20*a*) of the CZ bound.

Remark 8. Note that expression (45) attains its maximum when $\theta = \theta_{\text{crit}}$ if $\mu^- = 1$ or $\theta = -\theta_{\text{crit}}$ if $\mu^+ = 1$. In this regard, theorem 4 tells us that for a general μ^+, θ_{opt} lies between these two limiting cases.

To use theorem 4 to compute the CZ bound efficiently, we first need to calculate $\varphi^\pm_p$. Recall that for $(p,\theta) \in \mathcal{R} \setminus (2,0)$, φ^+_p and φ^-_p are the unique roots of equation (14) in the intervals $[|\theta|,\pi)$ and $(-\pi,-|\theta|]$, respectively. In the former case, we use Newton's method with π as the initial guess; and in the latter case, we use $-\pi$ as the initial guess instead. This method is quadratically convergent. Here we prove this claim for φ^+_p. The case of φ^-_p can be similarly proven. Note that from equations (A.3*f*) and (A.3*g*) in the proof of lemma 1 in the appendix, $f''_{p,\theta}(x) < 0$ for $(p,x) \in (0,2] \times [\pi/2,\pi]$ and $f'_{p,\theta}(\pi) \leqslant 0$. As $\varphi^+_p \in [|\theta|,\pi)$ for $p \in (0,1]$, lemma 4 implies that the root φ^+_p of equation (14) in the interval $[|\theta|,\pi)$ can always be found by Newton's method using the initial guess π for the case of $p \in (0,1]$.

For the case when the root $\varphi^+_p \in [0,\pi/2)$, we know from the proof of lemma 1 that this can only happen when $p \in (1,2]$ and $\theta \in (-\pi/2,0]$. In this case, equations (A.3*f*) and (A.3*g*) tell us that $f''_{p,\theta}(\pi/2) = \theta - \varphi_p(\theta) \leqslant 0$ and $f'_{p,\theta}(\pi/2) = 1 - p < 0$. From the proof of lemma 1 in the appendix, we know that $f'_{p,\theta}(x) = 0$ has exactly one root, say, x_1 in $(0,\pi/2)$. In addition, $f''_{p,\theta}(x) = 0$ implies $(x - \theta)\tan x = 2 - p$. Obviously, the LHS of this equation is a bijection from $[0,\pi/2)$ to $[0,+\infty)$. Together with the fact that $p \leqslant 2$, we conclude that $f''_{p,\theta}(x) = 0$ has exactly one root in $(0,\pi/2)$. Thus, $f''_{p,\theta}(x) \leqslant 0$ for all $x \in [x_1,\pi/2]$. Recall that $f''_{p,\theta}(x) \leqslant 0$ for $x \in [\pi/2,\pi]$ and $f'_{p,\theta}(\pi) < 0$. Applying lemma 4 to $f_{p,\theta}(x)$ in the interval $[x_1,\pi]$, we know that Newton's method converges using the initial guess π.

Since θ and φ^+_p are simple roots of equation (14), combined with equation (A.5), Newton's method is stable. Moreover, the necessary conditions for the loss of significance, in this case due to ill-conditioning, are that $\varphi^+_p \approx \theta \approx \pi/2$ and $p \approx 1$. To play safe, we may switch to bisection method in this situation. Nonetheless, our numerical experiment shows that Newton's method is highly accurate in this case as well. The same findings apply to the numerical computation of φ^-_p. Nevertheless, this ill-conditioning issue does affect the computation of expression (45). We shall discuss it in section 5.3 below.

With $\varphi^\pm_p$ now accurately and efficiently evaluated, we can find θ_{opt} by solving equation (46). From the proof of theorem 4, this can be done by bisection method using $[-\theta_{\text{crit}},\theta_{\text{crit}}]$ as the

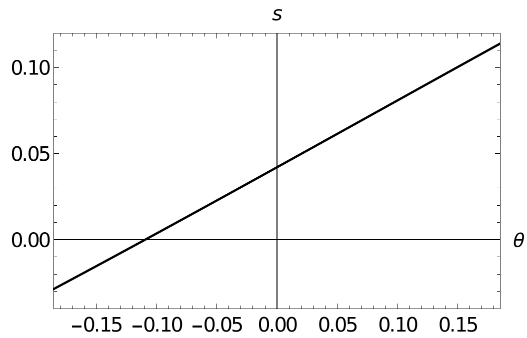

Figure 4. A typical $s(\theta)$ curve is very close to a straight line for all parameters used when $|\theta| \leqslant \theta_{\text{crit}}$. We set $p = 0.7$, $\epsilon = 0.2$ and $\mu^+ = 0.8$ in this plot.

initial interval. We can do much better than this in practice. As depicted in figure 4, $s_\epsilon(\theta)$ looks like a straight line for $|\theta| \leqslant \theta_{\text{crit}}$. Thus, Newton's method with an initial guess of, say, $\theta = 0$, will converge to θ_{opt} quadratically. Another advantage of this method is that we do not need to numerically compute θ_{crit}. In addition, for our parameter ranges, numerical stability is never an issue. As for round-off error, the only situation that requires attention is when $|\varphi_p^\pm| \approx \theta$. Here we may have to use the first few terms of the Taylor's series expansion of $\sin[(\varphi_p^\pm - \theta)/2]$ to accurately compute $\sin[(\varphi_p^\pm - \theta)/2]/|\varphi_p^\pm - \theta|^p$.

5.3. Computation of expression (45)

Recall that the $\mu^\pm$ corresponding to the optimized $\langle |E - E_r|^p \rangle$ may not be unique if $0 < p < 1$. In this case, we need to maximize expression (45) over all these $\mu^\pm$'s and hence the corresponding θ_{opt}'s. Furthermore, irrespective of the uniqueness of $\mu^\pm$, from equation (12), in order to evaluate expression (45) accurately, highly accurate θ_{opt} and $\varphi_p^+(\theta_{\text{opt}})$ are required if $\varphi_p^+(\theta_{\text{opt}}) \approx \pi$ or θ_{opt} to compensate for the loss of significance in evaluating $A^\pm_{p,\theta_{\text{opt}}}$ due to ill-conditioning and error propagation. Similarly for $\varphi_p^-(\theta_{\text{opt}})$. To compute expression (45) to a certain accuracy in these situations, we may have to evaluate θ_{opt} and $\varphi_p^\pm(\theta_{\text{opt}})$ to higher precision. This can be done by changing the stopping criterion and perhaps also by increasing the working precision. From equation (14), if $\varphi_p^+ \approx \pi$, then $p = O(\pi - \varphi_p^+)$, which is small. Conversely, if p is small, then $\varphi_p^+ = \pi - O(p)$. That is to say, we need to evaluate φ_p^+ to a higher working precision to avoid round-off error if $p \approx 0$. In fact, our numerical experiments suggest that using double precision arithmetic, rounding error is an issue, sometimes a serious one that gives totally wrong results, when $p \lesssim 10^{-5}$. So we switch to quadruple precision arithmetic for $p < 10^{-5}$ in our Mathematica code.

In summary, given p, ϵ and μ^+, the method outlined in the previous paragraph can compute expression (45) by numerically solving up to three equations, one for θ_{opt} and another two for $\varphi_p^\pm(\theta_{\text{opt}})$. (In case $\theta_{\text{opt}} = 0$, one only needs to solve φ_p^+ as it is equal to $-\varphi_p^-$.) And to evaluate the CZ bound in Inequality (20), one has to further numerically find $E_{r,\text{opt}}$ and hence μ^+ by solving one more equation. (In case μ^+ is not unique, one has to solve θ_{opt} and $\varphi_p^\pm$ for each μ^+.) Finally, one obtains the RHS of Inequality (20) by substitution. In contrast, the most efficient way to obtain the ML bound numerically is by solving just one single equation given ϵ [25]. Can we adapt that method here?

The reason why the ML bound can be obtained by solving just one equation is that we can recast the problem as finding a normalized initial state that saturates the ML bound. Since any such state must belong to the Hilbert space spanned by two energy eigenstates of the Hamiltonian, only one degree of freedom remains, namely, the amplitude square of the ground state energy component of the normalized initial state. More importantly, the exact evolution time can be written as an explicit function of this amplitude square as well as ϵ. Hence, computing the ML bound is reduced to the problem of maximizing certain evolution time, which can further be reduced to the problem of solving a non-linear equation of one variable [25].

Following the same logic, evaluating the CZ bound in this way has to optimize over a normalized initial state in the form of equation (23), which has two degrees of freedom, namely, $|a_+|^2$ and $|a_-|^2$. Unfortunately, the evolution time given ϵ is an implicit function of $|a_\pm|^2$'s that we do not know how to write in an explicit form. Thus, we can only proceed by solving a system of three Equations, namely, the one relating the evolution time with $|a_\pm|^2$'s and two equations determined by maximizing the evolution time through varying $|a_\pm|^2$'s. Consequently, there is no computational advantage over the method we have just presented.

5.4. *Computation of the CZ bound for fixed* p

With the above discussion, it is clear that for a fixed p, the CZ bound can be computed as follows.

1. Find $\langle |E - E_{r,\text{opt}}|^p\rangle$ and μ^+ either using the method in section 5.1 through determining $E_{r,\text{opt}}$ or by an oracle that returns $\langle |E - E_{r,\text{opt}}|^p\rangle$ and $\langle [(E - E_{r,\text{opt}})^+]^p\rangle$.
2. If $p \in (0,1]$, compute θ_opt using the method in section 5.2. Otherwise, set $\theta_\text{opt} = 0$.
3. Finally, compute expression (45) and hence the CZ bound using method in section 5.3.

Evaluating the LC bound can be done in almost the same way. The only exception is that θ_opt is always set to 0. For finite-dimensional quantum systems, this method is computationally accurate and efficient.

Last but not least, we remark that our analysis here focuses on a fixed p. In spite of the fact that both $\lim_{p\to 0^+}\langle [(E - E_r)^+]^p\rangle$ and $\lim_{p\to 0^+}\langle [(E_r - E)^+]^p\rangle$ exist for any given E_r, the existence of finite LC or CZ bounds as $p \to 0^+$ is not guaranteed. We shall report an interesting consequence of this observation in section 6.

5.5. *Computation of the optimized CZ bound*

Calculating the optimized CZ bound is straightforward to implement but difficult to analyze. Without additional information on $|\Psi(0)\rangle$, the powerful convex optimization method does not apply. All we can do is to use a modern general optimization algorithm, such as differential evolution and Nelder–Mead method, over the parameter p using the CZ bound for fixed p as the target function. Note that $\varphi_p^\pm$ vary smoothly with θ. If we further assume that $\langle |E - E_r|^p\rangle$, $\langle [(E - E_r)^+]^p\rangle$, $\langle [(E - E_r)^+]^{p-1}\rangle$ and $\langle [(E_r - E)^+]^{p-1}\rangle$ are continuous and monotonic functions of p, then we expect that any modern general optimization algorithm should work reasonably well both in speed and in accuracy. One of us has posted the Mathematica code to compute the optimized CZ bound [32]. Based on this code, our numerical experiments to be reported in section 6 show that this is indeed the case although vigorous mathematical analysis is beyond reach for a general $|\Psi(0)\rangle$. The same analysis applies also to the calculation of the optimized LC and LZ bounds. Once again, our numerical experiments find that modern general optimization algorithms work very well for these two optimized bounds.

5.6. Simple expression for the optimized CZ bound on two-dimensional quantum systems

Interestingly, numerical analysis in this section gives us a simplified expression for the optimized CZ bound on two-dimensional quantum systems. By shifting the reference level, we write the normalized initial state of such system as $a_1|E_1\rangle + a_0|E_0\rangle$ with $E_1 > E_0$.

For the case of $p \leqslant 1$, analysis in section 5.1 tells us that $E_{r,\mathrm{opt}}$ is either E_0 or E_1. For the first subcase, μ^+ defined in theorem 4 has to be 1; whereas for the second subcase, $\mu^+ = 0$. So from theorem 4 and remark 8,

$$\left(\frac{\tau}{\hbar}\right)^p \geqslant \frac{1}{(E_1 - E_0)^p} \frac{\cos\theta_{crit} - \sqrt{\epsilon}}{\min\left(A^+_{p,-\theta_{crit}}|a_1|^2, A^-_{p,\theta_{crit}}|a_0|^2\right)}, \tag{53}$$

with θ_{crit} given by the unique solution of equation (47).

If $1 \leqslant p \leqslant 2$, then $E_{r,\mathrm{opt}}$ obeys equation (43) so that the CZ bound becomes

$$\left(\frac{\tau}{\hbar}\right)^p \geqslant \frac{1 - \sqrt{\epsilon}}{(E_1 - E_0)^p A_{p,0}} \left(|a_0|^{-\frac{2}{p-1}} + |a_1|^{-\frac{2}{p-1}}\right)^{p-1}. \tag{54}$$

Thus, the optimized CZ bound for two-dimensional quantum systems can be expressed as

$$\frac{\tau}{\hbar} \geqslant \frac{1}{E_1 - E_0} \max\left\{ \max_{1\leqslant p\leqslant 2} \left[\frac{(1-\sqrt{\epsilon})\left(|a_0|^{-\frac{2}{p-1}} + |a_1|^{-\frac{2}{p-1}}\right)}{A_{p,0}}\right]^{\frac{1}{p}}, \max_{0<p\leqslant 1}\left[\frac{\cos\theta_{crit} - \sqrt{\epsilon}}{\min\left(A^+_{p,-\theta_{crit}}|a_1|^2, A^-_{p,\theta_{crit}}|a_0|^2\right)}\right]^{\frac{1}{p}}\right\}. \tag{55}$$

A notable feature of this expression is that its RHS is proportional to a factor that depends only on ϵ and $|a_0|$.

6. Performance analysis

Table 1 compares the minimum evolution times for various initial pure quantum states in energy representation using different QSLs. (Recall from section 2 that the dual ML bound is basically the ML bound of a time- and energy-reversed system. Thus, we omit the dual ML bound in our table because such comparison is already reflected in the relative performance between ML and CZ bounds over various initial states.) These initial states are specifically chosen to illustrate our points. From table 1, it is clear that the optimized CZ bound is the best for all cases which is closely followed by the optimized LC bound. This result is consistent with our conclusion in section 4 that the optimized CZ bound unifies all other bounds in the table. It also demonstrates that the MT, ML and optimized LZ bounds are mutually complementary, and so are the optimized LZ and optimized LC bounds.

Let us study table 1 in detail. The initial state of case number (a) is $|\Psi(0)\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. It saturates the MT bound for any given of $\epsilon \in [0,1]$. Table 1 shows that all the bounds we have covered give the saturation value of π when $\epsilon = 0$. This is consistent with our conclusion in theorem 2 that the optimized LC and hence the optimized CZ bounds are at least as good as the MT bound.

Table 1. Various QSL bounds for various initial states $|\Psi(0)\rangle$ and square root fidelities $\sqrt{\epsilon}$. The initial states used in this table from case (a) to (g) are $(|0\rangle+|1\rangle)/\sqrt{2}$, $\sum_{j=0}^{2047}|j\rangle/2^{11/2}$, $\sum_{j=1}^{2048}j^{-1}|j\rangle/\sqrt{\sum_{\ell=1}^{2048}\ell^{-2}}$, $\sqrt{0.1}|0\rangle+\sqrt{0.9}|1\rangle$, $\sqrt{0.3}|0\rangle+\sqrt{0.6}|1\rangle+\sqrt{0.1}|2\rangle$, $\sqrt{0.3}|0\rangle+\sqrt{0.6}|1\rangle+\sqrt{0.1}|\pi\rangle$ and $\sqrt{0.4}|0\rangle+\sqrt{0.45}|1\rangle+\sqrt{0.15}|2\pi\rangle$, respectively. Note that the LZ bound is optimized over p, the LC bound is optimized over p and E_r, whereas the CZ bound is optimized over p, θ and E_r. We do not tabulate the optimized values of E_r here because relatively little can be learned from it. Note that all QSL bounds obtained are finite except for the optimized LC and CZ bounds in case number (e) with $\sqrt{\epsilon}=0.19$. For the divergent case, the 'best estimation' of the optimized LC bound is $\approx 10^{4700}$ at $p\approx 10^{-6}$. And the 'the estimation' of the optimized CZ bound is $\approx 10^{50000000}$ at $p\approx 10^{-10}$ and $\theta\approx 10^{-11}$.

				optimized LZ		optimized LC		optimized CZ		
case	$\sqrt{\epsilon}$	MT bound	ML bound	bound	p_{opt}	bound	p_{opt}	bound	p_{opt}	θ_{opt}
(a)	0	3.1416	3.1416	3.1416	1.78	3.1416	1.2×10^{-5}	3.1416	8.8×10^{-4}	-5.6×10^{-4}
(b)	0	2.66×10^{-3}	1.53×10^{-3}	1.88×10^{-3}	2.00	2.84×10^{-3}	1.36	2.84×10^{-3}	1.36	0.00
(c)	0	0.0353	0.2181	0.4166	0.46	0.3961	0.44	0.4166	0.42	−0.28
(d)	0.1	4.9021	1.5432	2.1437	2.00	12.4204	1.00	12.4204	1.00	0.00
(e)	0.19	2.2994	1.5397	1.8485	2.00	∞^*	0.00^*	∞^*	0.00^*	0.00^*
	0.20	2.2824	1.5183	1.8268	2.00	3.1416	1.3×10^{-5}	3.1416	1.3×10^{-5}	2.9×10^{-6}
(f)	0.20	1.5800	1.3287	1.4586	1.75	2.5970	1.2×10^{-5}	2.5970	1.0×10^{-5}	2.2×10^{-6}
(g)	0.00	0.7461	1.1281	1.1795	0.67	1.3401	0.46	1.3410	0.46	0.03
	0.15	0.6746	0.9342	0.9323	0.89	1.0211	0.73	1.0221	0.74	−0.04
	0.35	0.5762	0.6932	0.6641	1.12	0.7525	1.02	0.7577	1.00	−0.10
	0.99	0.0672	0.0099	2.7×10^{-14}	0.19	0.0674	1.99	0.0674	1.99	0.00

The initial state considered in case (b) of table 1 is $\sum_{j=0}^{2047} |j\rangle/2^{11/2}$. The time for it to its orthogonal complement equals $\tau = \pi\hbar/1024 \approx 0.0030680\hbar$. In this case, both the optimized LC and CZ bounds are the best. They give about 92.5% of the actual evolution time whereas the MT bound is just about 86.6%. Here, both the optimized LC and CZ bounds give the same $p_{\text{opt}} \approx 1.36 > 1$.

Likewise, the (un-normalized) quantum state $\sum_{j=1}^{2048} j^{-1}|j\rangle$ used in case (c) is also 2048-dimensional. (Here the dimension refers to the minimum Hilbert space dimension of the Hamiltonian needed to support such an initial quantum state. We simply call this the Hilbert space dimension of the system and denote it by n.) Its values of p_{opt} for both the optimized LC and CZ bounds are $\approx 0.89 < 1$. We pick cases (a)–(c) to test how the computational times vary as the Hilbert space dimension of the system n increases for various QSLs in practice. Moreover, we compare the practical efficiency of our methods for both $p_{\text{opt}} < 1$ and $p_{\text{opt}} \geqslant 1$ in case n is large since the algorithms of finding $E_{r,\text{opt}}$ introduced in section 5.1 and their corresponding complexities are vastly different in these two cases. We use Mathematica code with just-in-time compilation installed in a typical desktop to compare their performance. For the MT and ML bounds, increasing n from 2 to 2048 has relatively little effect on the computational times. The runtimes for the ML bound are at most several ms in all three cases. In contrast, the runtimes for the MT bounds are about 20 μs, 0.9 ms and 40 ms for cases (a) to (c), respectively. For the unoptimized LZ bound, the runtimes are similar to those of the MT bound. Whereas for the optimized LZ bound, it increases from about 50 ms to about 0.3 s when n increases from 2 to 2048. As expected, longer times are needed to compute the bound for fixed p and much longer to optimize p as n increases. For example, for the unoptimized LC bound, the runtimes are less than 1 ms for case (a), about 70 ms for case (b) and about 0.1 s for case (c). And for the optimized LC bound, the runtimes are about 0.5 s, 150 s and 300 s for cases (a) to (c), respectively. Last but not least, for the unoptimized CZ bound, the increase is from about 3 ms for case (a) to about 70 ms for case (b) to about 0.1 s for case (c); while for the optimized CZ bound, the increase is from about 5 s for case (a) to 150 s for case (b) to about 300 s for case (c). To conclude, our experiment shows that the unoptimized LZ, LC and CZ bounds are all extremely efficient to evaluate. And up to our expectation, longer time is required to compute both the optimized and unoptimized versions of the LC and CZ bounds when $p_{\text{opt}} \leqslant 1$ because of the higher computational complexity cost partly due to the existence of n local minima in $\langle |E - E_r|^p \rangle$. But in all cases, their optimized versions are fast enough to be used in the field even when the Hilbert space dimension of the system n is of order of 1000. Here we also mention on passing that simply using generic optimization method to obtain the optimized LC and CZ bounds is in general not practical when n is large. This is particularly true when $p_{\text{opt}} \leqslant 1$. For example, computing the optimized CZ bound in case (c) using generic optimization takes about 1.3 hr even for probabilistic methods. This is roughly 15 times longer than our algorithm. Sometimes, generic optimization fails to produce an answer due to insufficient computer memory. To be fair, using differential evolution, a generic probabilistic optimization technique, the runtime of the optimized LC bound for case (c) can sometimes be shortened to about 13 s. We do not have a good explanation though.

We now investigate how these QSLs perform when it is not possible to evolve the given initial state to another state with fidelity ϵ in finite time. Consider case (d) with $\sqrt{\epsilon} = 0.1$ and case (e) with $\sqrt{\epsilon} = 0.2$. It is easy to show that the required evolution is not possible. We pick these two cases to illustrate two points. First, the optimized LC and CZ bounds can all diverge as $p \to 0^+$. (We also see in some other cases not listed in table 1 that the optimized LZ bound diverges as well.) Second, even for the case that these bounds cannot detect this impossible evolution, they generally give much higher QSLs. Next, we use case (f) to test how various QSLs handle another type of impossible evolution. Specifically, we choose $|\Psi(0)\rangle = \sqrt{0.3}|0\rangle + \sqrt{0.6}|1\rangle + \sqrt{0.1}|\pi\rangle$ so that it could reach $\sqrt{0.3}|0\rangle - \sqrt{0.6}|1\rangle + \sqrt{0.1}|\pi\rangle$, namely, the only state whose fidelity ϵ is 0.2^2 from it only in infinite time. Table 1 shows that none of the bounds correctly give a divergent result even though the optimized LC and CZ bounds give identical QSL that is significantly higher than the rest. This is not surprising for given only information on the pth moments of the absolute value of energy of this type of systems, one may not have enough information to conclude that the evolution cannot be completed in finite time. Note that the same conclusion can be drawn for case (g) with $\epsilon = 0$ that we will cover in detail later in this section.

As a variation of the theme, we consider case (e) with $\sqrt{\epsilon}$ around 0.2. The evolution time τ needed is π. (In fact, the evolution time is finite whenever $\sqrt{\epsilon} \geqslant 0.2$.) Interestingly, Table 1 tells us that both the optimized LC and CZ bounds give this exact result. More importantly, first order phase transition in the values of the optimized LC and CZ bounds are observed at $\sqrt{\epsilon} = 0.2$. This demonstrates the power of these two optimized bounds.

The last case we consider is case (g). Here we fix $|\Psi(0)\rangle = \sqrt{0.4}|0\rangle + \sqrt{0.45}|1\rangle + \sqrt{0.15}|2\pi\rangle$ and vary ϵ. Surely, table 1 shows that all bounds decrease as ϵ increases. In addition, we find that the optimized LC and CZ bounds are the best. They are generally better than the other QSLs by about 10%. (And in some other cases listed in table 1, they can be about 30% to 60% better, sometimes even a few times better.) Besides, when $p_{\text{opt}} \leqslant 1$, the optimized CZ bound is better than the optimized LC bound by about 1% because the optimized CZ bound has the freedom to pick a non-zero θ_{opt}. In addition, we see that p_{opt} increases as ϵ increases for the optimized LC and CZ bounds. Table 1 also demonstrates that p_{opt} can take on any value in $(0, 2]$, including the special case of $p_{\text{opt}} = 1$. These two trends are consistent with the fact that the evolution time τ decreases with increasing ϵ so that the optimized p_{opt} is likely to be the one with $\varphi^{\pm}_{p,\text{opt}}$ both getting closer and closer to θ_{opt}.

7. Conclusions and outlook

To summarize, we have proven the optimized CZ bound that includes all existing QSLs for time-independent Hamiltonian evolution as special cases. We also developed a precise and accurate numerical algorithm to compute this bound for quantum systems with underlying Hilbert space dimension $\lesssim$2000 and illustrated the usage of this bound through example initial states in table 1. This optimized CZ bound is at least as well as the existing ones and sometimes can be a few percent to a few times better.

It is instructive to see how this bound can be used as a performance metric in realistic situation. One possibility we have identified is in quantum control using piecewise constant pulse such as the one used in [33]. This would be our follow up project.

Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: https://community.wolfram.com/groups/-/m/t/3059 079.

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Appendix

Proof of lemma 1. To show the validity of Inequality (11) for $x > \theta$, it suffices to prove that $A_{p,\theta}$ exists and equals

$$A_{p,\theta} = \sup_{x>\theta} m_{p,\theta}(x) \equiv \sup_{x>\theta} \frac{\cos\theta - \cos x}{(x-\theta)^p}. \tag{A.1}$$

Since $m_{p,\theta}(\pi) > 0$ for all $\theta \in (-\pi, \pi/2]$, $A_{p,\theta} > 0$ if it exists. As $m_{p,\theta}(x) < 0$ for $\theta < 0$ and $\theta < x < -\theta$, we only need to consider those $x \geqslant -\theta$ for the supremum in equation (A.1) if $\theta < 0$. By fixing $b \in [-1, \cos\theta)$ for $\theta \in (-\pi, \pi/2]$, the set $S_{b,\theta} = \{x > \theta \colon \cos x = b\}$ is non-empty and $\min S_{b,\theta} \in [|\theta|, \pi]$. Observe that $m_{p,\theta}(x) > m_{p,\theta}(y)$ for all $x, y \in S_{b,\theta}$ with $x < y$ and $p > 0$. So, $\lim_{x\to\theta+} m_{p,\theta}(x)$ exists if $(p,\theta) \in \mathcal{R}$. Consequently, by extending the definition of $m_{p,\theta}(x)$ to $x = \theta$ by continuity in the case of $\theta \geqslant 0$, the supremum in equation (A.1) is in fact a maximum attained at a certain $\varphi_p(\theta) \in [|\theta|, \pi]$. Since $dm_{p,\theta}(\pi)/dx < 0, A_{p,\theta} > m_{p,\theta}(\pi)$, we can safely omit $x = \pi$ in this maximization. In this way, we obtain Inequality (11) for $(p,\theta) \in \mathcal{R}$.

We rewrite Inequality (11) as

$$g_{p,\theta}(x) \equiv \cos x - \cos\theta + A_{p,\theta}(x-\theta)^p \geqslant 0 \tag{A.2}$$

for all $x \geqslant \theta$. (Surely, Inequality (A.2) is trivially true for $x = \theta$.) Suppose the maximum of the RHS of equation (12) is reached when $x = \varphi_p(\theta)$. For the time being, we do not assume that $\varphi_p(\theta)$ is unique. We simply set $\varphi_p(\theta)$ to be any one of those x's that maximizes the RHS of equation (12). And we are going to prove its uniqueness in the next paragraph. Clearly, $x = \theta$ and $\varphi_p(\theta)$ are zeros of the equation $g_{p,\theta}(x) = 0$ with the latter being a multiple root. Hence, $g_{p,\theta}(\varphi_p) = g'_{p,\theta}(\varphi_p) = 0$. This gives the expressions for $A_{p,\theta}$ and $f_{p,\theta}$ in equations (13) and (14), respectively.

We now prove the properties of the solutions of equation (14) in lemma 1. Obviously, there is exactly one x maximizing equation (A.1) if these properties are correct. This is because more than one maximizing $x \in (|\theta|, \pi)$ means that there are at least two distinct $\varphi_p(\theta)$'s both in the same relevant domain satisfying equation (14). This contradicts with the property that $\varphi_p(\theta)$ is unique. We divide the remaining proof into the following five cases. And we make use of the following equations, which are derived from equation (14).

$$f_{p,\theta}(0) = p(1-\cos\theta), \tag{A.3a}$$

$$f_{p,\theta}(\theta) = 0, \tag{A.3b}$$

$$f_{p,\theta}(-\theta) = 2\theta\sin\theta, \tag{A.3c}$$

$$f_{p,\theta}\left(\frac{\pi}{2}\right) = \frac{\pi}{2} - \theta - p\cos\theta, \tag{A.3d}$$

$$f_{p,\theta}(\pi) = -p(1+\cos\theta), \tag{A.3e}$$

$$f'_{p,\theta}(\varphi_p) = (1-p)\sin\varphi_p + (\varphi_p - \theta)\cos\varphi_p \tag{A.3f}$$

and

$$f''_{p,\theta}(\varphi_p) = (2-p)\cos\varphi_p - (\varphi_p - \theta)\sin\varphi_p. \tag{A.3g}$$

Case (a): $(p,\theta) \in (0,1] \times (-\pi, 0)$. It is clear from equation (A.3g) that $f''_{p,\theta}(\varphi_p)$ is a smooth function of φ_p and $f''_{p,\theta}(\pi/2) \neq 0$. Hence, $f''_{p,\theta}(\varphi_p) = 0$ implies that

$$(\varphi_p - \theta)\tan\varphi_p = 2 - p \tag{A.4}$$

for $\varphi_p \in [0,\pi)$. Obviously, the LHS of equation (A.4) is a strictly increasing non-negative function in $[0,\pi/2)$ and a strictly increasing non-positive function in $(\pi/2,\pi]$, respectively. As a result, equation (A.4) has a unique simple root x_c in the interval $(0,\pi/2)$. Combined with $f''_{p,\theta}(0) > 0$ and $f''_{p,\theta}(\pi) < 0$, we conclude that $f''_{p,\theta}(x) > 0$ for all $x \in [0,x_c)$ and $f''_{p,\theta}(x) < 0$ for all $x \in (x_c,\pi)$.

As $f_{p,\theta}(0), f'_{p,\theta}(0) > 0$, we deduce from the sign of $f''_{p,\theta}(x)$ for $x \in [0,x_c)$ that $f_{p,\theta}(x) > 0$ for all x in this interval and $f'_{p,\theta}(x_c) > 0$. According to equation (A.3*d*), $f_{p,\theta}(\pi/2)$ decreases as θ increases from $-\pi$ to 0. Therefore, $f_{p,\theta}(\pi/2) \geqslant f_{p,0}(\pi/2) = \pi/2 - p > 0$. From the sign of $f''_{p,\theta}(x)$ for $x \in (x_c,\pi)$, we know that $f_{p,\theta}(x) > 0$ for all $x \in (x_c,\pi/2]$. Besides, $f'_{p,\theta}(x)$ is strictly decreasing in $(\pi/2,\pi)$ according to the analysis in the last paragraph. Together with $f_{p,\theta}(\pi) < 0$, we conclude that equation (14) has a unique simple root in $(\pi/2,\pi)$. This is because mean value theorem implies that equation (14) has a root in $(\pi/2,\pi)$. As the roots of equation (14) in this interval forms a closed set, the smallest root exists which we denote by x_r. Since $f_{p,\theta}(\pi/2) > 0$ and $f'_{p,\theta}(x)$ is strictly decreasing in $(\pi/2,\pi)$, we know that $f'_{p,\theta}(x_r) < 0$. Consequently, x_r is the unique root of equation (14) in $(\pi/2,\pi)$ because $f_{p,\theta}(x) > 0$ for all $x \in (\pi/2,x_r)$ and $f_{p,\theta}(x) < 0$ for all $x \in (x_r,\pi)$.

Lastly, as $f_{p,\theta}(-\theta) > 0$, this unique solution of equation (14) must lie in $[|\theta|,\pi)$ and hence in $[\max(|\theta|,\pi/2),\pi)$. This completes the proof of the properties of roots of equation (14) in this case.

Case (b): $(p,\theta) \in (0,1] \times (0,\pi/2]$. Note that $f_{p,\theta}(\theta) = 0$ and $f'_{p,\theta}(\theta) \geqslant 0$ with equality holds if and only if $p = 1$. Moreover, using the same argument to analyze $f''_{p,\theta}$ through equation (A.4) in the proof of case (a), there is a $\bar{x}_c \in (0,\pi/2)$ such that $f''_{p,\theta}(\bar{x}_c) = 0$, $f''_{p,\theta}(x) > 0$ for $x \in (\theta,\bar{x}_c)$ and $f''_{p,\theta}(x) < 0$ for $x \in (\bar{x}_c,\pi)$. Therefore, for $f_{p,\theta}(\theta+\delta), f'_{p,\theta}(\theta+\delta) > 0$ provided that $p \neq 1$ and $\delta > 0$ is sufficiently small. By Taylor's series expansion with remainder, the same is true for the case of $p = 1$. Using similar argument in the proof of case (a), we deduce that $f_{p,\theta}(\pi/2) \geqslant f_{p,\pi/2}(\pi/2) = 0$ with equality holds if and only if $\theta = \pi/2$.

From the same argument using the sign of $f''_{p,\theta}$ in case (a) and by using the fact that $f_{p,\theta}(\pi) < 0$, we conclude that $f_{p,\theta}(x) > 0$ for all $x \in (\theta,\pi/2)$. Besides, equation (14) has a unique simple root in $[\pi/2,\pi)$.

Case (c): $(p,\theta) \in (1,2] \times (-\pi,0)$. Using the same argument on $f''_{p,\theta}$ in the proof of case (a), we know that there is a $\bar{\bar{x}}_c \in (0,\pi/2)$ such that $f''_{p,\theta}(\bar{\bar{x}}_c) = 0$, $f''_{p,\theta}(x) > 0$ for $x \in [0,\bar{\bar{x}}_c)$ and $f''_{p,\theta}(x) < 0$ for $x \in (\bar{\bar{x}}_c,\pi/2)$. Note that $f_{p,\theta}(0), f_{p,\theta}(-\theta)$ and $f'_{p,\theta}(0) > 0$. So using the same argument as in the proof of case (a), we know that $f_{p,\theta}(x) > 0$ for all $x \in [0,|\theta|]$. Together with the fact that $f_{p,\theta}(\pi) < 0$, we conclude that equation (14) has a unique simple root in $[|\theta|,\pi)$.

Case (d): $(p,\theta) \in (0,2) \times \{0\}$. In this case, $f_{p,0}(0) = f'_{p,0}(0) = 0$ and $f''_{p,0}(0) > 0$. Hence, $f_{p,0}(\delta), f'_{p,0}(\delta) > 0$ for a sufficiently small $\delta > 0$. Together with $f_{p,0}(\pi) < 0$, we can use the same argument as in the proof of case (a) to deduce the existence of a unique simple root for equation (14) in $(0,\pi)$. Furthermore, if $p \in (0,1]$, using the argument in the proof of case (a), we know that $f_{p,0}(\pi/2) > 0$. Hence, the solution of equation (14) can be further restricted to $[\pi/2,\pi)$.

Case (e): $(p,\theta) = (2,0)$. The argument is similar to that in the proof of case (d). Here, it is straightforward to check that $f^{(j)}_{p,0}(0) = 0$ for $j = 0,1,2,3$. Besides, $f^{(4)}_{p,0}(0) < 0$. Therefore, 0 is a root of equation (14) of order 4. From equation (A.3*g*), $f''_{p,0}(x) < 0$ for $x \in (0,\pi)$. Therefore, $f'_{p,0}(x) < 0$ and $f_{p,0}(x) < 0$ for $x \in (0,\pi)$. In other words, 0 is the only root of equation (14) in $[0,\pi)$. This completes the proof of case (e). □

Proof of corollary 2. Here we only prove properties of those functions involving $\varphi_p^+(\theta)$. As $\varphi_p^-(\theta) = -\varphi_p^+(-\theta)$, properties of those functions involving $\varphi_p^-(\theta)$ follows from the properties of the corresponding functions of $\varphi_p^+(\theta)$. Recall from lemma 1 that equation (14) has a unique solution $\varphi_p^+(\theta) \in [-\pi/2, \pi)$ whenever $p \in (0,1]$ and $\theta \in [-\pi/2, \pi/2]$. Therefore, $\varphi_p^+ \pm \theta \in [0, 3\pi/2)$. Moreover, the solution of equation (14), namely, $\varphi_p^+(\theta)$, is the one that maximizes the RHS of equation (12). Thus, applying the implicit function theorem to equation (14), we know that φ_p^+ is differentiable and equals

$$\frac{\mathrm{d}\varphi_p^+}{\mathrm{d}\theta} = \frac{\sin\varphi_p^+ - p\sin\theta}{\left(\varphi_p^+ - \theta\right)\cos\varphi_p^+ + (1-p)\sin\varphi_p^+} \tag{A.5}$$

provided that the denominator of this equation is non-zero.

We claim that this denominator is non-positive for all $|\theta| \leqslant \pi/2$ and $p \in (0,1]$ with equality holds if and only if $p = 1$ and $\theta = \pi/2$. In these parameter ranges, lemma 1 implies that $\varphi_p^+ \in [\pi/2, \pi)$ and $\varphi_p^+ \geqslant |\theta|$ with equality holds if $\theta = \pi/2$. By multiplying the denominator of equation (A.5) by $\sin\varphi_p^+$ and by using equation (14), it suffices to prove that

$$\kappa(p,\theta) = \sin^2\varphi_p^+ - p + p\cos\theta\cos\varphi_p^+ \leqslant 0. \tag{A.6}$$

(Note that through equation (14), we may regard κ as a function of p and θ.) From equation (14), we know that

$$\frac{\partial\theta}{\partial p} = \frac{\cos\varphi_p^+ - \cos\theta}{(1-p)\sin\theta}. \tag{A.7}$$

Hence,

$$\frac{\mathrm{d}\kappa}{\mathrm{d}p} = \cos\theta\cos\varphi_p^+ - 1 - \frac{p\cos\varphi_p^+\left(\cos\varphi_p^+ - \cos\theta\right)}{1-p} < 0 \tag{A.8}$$

whenever $|\theta| < \pi/2$. Therefore,

$$\kappa(p,\theta) < \lim_{q\to 0^+}\kappa(q,\theta) = \lim_{q\to 0^+}\sin^2\varphi_q(\theta) = 0 \tag{A.9}$$

for all $\theta \in [-\pi/2, \pi/2)$. Here we obtain the last equality by solving equation (14) in the limit of $q = 0^+$. From equation (14), $[\varphi_p^+(\pi/2) - \pi/2]\tan\varphi_p^+(\pi/2) = -p$. Using the analysis on the property of equation (A.4) in the proof of lemma 1, we conclude that $\varphi_p^+(\pi/2) \geqslant \pi/2$ with equality holds if and only if $p = 1$. So, $\kappa(p,\pi/2) \leqslant \lim_{q\to 0^+}\kappa(q,\pi/2) = \sin^2\varphi_0^+(\pi/2) - p = 0$ with equality holds if and only if $p = 1$. In summary, $\kappa(p,\theta) \leqslant 0$ for $p \in (0,1]$ and $|\theta| \leqslant \pi/2$. This proves our claim that the denominator of equation (A.5) is non-positive and equality holds if and only if $(p,\theta) = (1,\pi/2)$.

As φ_p^+ is differentiable for $|\theta| \leqslant \pi/2$, so to prove that $\varphi_p^+ - \theta$ is a strictly decreasing function of θ is equivalent to show that $\sin\varphi_p^+ - p\sin\theta > (\varphi_p^+ - \theta)\cos\varphi_p^+ - (1-p)\sin\varphi_p^+$. Multiplying this inequality by $\sin\varphi_p^+$ and using equation (14), this is equivalent to proving that

$$2\sin^2\varphi_p^+ + p\left[\cos 2\varphi_p^+ - \cos\left(\varphi_p^+ - \theta\right)\right] > 0. \tag{A.10}$$

Clearly, this inequality holds if $\cos 2\varphi_p^+ \geqslant \cos(\varphi_p^+ - \theta)$. And for the case of $\cos 2\varphi_p^+ < \cos(\varphi_p^+ - \theta)$, it suffices to show that

$$0 < 2\sin^2\varphi_p^+ + \cos 2\varphi_p^+ - \cos\left(\varphi_p^+ - \theta\right) = 1 - \cos\left(\varphi_p^+ - \theta\right). \tag{A.11}$$

Since $\varphi_p^+ > \theta$ unless $\theta = \pi/2$, Inequality (A.11) is satisfied except possibly when $\varphi_p^+ = \theta = \pi/2$. And in this case, equation (A.5) becomes $d\varphi_p^+/d\theta = 1$. Therefore, $\varphi_p^+ - \theta$ is a strictly decreasing function of θ.

By the same token, we prove that $\varphi_p^+ + \theta$ is an increasing function of θ by showing that

$$\begin{aligned} & \sin\varphi_p^+ - p\sin\theta + \left(\varphi_p^+ - \theta\right)\cos\varphi_p^+ - (1-p)\sin\varphi_p^+ < 0 \\ \iff & \cos\left(\varphi_p^+ + \theta\right) - \cos 2\varphi_p < 0 \\ \iff & \sin\left(\frac{3\varphi_p^+ + \theta}{2}\right)\sin\left(\frac{\varphi_p^+ - \theta}{2}\right) < 0. \end{aligned} \tag{A.12}$$

So, it suffices to prove that $3\varphi_p^+ + \theta \in (2\pi, 4\pi)$. Let us write $3\varphi_p^+ + \theta = 3(\varphi_p^+ - \theta) + 4\theta$. Since $\varphi_p^+ - \theta$ is a strictly decreasing function of θ whose range is in $[0, 3\pi/2)$, we conclude that $3\varphi_p^+ + \theta \in (2\pi, 5\pi/2] \subset (2\pi, 4\pi)$.

□

Proof of lemma 2. Let $x \in (0,\pi)$. Since $x > \sin x$, we have $2\cot(x/2) < x\csc^2(x/2)$. This means $\mathrm{d}h/\mathrm{d}x < 0$ and hence h is strictly decreasing in $[0,\pi]$. Thus, $h\colon [0,\pi] \mapsto [0,2]$ is a homeomorphism. □

Proof of lemma 3. For the case of $\epsilon = 1$, the argument in the LHS of equation (19) equals 0 for all $x \in (0,\pi)$. Thus, equation (19) holds in this case.

For the case of $\epsilon \in [0,1)$, we consider the function

$$u(x) = \ln x + \frac{\ln\left(\frac{1-\sqrt{\epsilon}}{2}\right) - 2\ln\sin\frac{x}{2}}{x\cot\frac{x}{2}}, \tag{A.13}$$

which is smooth for $x \in (0,\pi)$. Clearly, $u(x)$ is the logarithm of the argument in the LHS of equation (19). In addition,

$$\frac{\mathrm{d}u}{\mathrm{d}x} = \frac{1}{x^2}\left(\ln\frac{1-\sqrt{\epsilon}}{2} - 2\ln\sin\frac{x}{2}\right)\left[\frac{x\sec^2\frac{x}{2}}{2} - \tan\frac{x}{2}\right]. \tag{A.14}$$

Note that the first factor in the RHS of equation (A.14) is non-zero in $(0,\pi)$. For the third factor to vanish, $x = \sin x$. So, the third factor is non-zero in $(0,\pi)$, too. As for the second factor in the RHS of equation (A.14), it has a unique zero in $(0,\pi)$, namely, at $x = \cos^{-1}(\sqrt{\epsilon})$. Since

$$\left.\frac{\mathrm{d}^2u}{\mathrm{d}x^2}\right|_{x=\cos^{-1}(\sqrt{\epsilon})} = \frac{1}{[\cos^{-1}(\sqrt{\epsilon})]^2}\left[1 - \frac{\cos^{-1}(\sqrt{\epsilon})}{\sqrt{1-\epsilon}}\right] < 0, \tag{A.15}$$

$u(x)$ and hence $\exp[u(x)]$ attain their global maxima in the interval $(0,\pi)$ at $x = \cos^{-1}(\sqrt{\epsilon})$. As $\exp\{u(\cos^{-1}[\sqrt{\epsilon}])\} = \cos^{-1}(\sqrt{\epsilon})$, we conclude that equation (19) is valid for $\epsilon \in [0,1)$. □

Proof of lemma 4. Denote the root by x_r. Since this Lemma is trivially true when $x_r = b$, we may assume that $x_r < b$ and $w(b) < 0$. By Taylor's series expansion with remainder, $0 = w(x_r) \leqslant w(b) + w'(b)(x_r - b)$ or $x_r \leqslant x_1 \equiv b - w(b)/w'(b)$. We claim that $w(x_1) < 0$. Suppose the contrary, $w(x) = 0$ has another root $\bar{x}_r > x_1$. Nonetheless, the above Taylor's series argument implies that $\bar{x}_r \leqslant x_1$, which is absurd. Note that $w'(x_1) < 0$. If not, $w'(x) \geqslant 0$ for all $x \in [a, x_1)$ because $w''(x) \leqslant 0$. Then, by mean value theorem, $w(x) \leqslant w(x_1) < 0$ contradicting the condition that $w(a) \geqslant 0$. Replacing b by x_1 and repeating the above argument, this Lemma can be proven by recursion. □

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