

# Quantum Liouville theorem based on Haar measure

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Liouville theorem (L theorem) reveals robust incompressibility of the distribution function in phase space, given arbitrary potentials. However, its quantum generalization, Wigner flow, is compressible, i.e., L theorem is only conditionally true (e.g., for perfect Harmonic potential). We develop quantum L theorem (rigorous incompressibility) for arbitrary potentials (interacting or not) in Hamiltonians. Haar measure, instead of symplectic measure  $dp \wedge dq$  used in Wigner's scheme, plays a central role. The argument is based on general measure theory, independent of specific spaces or coordinates. Comparison of classical and quantum is made: for instance, we address why Haar measure and metric preservation do not work in the classical case. Applications of the theorems in statistics, topological phase transition, ergodic theory, etc., are discussed.

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## I. INTRODUCTION

In classical physics, Liouville theorem (L theorem) asserts that distribution function  $\rho$  in phase space  $\{p, q\}$  is constant along evolution trajectories [1,2]. Intuitively speaking, whether an object is soft or hard in real space, it is equally incompressible in  $\{p, q\}$ . If the volume in real space  $\Delta q$  is changed, its momentum volume  $\Delta p$  will adjust to maintain  $\Delta p \cdot \Delta q$  constant. L theorem reveals the elegance of classical dynamics (which is largely concealed in Newtonian and Lagrangian mechanics [2]) and serves as a cornerstone of statistical mechanics [1].

Formally speaking, classical L theorem is about rigorous incompressibility in phase space  $\{p, q\}$ , given Hamilton's equations (HEs) and local probability conservation; its quantum generalization, Wigner flow [3], is compressible [3,4], though, except for situations such as free particles, a perfect Harmonic potential. In this paper, we discover a pathway to establish a rigorous quantum L theorem based on Haar measure [5,6], while the previous symplectic measure  $dp \wedge dq$  [2] proves inappropriate and replaceable.

This paper develops arguments in three steps. First, define incompressibility and measure preservation; show their equivalence (Theorem 1 for both classical and quantum), such that building incompressibility is converted to seeking invariant measure. Second, present measure-preserving theorem (quantum L theorem) and metric-preserving theorem (Theorems 2 and 3, only for quantum). Third, note the theorems' values in nonequilibrium [7–13], topological transition [14–22], gapless problems [23,24], strong interaction [25], Floquet systems [26–29], and ergodic theory [5,20].

## II. EQUIVALENCE OF INCOMPRESSIBILITY AND MEASURE-PRESERVATION

Intuitively, measure  $m$  is the length, area, and volume of a space, depending on the dimension. Formally, measure is

a function  $m : \mathfrak{B}_X \rightarrow \mathbb{R}$  based on topological space  $X$ , which gives the volume of arbitrary (measurable) subsets of  $X$  [5,6].  $\mathfrak{B}_X$  is the  $\sigma$  algebra of  $X$ , i.e., a set of subsets of  $X$  that satisfies (i)  $X \in \mathfrak{B}_X$ , (ii) if  $B \in \mathfrak{B}_X$ ,  $X/B \in \mathfrak{B}_X$ , and (iii) if  $B_n \in \mathfrak{B}_X$ ,  $\bigcup_{n=1}^{\infty} B_n \in \mathfrak{B}_X$  to rule out nonmeasurable subsets (e.g., the Vitali set [6]).

**Definition 0.** Dynamic evolution is transformation group  $\{T_t | t \in \mathbb{R}\}$  formed by invertible (bijective) maps  $T_t : X \rightarrow X$ , where  $X$  is a topological space, and a point in  $X$  represents a physical state.

**Remarks.** Definition 0 is for both classical and quantum, as evolutions in both cases are invertible. Hilbert space  $\mathcal{H}$  is a vector space more than a topological space.

**Definition 1.** Measure preservation (or invariance) is a property of a measure function  $m : \mathfrak{B}_X \rightarrow \mathbb{R}$ , namely,

$$m(T(B)) = m(B), \quad \forall T \in \{T\}, \forall B \in \mathfrak{B}_X, \quad (1)$$

associated with dynamic evolution  $\{T_t | t \in \mathbb{R}\}$ . Measure function  $m$  can be expressed in local differential forms

$$m \sim \mu(x^1, \dots, x^N) \cdot dx^1 \wedge \dots \wedge dx^N, \quad (2)$$

where  $\mu(x^1, \dots, x^N)$  is a function  $X \rightarrow \mathbb{R}$  and  $\wedge$  is the exterior product. Since  $\mu$  is another form of  $m$ , we call both of them measure functions.  $x^1, \dots, x^N$  are coordinates in  $N$ -dimension space  $X$ . For example, in a two-dimension phase space  $\{p, q\}$ , symplectic measure has  $(x^1, x^2) = (p, q)$  and  $\mu(p, q) = 1$ ; in the space of  $SO(3)$  group ( $N = 3$ ), it has  $(x^1, x^2, x^3) = (\phi, \theta, \psi)$  and Haar measure function  $\mu(\phi, \theta, \psi) = \sin(\theta)$  [6], where  $\phi, \theta, \psi$  are Euler angles. Measure transformation is defined by

$$\mu(x^1, \dots, x^N) dx^1 \wedge \dots \wedge dx^N = \mu'(x^{1'}, \dots, x^{N'}) dx^{1'} \wedge \dots \wedge dx^{N'}. \quad (3)$$

$x^1, \dots, x^N$  and  $x^{1'}, \dots, x^{N'}$  stand for two sets of coordinates. The counterpart of invariance Eq. (1) in  $\mu$  is

$$\mu(x^1, \dots, x^N) = \mu'(x^{1'}, \dots, x^{N'}). \quad (4)$$

**Definition 2.** Incompressibility is a property associated with a specific measure function  $\mu$  and dynamic evolution  $\{T_t | t \in \mathbb{R}\}$  (Definition 0) that for *arbitrary* distribution function  $\rho(x^1, \dots, x^N; t)$ ,

$$\rho(x^1, \dots, x^N; t) = \rho(x^{1'}, \dots, x^{N'}; t'), \quad (5)$$

where  $x^i = x_{\{(x^j)_0\}}^i(t)$  and  $x^{i'} = x_{\{(x^j)_0\}}^{i'}(t')$ .  $x_{\{(x^j)_0\}}^i(t)$  are solutions of equations of motion subject to initial conditions  $\{(x^j)_0\} := \{(x^1)_0, \dots, (x^N)_0\}$ . Equivalently, we may introduce a single-variable function:

$$\rho_{\{(x^j)_0\}}(t) := \rho(x_{\{(x^j)_0\}}^1(t), \dots, x_{\{(x^j)_0\}}^N(t); t). \quad (6)$$

Incompressibility is expressed as

$$\dot{\rho}_{\{(x^j)_0\}}(t) = 0. \quad (7)$$

The time-dependent function  $\rho_{\{(x^j)_0\}}(t) : \mathbb{R} \rightarrow \mathbb{R}^+$  stands for probability density in the vicinity of a system setting out from initial states  $\{(x^j)_0\}$ . The equivalence of Eqs. (5) and (7) is evident. We simply plug in Eq. (5) with  $\forall t, t', t'' \dots \in \mathbb{R}$ . The equality holds for arbitrary time, which is exactly  $\dot{\rho}_{\{(x^j)_0\}}(t) = 0$ .

Now we present Theorem 1: equivalence between incompressibility and measure-preserving.

**Theorem 1.** Impressibility subject to measure function  $\mu$  and dynamic evolution  $\{T_t | t \in \mathbb{R}\}$  defined on space  $X$  is equivalent to the measure function  $\mu$  being invariant under  $\{T_t | t \in \mathbb{R}\}$ .

$$\begin{aligned} & \sum_k^N \int \rho((x^1)_0, \dots, (x^N)_0; 0) \cdot \partial_{x^k} [\delta(x^k - x_{\{(x^j)_0\}}^k(t))] \cdot \frac{d}{dt} (x^k - x_{\{(x^j)_0\}}^k(t)) \cdot \prod_{i \neq k}^{N-1} \delta(x^i - x_{\{(x^j)_0\}}^i(t)) \\ & \quad \cdot \mu_0((x^1)_0, \dots, (x^N)_0) \cdot d(x^1)_0 \wedge \dots \wedge d(x^N)_0 \\ &= - \sum_k^N \dot{x}_{\{(x^j)_0\}}^k(t) \cdot \partial_{x^k} \int \rho((x^1)_0, \dots, (x^N)_0; 0) \cdot \prod_i^N \delta(x^i - x_{\{(x^j)_0\}}^i(t)) \cdot \mu_0((x^1)_0, \dots, (x^N)_0) \cdot d(x^1)_0 \wedge \dots \wedge d(x^N)_0 \\ &= - \sum_k^N \dot{x}_{\{(x^j)_0\}}^k(t) \partial_{x^k} \rho(x^1, \dots, x^N; t). \end{aligned} \quad (11)$$

Thus, we deduce incompressibility (Definition 2):

$$\dot{\rho}_{\{(x^j)_0\}}(t) = \partial_t \rho + \sum_k^N \dot{x}_{\{(x^j)_0\}}^k(t) \partial_{x^k} \rho = 0. \quad (12)$$

To show the inverse, we simply need to reverse the derivation from the last to the beginning. Thus, incompressibility and measure-preserving are equivalent. ■

**Remarks.** In Theorem 1,  $\rho$  is arbitrary, while  $\mu$  is particular; that is, incompressibility is a property of a given  $\mu$  and  $\{T_t | t \in \mathbb{R}\}$ , not of  $\rho$ . Without measure invariance,  $\partial_t \rho$  will contain extra factors [compared with Eq. (11)], and incompressibility is false (Appendix A). Theorem 1 converts incompressibility to seeking invariant measures given evolution transformations  $\{T_t | t \in \mathbb{R}\}$ . Then, we may take advantage of arguments in measure theory [5,6] (e.g., existence and

*Proof.* The distribution function evolves with local probability conservation (Appendix A):

$$\begin{aligned} & \rho(x^1, \dots, x^N; t) \\ &= \int \rho((x^1)_0, \dots, (x^N)_0; 0) \cdot \prod_i^N \delta(x^i - x_{\{(x^j)_0\}}^i(t)) \\ & \quad \cdot \mu_0(x_{\{(x^j)_0\}}^1, \dots, x_{\{(x^j)_0\}}^N) \cdot dx_{\{(x^j)_0\}}^1 \wedge \dots \wedge dx_{\{(x^j)_0\}}^N. \end{aligned} \quad (8)$$

Equation (8) is generic evolution, either incompressible or not. It links  $\rho(x^1, \dots, x^N; t)$  with  $\rho(x^1, \dots, x^N; 0)$ . We have defined the time-dependent measure  $\mu_t(x^1, \dots, x^N) := \mu_0(x_{\{(x^j)_0\}}^1(-t), \dots, x_{\{(x^j)_0\}}^N(-t)) \cdot \mathcal{J}_t(x^1, \dots, x^N)$ , where  $\mu_0 = \mu_{t=0}$  and  $\mathcal{J}_t := \partial((x^1)_0 \dots (x^N)_0) / \partial(x^1 \dots x^N)$  is a Jacobian matrix linking two sets of coordinates. Measure preserving Eqs. (1) and (4) gives

$$\begin{aligned} & \mu_0(x_{\{(x^j)_0\}}^1(t), \dots, x_{\{(x^j)_0\}}^N(t)) \cdot dx_{\{(x^j)_0\}}^1(t) \wedge \dots \wedge dx_{\{(x^j)_0\}}^N(t) \\ &= \mu_0((x^1)_0, \dots, (x^N)_0) \cdot d(x^1)_0 \wedge \dots \wedge d(x^N)_0. \end{aligned} \quad (9)$$

Take the derivative of Eq. (8) to estimate  $\partial_t \rho(x^1, \dots, x^N; t)$ , and Eq. (9) into  $\partial_t \rho$ :

$$\begin{aligned} & \partial_t \rho(x^1, \dots, x^N; t) \\ &= \sum_k^N \int \rho((x^1)_0, \dots, (x^N)_0; 0) \cdot \partial_t [\delta(x^k - x_{\{(x^j)_0\}}^k(t))] \\ & \quad \cdot \prod_{i \neq k}^{N-1} \delta(x^i - x_{\{(x^j)_0\}}^i(t)) \cdot \mu_0((x^1)_0, \dots, (x^N)_0) \\ & \quad \cdot d(x^1)_0 \wedge \dots \wedge d(x^N)_0. \end{aligned} \quad (10)$$

Then, apply the chain rule:

uniqueness of invariant measures or metrics). This leads to the second step: build quantum L theorem.

### III. PRESERVATION THEOREMS FOR MEASURE AND METRIC

We recap two conditions for classical L theorem: local probability conservation (continuity condition) and HEs. Continuity gives

$$\begin{aligned} \dot{\rho}_{p,q}(t) &= \partial_t \rho(p, q; t) + \partial_p \rho(p, q; t) \cdot \dot{p}_{p,q}(t) \\ & \quad + \partial_q \rho(p, q; t) \cdot \dot{q}_{p,q}(t). \end{aligned} \quad (13)$$

Continuity  $\partial_t \rho(\mathbf{r}; t) = -\nabla \cdot (\mathbf{J}(\mathbf{r}; t)) = -\nabla \cdot (\rho(\mathbf{r}; t) \mathbf{v}(\mathbf{r}; t))$ . Here, spatial coordinates  $\mathbf{r} \rightarrow (p, q)$  and  $\nabla \rightarrow \hat{e}_p \partial_p + \hat{e}_q \partial_q$ .

Current density becomes

$$\mathbf{J}(p, q; t) = \rho(p, q; t)(\dot{p}_{p,q}(t)\hat{e}_p + \dot{q}_{p,q}(t)\hat{e}_q). \quad (14)$$

Plugging Eq. (14) into Eq. (13):

$$\dot{\rho}_{p,q}(t) = -\rho(p, q; t)(\partial_p \dot{p}_{p,q}(t) + \partial_q \dot{q}_{p,q}(t)). \quad (15)$$

The second condition is satisfaction of HEs:  $\dot{q}_{p,q}(t) = \partial_p H(p, q)$  and  $\dot{p}_{p,q}(t) = -\partial_q H(p, q)$ . Combined with Eq. (15), we have  $\dot{\rho}_{p,q}(t) = 0$ .

Quantum generalization by Wigner inherits phase space  $\{p, q\}$  [3], although the uncertainty principle casts doubt on this notion. Given that HEs are substituted by the Schrödinger equation (SE), the hope is that by judicious maps [e.g., Wigner function Eq. (16)], incompressibility should remain:

$$\rho_W(p, q) = \frac{1}{2\pi} \int dq' \varphi^* \left( q - \frac{\hbar}{2} q' \right) e^{-iq'p} \varphi \left( q + \frac{\hbar}{2} q' \right). \quad (16)$$

The wave function  $\varphi(q)$  is mapped to  $\rho_W(p, q)$  [30]. By evaluating the partial derivative  $\partial_t \rho_W(p, q)$  combined with the SE, one obtains [31]

$$\partial_t \rho_W = -\partial_q \rho_W \dot{q} + \sum_{\lambda}^{\text{odd}} \frac{(\hbar/2i)^{\lambda-1}}{\lambda!} \frac{\partial^\lambda V}{\partial q^\lambda} \frac{\partial^\lambda \rho_W}{\partial p^\lambda}, \quad (17)$$

where  $\lambda$  goes over all odd integers. Given terms of  $\lambda \geq 3$  all vanish, Eq. (17) leads to  $\partial_t \rho_W = -\partial_q \rho_W \dot{q} - \partial_p \rho_W \dot{p}$ , i.e.,  $\dot{\rho}_W = 0$ . However, this relies on  $\partial^\lambda V / \partial q^\lambda = 0$  for  $\lambda \geq 3$ . In other words, incompressibility only holds for perfect Harmonic oscillators. Thus, L theorem is only true for classical not for quantum.

Recall that classical L theorem involves: (1) Dynamics are formulated with a group of invertible maps on a topological phase space  $X$ . (2) Topological space  $X$  is phase space  $\{p_i, q_i\}_N$ . (3) Incompressibility is linked to symplectic measure  $\prod_i dp_i \wedge dq_i$  equipped on  $X$ . (4) Robustness: incompressibility is derived *only* from local probability conservation and equations of motion.

Wigner's generalization inherits (2) and (3), but modifies (4) by replacing HEs by SEs (as equations of motion). However, (4) is still violated, as incompressibility further relies on potentials. Point (1) needs more remarks. Quantum mechanics is established on Hilbert space  $\mathcal{H}$ , more than a topological space like  $\{p_i, q_i\}_N$ . The magnitude of a state vector in  $\mathcal{H}$  stands for probability, and superposition of two state vectors yields another. However, for 2D  $\{p, q\}$ , say,  $p = 0, q = 0$ ,  $\|(p, q)\| = 0$ , which does not mean zero probability; it is meaningless to add two points:  $(p, q) + (p', q')$ . Thus, quantum fails point (1). Wigner recovered (1) by introducing the Wigner function [Eq. (16)], which transcribes  $\mathcal{H}$  to  $\{p_i, q_i\}_N$  and justifies  $\{p_i, q_i\}_N$  despite the uncertainty principle. The transformation is invertible (no loss of information) [3] and the wave function is holographic in the distribution function  $\rho_W$  on  $\{p_i, q_i\}_N$ . It also casts equations of motion into phase space, known as Moyal brackets [32].

Wigner hoped to achieve a quantum analog with minimum modifications: maintaining (1)–(3) [in fact, partially for (1)], while sacrificing (4). However, the scheme relies on potentials and encounters problems in negative probability [3,32], quantization [33], etc. We present a different pathway. The

proposal is aligned with Wigner's spirit of mapping  $\mathcal{H}$  to topological space [3,4,32], but  $\{p_i, q_i\}_N$  is no longer the choice since uncertainty is averse to it. Additionally, just like classical L theorem arises from HEs, quantum L theorem should directly arise from the SE, without referring to Hamiltonian's forms, to respect point (4)—robustness. Hence, we inherit points (1) and (4), while modifying (2) and (3): for (2),  $\mathcal{H}$  is mapped to the unitary group's parameter space instead of  $\{p_i, q_i\}_N$ ; for (3), symplectic measure is replaced with Haar measure. Remember measure function  $\mu$  is external equipment (thus to be chosen), rather than intrinsic for a space.

**Theorem 2.** If the evolution  $\{T_t | t \in \mathbb{R}\}$  is a unitary group  $G$ , the distribution function  $\rho_H$  defined topological space of  $G$  equipped with its Haar measure is constant along the evolution trajectory.

*Proof.* We need two conditions. The continuity Eq. (14) is now replaced by the more general Eq. (8), and  $\partial_t \rho = -\nabla \cdot \mathbf{J}$  is about choosing symplectic measure  $\mu \equiv 1$ . The second condition, equations of motion, i.e., SE, enters via evolution  $T_t = U(t, 0)$  being unitary. That is,  $\{T_t | t \in \mathbb{R}\}$  must belong to the unitary group, which is a compact group. To be specific, two features of SE ensure  $T_t$  to be unitary: SE takes the form of diffusion equation (with imaginary coefficients), and the Hamiltonian operator is Hermitian:  $H = H^\dagger$ .

Since Haar measure uniquely exists, i.e.,  $\mu_t = \mu_0$  for  $\{U(t, 0) | t \in \mathbb{R}\}$ , we may always find a unique Haar measure  $\mu_H$  invariant for  $U(t, 0)$ . Theorem 1 states that invariant measure is equivalent to the invariant distribution function  $\rho_H$ . Quantum L theorem can be expressed as

$$\dot{\rho}_H(t) = 0, \quad (18)$$

where the subscript  $H$  refers to the density based on Haar measure  $\mu_H$  to distinguish from the density (quasiprobability) defined by Wigner function, which has  $\dot{\rho}_W(t) \neq 0$ . ■

**Remarks.** Classical L theorem is proved by explicitly finding  $\mathbf{J}$  [Eq. (14)] based on determined space  $\{p, q\}$  and measure  $dp \wedge dq$ . Quantum L theorem is based on Haar measure, which refers to a class of measures, i.e., it varies with groups and for each *compact* group it is unique (either analytically or numerically achievable) [6]. Proof of quantum L theorem involves generic argument about Haar measure, rather than referring to specific coordinates or spaces. Similar to classical, quantum L theorem only relies on two conditions: equations of motion, i.e., SE, and local probability conservation. The former enters via  $T_t = U(t, 0)$ ; the latter is via Eq. (8).

**Theorem 3.** The metric in group parameter space will remain constant during evolution.

*Remarks.* The metric is the distance between two points. Theorem 3 holds because there always exists (a possibly nonunique) invariant metric associated with an invariant Haar measure. Thus, the measure and metric (volume and distance) will be simultaneously respected. Refer to Chap. 8 of Ref. [6] for existence proof of the invariant metric.

Why is the invariant metric absent in classical dynamics [Figs. 1(a) and 1(b)]? Why can't Haar measure approach be applied to  $\{p, q\}$ ? To clarify these questions, we need to see there are some physical principles. (a) Dynamics are formulated with a group of invertible maps  $\{T\}$  on a topological phase space  $X$ . (b) The topological space  $X$  on which  $\{T\}$  is

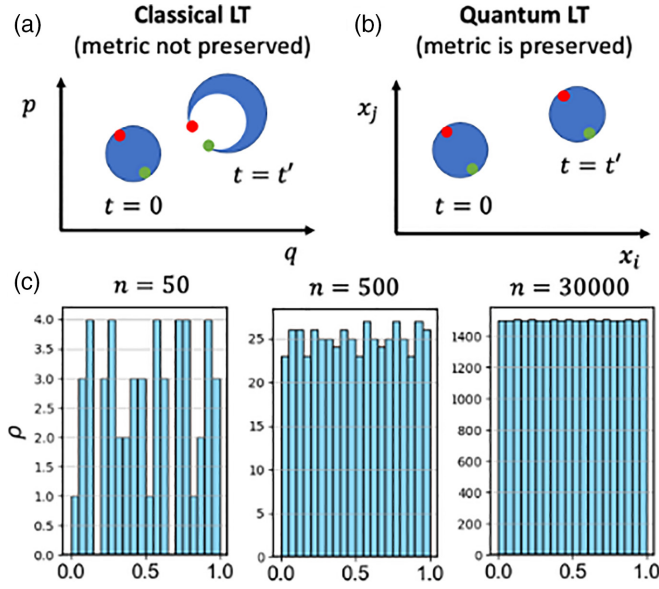


FIG. 1. (a) Classical preserves volume but not distance (e.g., red and green points), like kneading dough. (b) Quantum preserves both volume and distance. (c) At  $t \rightarrow \infty$ ,  $\rho \rightarrow$  constant against normalized coordinates (in achievable regions).  $\Phi = \Omega = 0$ ,  $\Theta = \pi/4$  (Appendix A) are chosen with a bin number of 20.

defined should be the physical space, i.e., a point in  $X$  stands for a physical state. (c) Measure function equipped on  $X$  is invariant with  $\{T\}$ , i.e.,  $m(T(B)) = m(B)$  for  $\forall B \in \mathfrak{B}_X$ ,  $\forall T \in \{T\}$ .

Haar measure is a special invariant measure subject to the constraint  $\{T\} = X = G$ , which leads to its uniqueness. If we define Haar measure on  $\{p, q\}$ , every point  $(p, q)$  should stand for a transformation of  $G$ , leading to  $G$  no more than a translation group. That means point  $(p, q)$  stands for translating an arbitrary point  $(p_0, q_0)$  to  $(p_0 + p, q_0 + q)$ ; to be invariant Haar measure is  $\mu_H \equiv 1$ . But do not think  $\mu_H(p, q) \equiv 1$  is the same as symplectic measure  $\mu(p, q) \equiv 1$ . The difference is that the Haar measure has  $\{T\}$  to be translations, totally irrelevant to the system's evolution [principle (a) above is violated]. The symplectic measure's  $\{T\}$  is determined by HEs, expressed by the map  $p = p_{p_0, q_0}(t)$ ,  $q = q_{p_0, q_0}(t)$ . Thus, it is not the case that Haar measure cannot be imposed on classical space  $\{p, q\}$ , but rather that principle (a) cannot be simultaneously respected. Quantum L theorem is nontrivial not only for being rigorously incompressible [principle (c)], but also that principles (a)–(c) can simultaneously be fulfilled.

Finally, we note applications of the theorems. It transpires that L theorem's classical implications [1] can be transplanted to quantum, like uniform distribution  $\rho$  over equal-energy surface in  $\{p_i, q_i\}_N$ . We plot the counterpart in parameter space [Fig. 1(c)]. We use a spin model in a cyclic evolving magnetic field, whose evolution operator  $\mathcal{U}$  is given in Appendix A [also Eq. (3) of Ref. [20]]. We consider  $\mathcal{U}^n$  with  $n \rightarrow \infty$ . Note that the cyclic Hamiltonian  $H$  is merely for demonstrating; incompressibility is independent of being cyclic.

Incompressibility is required to apply the theorems and tools developed in ergodic theory [5]. Quantum L theorem offers a valuable nonperturbation approach to exploring areas where perturbation is invalid, such as at the topological phase transition (gap closing) [18–21, 34], at the quantum

TABLE I. Measure and metric invariance for Wigner flow, classical and quantum L theorem, and their valid conditions. HE (SE) means obeying Hamilton (Schrödinger) equations.

	Measure	Metric	Valid condition
Wigner flow	no ( $dp \wedge dq$ )	no	$\partial_q^n V = 0$ for $n > 2$
Classical L theorem	yes ( $dp \wedge dq$ )	no	HE
Quantum L theorem	yes (Haar)	yes	SE

critical point [23, 24], or electrons with strong interaction or correlation [25] or driven by strong or fast ultrafast lasers [7–13, 35, 36]. Refer to Appendix B for theorem's application, interpretation, and experimental observation.

The present argument can be extended to infinite dimensions. The trick is expressing infinite  $X$  as a product of one finite and one infinite space, then projecting dynamics into the finite-dimension quotient space. Extending to infinite space is crucial; the position operator is an infinite-dimension operator and plays central roles in transport theory [37, 38].

#### IV. CONCLUSION

We have demonstrated the equivalence between incompressibility and measure preservation (Theorem 1); prove a quantum Liouville theorem [Theorem 2, Eq. (18)] and metric theorem (Theorem 3), confirmed by numerical results [Fig. 1(c)]. L theorem is now rigorously true for both classical and quantum, independent of Hamiltonians (whether  $H$  is interacting or time dependent). L theorem arises from two conditions: local probability conservation and (classical or quantum) equations of motion, while distinctions are highlighted in Table I. Quantum L theorem provides precise nonperturbation arguments, useful in numerous research fields.

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#### APPENDIX A: PROOF NOTES

The 2D phase space  $\{p, q\}$  is used to demonstrate the meaning of generic denotations. Here,  $p_{p_0, q_0}(t)$  and  $q_{p_0, q_0}(t)$  give the evolution trajectory from initial conditions  $p_0, q_0$ . For example, for the 1D Harmonic oscillator (whose phase space is 2D,  $\omega = \sqrt{k/m}$ ),

$$\begin{aligned} p_{p_0, q_0}(t) &= \cos(\omega t) p_0 - m\omega \sin(\omega t) q_0, \\ q_{p_0, q_0}(t) &= \cos(\omega t) q_0 - \frac{1}{m\omega} \sin(\omega t) p_0. \end{aligned} \quad (\text{A1})$$

Conversely, we can express  $p_0, q_0$  in  $p, q$  and  $t$ :  $p_0 = p_{p, q}(-t)$ ,  $q_0 = q_{p, q}(-t)$ . Then we may evaluate the  $2 \times 2$  Jacobian matrix  $\mathcal{J}_t^{(p_0, q_0)}(p, q)$  to link the integrals under two distinct sets of coordinates.

$dx_{(x^j)_0}^1(t) \wedge \dots \wedge dx_{(x^j)_0}^N(t)$  and  $d(x^1)_0 \wedge \dots \wedge d(x^N)_0$  in Eq. (9) become  $dp_{p_0, q_0}(t) \wedge dq_{p_0, q_0}(t)$  and  $dp_0 \wedge dq_0$ . Note that we do *not* take  $dx_{(x^j)_0}^i(t)$  as the time derivative of function  $x_{(x^j)_0}^i(t)$  because  $t$  is just a label of the set of  $N$  coordinates. That is,  $dx_{(x^j)_0}^1(t) \wedge \dots \wedge dx_{(x^j)_0}^N(t)$  is holistic, and a single  $dx_{(x^j)_0}^i(t)$  term is meaningless.

How is Eq. (8) obtained? Consider a single particle moves in space:  $\rho = \prod_i^N \delta(x^i - x_{(x^j)_0}^i(t))$ . If it follows a probability distribution (or if we have a swarm of particles), we make a weighted superposition:  $\rho = \int \rho_0((x^1)_0 \dots (x^N)_0) \prod_i^N \delta(x^i - x_{(x^j)_0}^i(t))$ . Finally, if the space is of nonuniform measure (just imagine gravitational force might distort Euclidean space), we need to further multiply a local measure field  $\mu_0$  and finally obtain Eq. (8). Physically, Eq. (8) is a generic expression of local probability conservation (for arbitrary coordinates). If  $\mu$  is constant, we obtain the familiar Eq. (15).

Another common mistake is confusion of  $\rho(x^1, \dots, x^N)$  with  $\rho_{\{(x^j)_0\}}(t)$ : the former is a multiple variable; the latter is a single variable (time). A partial derivative may only act on the former, and the time derivative (e.g.,  $\dot{\rho}$ ) only acts on the latter. Recognizing them is crucial for proof derivation.

Measure invariance [Eqs. (1) and (4)] is indispensable for the proof. If invariance is lacking, we shall obtain the following:

$$\begin{aligned} & \rho(x^1, \dots, x^N; t) \\ &= \int \rho((x^1)_0, \dots, (x^N)_0; 0) \cdot \prod_i^N \delta(x^i - x_{(x^j)_0}^i(t)) \\ & \quad \cdot \mu_0((x^1)_0, \dots, (x^N)_0) \frac{\mu_0(x_{(x^j)_0}^1(t), \dots, x_{(x^j)_0}^N(t))}{\mu_t(x_{(x^j)_0}^1(t), \dots, x_{(x^j)_0}^N(t))} \\ & \quad \cdot d(x^1)_0 \wedge \dots \wedge d(x^N)_0. \end{aligned} \quad (A2)$$

As such,  $\dot{\rho}_{\{(x^j)_0\}}(t) \neq 0$ , i.e., it is compressible.

An example of invariant measure is the Haar measure of  $SO(3)$ . Rotation links two sets of coordinates:  $d\phi' d\theta' d\psi' = \mathcal{J} \cdot d\phi d\theta d\psi$ , where the Jacobian matrix is  $\mathcal{J} = \partial(\phi', \theta', \psi') / \partial(\phi, \theta, \psi)$ . Calculation is somewhat tedious, but

$$d\phi' d\theta' d\psi' = \frac{\sin(\theta)}{\sin(\theta')} d\phi d\theta d\psi. \quad (A3)$$

That is,  $\mu = \mu' = \sin(\theta)$  and  $\mu_H(\phi, \theta, \psi) = \sin(\theta)$ . Mind that invariant measure is different from uniform measure, which has  $\mu$  constant. In general dimensions, the definition is given by Eq. (4).

L theorem indicates that in the long-time limit, in the achieved phase space,  $\rho$  is constant (ergodicity). The evolution operator is [20]

$$\mathcal{U} = \begin{pmatrix} \cos(\Theta/2)e^{-i\Phi} & -\sin(\Theta/2)e^{-i(\Omega-\Phi)} \\ \sin(\Theta/2)e^{i(\Omega-\Phi)} & \cos(\Theta/2)e^{i\Phi} \end{pmatrix}. \quad (A4)$$

Parameters  $\Phi, \Theta, \Omega$  arise from band parameters: gap, driving frequency, etc. [20]. However, here we only need to take them as parameters of  $H$ . The parameters  $\Phi, \Theta, \Omega$  are equivalent to Euler angles (the coordinate transformation can be found in Appendix C of Ref. [20]), and the Haar measure is  $\sin(2\Theta)d\Phi \cdot d\Theta \cdot d\Omega$ . Then we evaluate  $\mathcal{U}^n$ , with an initial  $|0\rangle = (1, 0)^T$ , which gives  $|\varphi_n(\Phi, \Theta, \Omega)\rangle := \mathcal{U}^n|0\rangle$ . Then let  $n \rightarrow \infty$ , i.e.,  $t \rightarrow \infty$ . And examine the distribution  $\rho$  over topological space  $X = \{\Phi, \Theta, \Omega\}$  against Haar measure [Fig. 1(c)].

Here we can see difference between Hilbert space  $\mathcal{H}$  and the topological space  $X$ .  $|\varphi_n(\Phi, \Theta, \Omega)\rangle$  is vector in  $\mathcal{H}$ , i.e., the 2D vector on  $\mathbb{C}$ . However, the three-component  $(\Phi, \Theta, \Omega)$  cannot be added like a vector (although it is extracted from vectors in  $\mathcal{H}$ ), but rather like points in topological space  $X$ .

## APPENDIX B: THE THEOREM'S PHYSICAL INTERPRETATION AND APPLICATION

### 1. The utility of quantum L theorem

Why do we need quantum L theorem? Does it provide information beyond the SE? Although SE and initial conditions carry all dynamic information, it is usually unsolvable. Quantum L theory is not to provide new information but to access information from SE (e.g., asymptotic, or statistical behavior) without the need to solve it.

The mechanism is, because  $\rho_H$  is constant along the achievable regions, if one's interest is statistical or asymptotic behavior (most observables belong to this type), one may switch from solving the true evolution path in Hilbert space to solving the achievable region in unitary group parameter space against Haar measure. We do not care about the temporal order of the system traversing these regions, but only the region, which is a more tractable problem.

In fact, similar strategies have been used by classical L theorem and classical statistics: it does not matter how the system covers phase space  $\{p, q\}$ , but only the achievable regions and the corresponding probability density. As such, solving  $N$ -particle Hamiltonian equations is eluded, and statistical behaviors of unsolvable large system could be formulated.

### 2. Application examples

Quantum L theorem needs some models to demonstrate its power to yield concrete results. Just like when classical L theorem (occupancy  $e^{-\beta T}$  deduced from it) is applied to transports, one gets conductivity rules (e.g., temperature dependence); when it is applied to free particle models, one gets dilute gas behaviors.

In spin and band models [20], solving the reachable region corresponds to finding the ergodic subgroup (Appendix C of Ref. [20]), via which one can obtain analytic solutions of spin or interband pumping (quantum L theorem was then termed a measure-preserving formalism and is now formalized into Theorem 2). Without quantum L theorem, pumping probability  $p_G$  is expressed with an infinite series, evaluated by  $\mathcal{U}^n$

with  $n \rightarrow \infty$ .  $p_n$  exhibits as a complicated series:

$$\begin{aligned}
 p_1 &= \sin^2\left(\frac{\Theta}{2}\right), \\
 p_2 &= \frac{1}{2}\left(p_1 + \left| -\sin\left(\frac{\Theta}{2}\right)\cos\left(\frac{\Theta}{2}\right) - e^{2i\Phi}\sin\left(\frac{\Theta}{2}\right)\cos\left(\frac{\Theta}{2}\right) \right|^2\right), \\
 p_3 &= \frac{1}{3}\left(2p_2 + \left| \cos\left(\frac{\Theta}{2}\right)\left(-\sin\left(\frac{\Theta}{2}\right)\cos\left(\frac{\Theta}{2}\right) - e^{2i\Phi}\sin\left(\frac{\Theta}{2}\right)\cos\left(\frac{\Theta}{2}\right)\right) \right. \right. \\
 &\quad \left. \left. - \sin\left(\frac{\Theta}{2}\right)\left(-\sin^2\left(\frac{\Theta}{2}\right) + e^{-2i\Phi}\cos^2\left(\frac{\Theta}{2}\right)\right) \right|^2\right), \\
 p_4 &= \frac{1}{4}(3p_3 + \dots).
 \end{aligned} \tag{B1}$$

Since  $p_G = p_\infty$ , one can imagine what horrible expression it will be. But with quantum L theorem, one can prove  $p_G$  converge to a compact analytic solution:

$$p_G = \frac{\sin^2\left(\frac{\Phi}{2}\right)}{2(1 - \cos^2\left(\frac{\Phi}{2}\right)\cos^2(\Phi))}. \tag{B2}$$

Via the analytic solution above, one may deduce a concept geometric pumping in both spin and band scenarios [20], whose defining feature is pumping probability only depends on geometric and topological parameters irrelevant to energetic ones. Thus, quantum L theorem also helps establish unique physical concepts.

### 3. Experiment

Empirical information can be obtained by testing the phenomena predicted by quantum L theorem. Quantum L theorem is not a specific observable but is a law that influences broad phenomena. Take geometric pumping as an example. (It is not the only case; because a TPT model is solved with the theorem, we use this to demonstrate.)

Passing from classical statistics to fermion and boson statistics, a crucial thing is to lower temperature to make quantum effect emerge; we only need to examine conventional observables but in search of abnormality against classical interpretation. Similarly, detecting quantum L theorem does not need very fancy measurement. A simple path is to perform measurements around the topological phase transition (TPT), i.e., at band or level degeneracy.

For example, we apply quantum L theorem to a two-band model that undergoes periodic gap closing and we obtain exact analytic solutions. For details of the model and the solving process, one can refer to Ref. [20]. Here we just quote the result: if gap closing changes the topological state of bands, a  $1/2$  electron will be pumped to the upper band at gap closing  $k_0$ ; if gap closing does not alter the topological state, no electron will be pumped.

To test this prediction by quantum L theorem, we need (i) a topological insulator at the vicinity of TPT (in practice, that means the insulator's gap cannot be too large); (ii) a means of realizing periodic TPT; (iii) a means of measuring the amount of pumping charge (hopefully with capability of time resolution).

For (i), we can choose  $\text{ZrTe}_5$ , a topological insulator ( $Z_2$  type) features a single band cone at  $\Gamma$  in B.Z. [19,21], with gap 10–100 meV. For (ii), we can use phonons to drive the band and periodically close the band gap to realize periodic TPT. In  $\text{ZrTe}_5$ , this can be done by, e.g.,  $A_{1g}$  phonon mode ( $\sim 1.2$  THz). For (iii), we can use an ultrafast spectrum or pump-probe techniques [19,21]). The amount of charge being pumped will be proportional to the change of reflectivity  $\Delta R$  or transition  $\Delta E$  (compared with the ground state), i.e.,  $\Delta R$  (or  $\Delta E$ )  $\propto Q_{\text{pump}}$  [19].

Since geometric pumping is fractional and relies on the presence of TPT, we anticipate (a) the pumping might happen even at subgap excitation, i.e., driving frequency is less than the average gap  $\hbar\omega \ll \Delta$ ; (b) such pumping disappears given TPT is absent; or (c) the saturated  $Q_{\text{pump}}$  is lower than energetic pumping by quasiparticles.

### 4. Advantages and limitations of quantum L theorem compared with classical L theorem and Wigner function

Quantum L theorem arises from modifying the Wigner function, fixing a major shortcoming for Wigner function: loss of incompressibility. Moreover, the metric preservation (Theorem 3) renders a rigid-body motion for the wave package, i.e., for an arbitrary wave package, it will not disperse, which provides another pathway of understanding the long lifetime of wave packages other than soliton approaches. On the other hand, since the Wigner function involves position  $q$ , it can handle real-space problems, e.g., transport, under a semiquantum picture ( $p, q$  are both definite). The quantum L theorem currently works for space of finite dimensions, because the dimension  $N$  of the  $U(N)$  group must be finite. Thus, the position-related problem (the position is an infinite-dimension quantum operator) is still unachievable for the current version of quantum L theorem.

That is why we try to generalize the theorem to infinite dimensions. At the end of the main text, we forecasted our next work by saying: “The present argument can be extended to infinite dimensions. The trick is expressing infinite  $X$  as a product of one finite and one infinite space,” which gives a prospective of simultaneously realizing three aspects: (i) quantum, (ii) infinite dimensions of Hilbert space, (iii) incompressibility; in comparison with classical L theorem only fulfilling (ii) and (iii), and Wigner function only fulfilling (i)

and (ii). It is intriguing to see to what an extent quantum L theorem can cover Wigner function's jobs. Nonetheless, the current theorem already shows its advantage in treating quantum degrees of freedom, e.g., spin, interband scenarios, which are unachievable for Wigner function.

### 5. Does Haar measure have a physical meaning?

In this section, we link the Haar measure with the physical probability. In view of the fundamentality and controversy related to quantum interpretation, for example, even the notion of probability might have different interpretations (Chap. 11 of Ref. [41]), which leads to different logic lines, and we must stress the present concern about Haar measure is merely that it is physically suitable or convenient, and the probability density associated to it means a common sense; a deeper understanding must be established upon the full understanding of quantum measurements [41], which is apparently beyond the scope of this paper.

A physical meaning such as probability density is usually assigned to a density field; one does not usually give a separate physical meaning to a measure function, as it is an ingredient in defining a density field. It is not always possible to extend the wondering of what the physical meaning is along an array of math decomposition. However, as a heuristic, one may imagine measure as a ruler to determine a density; different rulers will give different density readings, but the different readings correspond to the same physical state. That is, different measure functions are linked by transformations; choosing a different measure function does not alter the physics.

Thus, in a sense, different definitions of density are on equal status, if one can accept the density defined in real space  $\Delta q$  or density defined in phase space by  $\Delta q \Delta p$ , one should accept the density defined with Haar measure without doubts. Each density corresponds to a particular choice of space and measure function equipped on the space (such a space is called *measure space* in measure theory).

Given every measure (and associated density) is equal, what makes Haar measure (symplectic measure) uniquely outstanding in quantum (classical)? That is, a good measure function should be a time-independent (static) one that can maintain incompressibility for arbitrary systems, which mean arbitrary initial states, arbitrary potentials, and arbitrary number of particles. A poorly selected measure function can possibly maintain incompressibility, but it must adjust its form based on the motion of particles (thus a time-dependent function), which will be trivial. That is why in Eq. (8) the measure function field is a static  $\mu_0$  rather than  $\mu_t$ . Thus, constructing an incompressible formulation is an incomplete (thus kind of misleading) statement for L theorem; one should keep in mind using a static measure function. Understanding these constraints in constructing incompressibility, it is easy to understand why a measure needs to be of very nice mathematical properties, which are not optional or preferred, but mandatory.

Choosing a good measure function like Haar measure in quantum or symplectic measure in classical helps reveal stable points of a dynamic system (thus leading to stable observables), while a poorly chosen measure will probably give the illusion that the system is still unstable. For example, if we

choose a nonuniform measure in  $\{p, q\}$  space, at equilibrium, the density still keeps changing.

There are infinite ways of defining a density (i.e., choosing a measure function), but there is only a single one among them that correctly reflects physical stable states; and that density (also the associated measure function) can be considered physically meaningful or convenient.

Note that building a complete logic for quantum [41] is not covered by this paper. We focus on more certain arguments and achievable aspects. (1) The physical probability is most commonly described by a density field, which is defined upon a specific measure function (Haar measure is one possible choice). (2) A physically suitable and convenient (also mathematically nontrivial) measure function should be a static one and invariant under physical evolution. (3) Based on this criteria, symplectic measure and Haar measure become (potentially uniquely) outstanding for classical and quantum, respectively. (4) Haar measure will help simplify calculations, analytically solve models, and allude to unique physical concepts or phenomena, as demonstrated here. These are indicators (although not proof) for Haar measure having physical meanings and significance.

Now we can connect the above physical discussions back to the formal (maybe a little abstract) presentation in the main text. As we mentioned, being static boils down to the fact in Eq. (8) that the measure field is a static field not being allowed to change over time. Whether it is time independent and whether the arbitrariness (in initial conditions, potentials, etc.) is true boil down to transformation properties of measure function (Definition 1) under the evolution group (Definition 0) determined by the equation of motions in classical or quantum scenarios.

Fundamentally, these considerations boil down to the three principles (a)–(c) raised after Theorem 3. We apply the three principles to an analysis on inapplicability of Haar measure to classical. To be concrete, as we mentioned, the simultaneous satisfaction for the three principles makes  $dp \wedge dq$  outstanding for classical and Haar measure outstanding for quantum. The reverse inapplicability (symplectic applied to quantum) is exactly the failing of incompressibility for the Wigner function.

Back to the question of whether Haar measure has physical meanings, we make two nondecisive but constructive comments. (1) A physically suitable measure should be invariant under evolution transformation (Definition 0), just like people believe a valid relativistic quantum theory should be invariant under Lorentz group, although reconciling quantum with relativity theory still eludes us. (2) A physical measure should be useful. We have given preliminary evidence for Haar measure, and there is more to explore. For example, Haar measure is useful in understanding the long lifetime of particles, as the wave package picture suffers from dispersion. Given such evidence is accumulated, one may promote quantum L theorem (the measure conservation) to a more fundamental state.

### 6. A guideline for the physics and math background

To bridge the gap between physics and math, we provide a guideline. There are three tiers. First, for convinced and proficient readers, they can quote the result as the time evolution

being unitary and the Haar measure remaining invariant under time evolution—the invariant Haar measure implies the corresponding distribution remains constant over time. Second, for readers interested in techniques of the proof, the kernel knowledge includes: (i) The derivation of classical L theorem—refer to Chap. 1 of Gibbs’s book [39]. (ii) Chapters 1 and 2 of Bogoliubov’s book [40], because our derivation of Theorem 1 could be considered a generalization of Bogoliubov’s proof of classical L theorem by including a local measure field. (iii) invariant measure and Haar measure. The most illuminating

examples to quickly capture these topics are Haar measure of the SU(2) or SO(3) group, the measure function associated to rational and irrational numbers on the real number axis, and Vitali set as examples to understand nonmeasurable sets. (iv) Derivation regarding Wigner functions [e.g., Eqs. (16) and (17)] is found in Ref. [3]. We also provide references for more ambitious readers who are aimed to explore the uniqueness of Haar measure, [6] applications of quantum L theorem intertwining with ergodic theory [5], or general topics in measure theory.

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