

Entropy for quantum pure states and quantum H theoremXizhi Han (韩希之)¹ and Biao Wu (吴飙)^{1,2,3,*}¹*International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China*²*Collaborative Innovation Center of Quantum Matter, Beijing 100871, China*³*Wilczek Quantum Center, College of Science, Zhejiang University of Technology, Hangzhou 310014, China*

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We construct a complete set of Wannier functions that are localized at both given positions and momenta. This allows us to introduce the quantum phase space, onto which a quantum pure state can be mapped unitarily. Using its probability distribution in quantum phase space, we define an entropy for a quantum pure state. We prove an inequality regarding the long-time behavior of our entropy's fluctuation. For a typical initial state, this inequality indicates that our entropy can relax dynamically to a maximized value and stay there most of time with small fluctuations. This result echoes the quantum H theorem proved by von Neumann [*Zeitschrift für Physik* **57**, 30 (1929)]. Our entropy is different from the standard von Neumann entropy, which is always zero for quantum pure states. According to our definition, a system always has bigger entropy than its subsystem even when the system is described by a pure state. As the construction of the Wannier basis can be implemented numerically, the dynamical evolution of our entropy is illustrated with an example.

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I. INTRODUCTION

Statistical mechanics, studying thermal properties of a many-body system from microscopic perspective, have gained huge success in the past century. However, the basic principles of statistical mechanics have not been fully understood; the establishment of microcanonical ensemble has to rely on hypotheses [1]. Since microscopic particles—elements of a macroscopic system—are governed by the Schrödinger equation, one feels obliged to address the problem with quantum mechanics. Von Neumann was among the first physicists trying to use quantum mechanics to understand the basic principles of statistical mechanics. In a 1929 paper [2], von Neumann proposed a method to construct commutable macroscopic momentum and position operators and, therefore, quantum phase space. Within this framework, he introduced an entropy for quantum pure state and proved two theorems, which he called quantum ergodic theorem and quantum H theorem, respectively. These results are remarkable advances in the establishment of the microcanonical ensemble, the foundation of statistical mechanics, without hypothesis. However, von Neumann's beautiful results have been largely forgotten likely due to misunderstanding [3].

Probably due to the developments in ultracold atomic gas experiments [4–6], we have recently seen tremendous efforts to study the foundation of statistical mechanics. Many new and beautiful results are obtained [7–29]. These efforts have also led to renewed interest in von Neumann's forgotten work; the English version of his paper is now available [30]. Von Neumann's quantum ergodic theorem has been reexamined recently [31]. In particular, a different version of quantum ergodic theorem was proved by Reimann [16,32]. Reimann's ergodic theorem does not involve any coarse-graining and can be subjected to numerical study [33]. In contrast, much less progress has been made on the quantum H theorem and the associated key concepts, such as macroscopic momentum and

position operators, and entropy for quantum pure states, which were introduced in 1929.

In this work we define a different entropy for quantum pure states and study its long-time dynamical fluctuation in an attempt to improve on von Neumann's quantum H theorem [2]. Von Neumann proved his theorem with the following steps: (i) construct commutable macroscopic position and momentum operators; (ii) define an entropy for pure quantum states with coarse-graining; (iii) investigate the long-time behavior of the entropy.

We follow von Neumann's steps with new theoretical tools and perspectives. For step (i), we use Kohn's method [34] to construct a complete set of Wannier functions that are localized both in position and momentum space. Such a construction can be implemented numerically with great efficiency. With these Wannier functions, we are able to construct commutable macroscopic position and momentum operators and, therefore, a quantum phase space, which is divided into cells of size of the Planck constant and each of these Planck cells is assigned a Wannier function. The success of step (i) allows us to map unitarily a pure quantum state onto the phase space.

We accomplish step (ii) by defining an entropy for a quantum pure state based on its probability distribution on the phase space. Here we do not use coarse-graining used by von Neumann in the context of macroscopic observables. For our entropy, the total system always has a larger entropy than its subsystems even if the total system is described by a quantum pure state. This is not the case for the conventional von Neumann's entropy for mixed states.

For step (iii), we introduce an ensemble entropy for a pure state and prove an inequality regarding the dynamical fluctuation of our entropy, which is similar to von Neumann's quantum H theorem. This inequality includes a constant C that characterizes the correlation of probability fluctuations between different Planck cells. When the correlation is small, the inequality dictates that our entropy relax dynamically to the ensemble entropy and stay at this value most of the time with small fluctuations for macroscopic systems. Our analysis shows that C is small as long as the energy

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shell of microcanonical ensemble is not too narrow and not sporadically populated. As a result, a better understanding of the microscopic origin of the second law of thermodynamics is achieved. The long-time dynamical evolution of our entropy is illustrated numerically with an example.

II. QUANTUM PHASE SPACE

To establish quantum phase space, von Neumann proposed to construct a macroscopic position operator \mathbf{Q} and a macroscopic momentum operator \mathbf{P} that satisfy [30]

$$[\mathbf{Q}, \mathbf{P}] = 0, \quad (1)$$

$$\mathbf{Q} \sim \mathbf{q}, \quad \mathbf{P} \sim \mathbf{p}, \quad (2)$$

where \mathbf{q} and \mathbf{p} are usual microscopic position and momentum operators, respectively, that have the commutator $[\mathbf{q}, \mathbf{p}] = i\hbar$. Equation (2) indicates that the macroscopic position and momentum operators are not identical but close to their microscopic counterparts. Mathematically it is equivalent to finding a complete set of normalized orthogonal wave functions $\{w_j\}$ localized in both position and momentum spaces. The macroscopic position and momentum operators can then be expressed as

$$\mathbf{P} = \sum_j |w_j\rangle \langle w_j| \mathbf{p} |w_j\rangle \langle w_j|, \quad (3)$$

$$\mathbf{Q} = \sum_j |w_j\rangle \langle w_j| \mathbf{q} |w_j\rangle \langle w_j|. \quad (4)$$

Equation (2) implies that the i th-order central moments,

$$\Delta^{(i)} p_j \equiv \langle w_j | (\mathbf{p} - \langle \mathbf{p} \rangle_j)^i | w_j \rangle^{1/i}, \quad (5)$$

$$\Delta^{(i)} q_j \equiv \langle w_j | (\mathbf{q} - \langle \mathbf{q} \rangle_j)^i | w_j \rangle^{1/i}, \quad (6)$$

should be relatively small for all $i \geq 2$. $\langle f \rangle_j$ denotes $\langle w_j | f | w_j \rangle$. For convenience, we often denote $\Delta^{(2)}$ simply by Δ .

For one-dimensional system in which $\mathbf{q} \equiv \mathbf{x}$, $\mathbf{p} \equiv \hbar \mathbf{k} = -i\hbar \partial_x$, von Neumann proposed to find $\{w_j\}$ by Schmidt orthogonalizing a set of Gaussian wave packets of width ζ [2],

$$g_{j_x, j_k} \equiv \exp \left[-\frac{(x - j_x x_0)^2}{4\zeta^2} + i j_k k_0 x \right], \quad (7)$$

where j_x, j_k are integers. When $x_0 k_0 = 2\pi$, this set of Gaussian packets is complete. We are at liberty to choose x_0, k_0 , and ζ as long as $x_0 k_0 = 2\pi$ is satisfied. Unless otherwise specified, parameters are chosen as $x_0 = 1, k_0 = 2\pi$, and $\zeta = (2\pi)^{-1}$.

This method, which is called ‘‘cumbersome’’ by von Neumann [30], suffers from two major drawbacks. First, it is not feasible numerically due to its high computational cost and sensitivity to the order of the orthogonalization procedure. Second, von Neumann argued [2] that the existence of \mathbf{P} and \mathbf{Q} corresponds to the fact that the position and momentum can be measured simultaneously in macroscopic measurements. As there is no difference among measuring positions at different spatial points, we expect that the constructed $\{w_j\}$ have spatial translational symmetry. However, the wave

packets constructed with von Neumann’s method have no such symmetry.

A. Wannier basis

Kohn suggested a method to construct Wannier functions out of Gaussian wave packets [34]. We adapt Kohn’s approach to orthogonalize the Gaussian packets in Eq. (7) and construct a complete set of Wannier functions $\{w_j\}$ whose translational symmetry is guaranteed. The detailed procedure of construction is elaborated as follows.

(1) Choose an initial set of localized wave packets such as the Gaussian wave packets $g_{j_k}(x) \equiv g_{0, j_k}(x)$ in Eq. (7). Find their Fourier transform $\tilde{g}_{j_k}(k) \equiv \mathcal{F}\{g_{j_k}(x)\} \equiv \frac{1}{\sqrt{2\pi}} \int g_{j_k}(x) e^{-ikx} dx$.

(2) At a fixed k , for every j_k , $[\tilde{g}_{j_k}(k + 2n\pi)]_{n \in \mathbb{Z}}$ is a normalizable vector; we denote it by $u_{k, j_k}(n)$. Apply Schmidt orthogonalization procedure $v_0 = u_0$ (the subscript k is omitted), normalize $v_0, v_1 = u_1 - (u_1, v_0)v_0$, normalize v_1 , and repeat for u_2, u_3, \dots . We eventually get an orthonormal basis $\{v_{k, j_k} \in l^2(\mathbb{Z})\}_{j_k \in \mathbb{Z}}$. Define $\tilde{w}_{j_k}(k + 2n\pi) \equiv v_{k, j_k}(n)/\sqrt{2\pi}$.

(3) For every k (discrete in numerical calculations) on $[0, 2\pi)$, repeat step 2. According to Proposition 1 in Appendix A, $w_{j_x, j_k}(x) \equiv w_{j_k}(x - j_x)$ [w_{j_k} is the Fourier transform of \tilde{w}_{j_k}] are orthonormal. $\{w_j\}$ is the desired orthonormal basis [j denotes (j_x, j_k)].

We have thus established a quantum phase space that is different from the classical phase space: (1) It is divided into phase cells of size Planck constant h (for one-dimensional system) as illustrated in Fig. 1(a); we call such a cell Planck cell for brevity. (2) Each Planck cell is assigned a Wannier function w_j , which is localized near site $(x = j_x, k = 2j_k\pi)$. We are now able to map a pure wave function unitarily onto phase space. There has been tremendous efforts to formulate quantum mechanics in phase space based on Wigner’s quasidistribution function and Weyl’s correspondence [35]. However, Wigner’s quasidistribution is not positive-definite and cannot be interpreted as probability in phase space. According to our construction, for a wave function ψ , $|\langle \psi | w_j \rangle|^2$ is its probability at Planck cell j as $\{w_j\}$ is a set of complete orthonormal basis.

The generalization to higher dimensions is straightforward. With the one-dimensional $\{w_j(x)\}$ that we have constructed, we simply define

$$w_{j_1 j_2 \dots j_n}(x_1, x_2, \dots, x_n) \equiv w_{j_1}(x_1) w_{j_2}(x_2) \dots w_{j_n}(x_n). \quad (8)$$

Then $\{w_{j_1 j_2 \dots j_n}\}$ is the localized orthonormal basis for an n -dimensional system.

Numerical results of one-dimensional Wannier functions are provided in Fig. 1. A Wannier function localized near $(x = 3, k = 20\pi)$ is plotted in the k and x spaces, respectively, in Figs. 1(c) and 1(d). This Wannier function is obtained with the above procedure using the Gaussian wave packets g_{j_x, j_k} as initial functions. And the order of Schmidt orthogonalization in our procedure is chosen to be $j_k = 0, 1, -1, 2, -2, \dots$. The result does not sensitively depend on the order.

Our numerical computation finds that the Wannier function spreads out slowly with increasing momentum k . From Fig. 1(b) we can see that both $\Delta^{(i)} k_j$ and $\Delta^{(i)} x_j$, which characterize the spreads of the Wannier function, diverge as

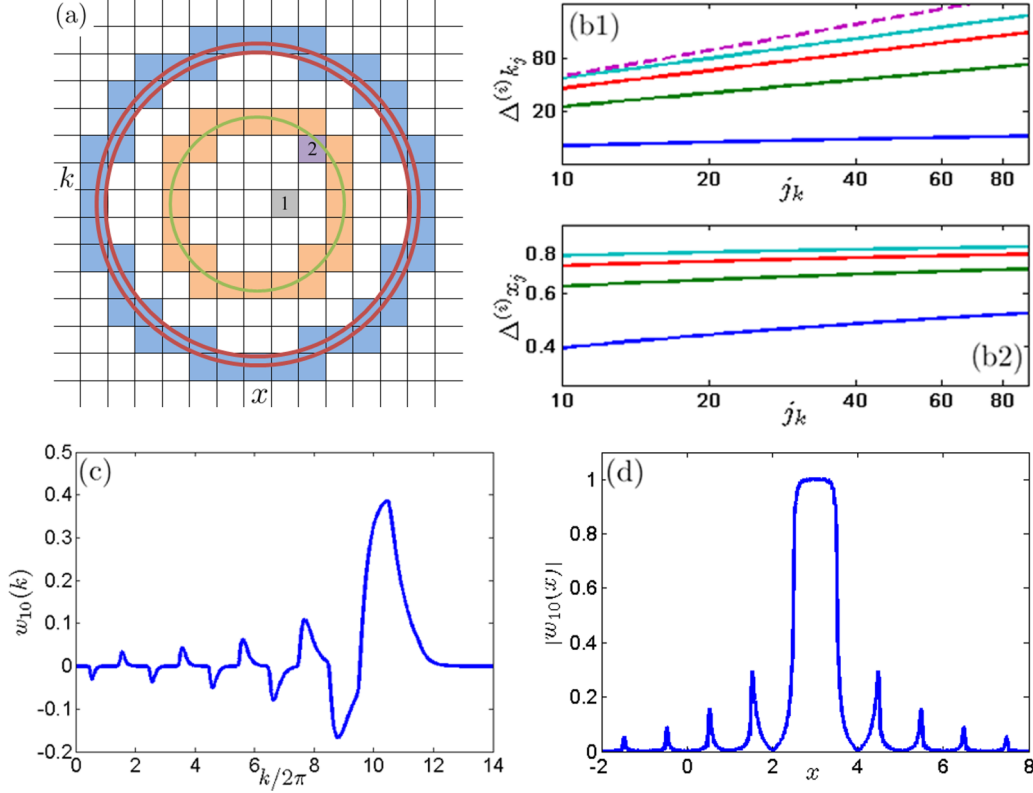


FIG. 1. (Color online) Illustration of quantum phase space. (a) Schematic plot of quantum phase space. (b) Spreads of Wannier functions as a function of j_k . Both axes are in logarithmic scales. Solid lines are for $i = 8, 6, 4, 2$, from top to bottom, respectively. The dashed line of slope 1 is drawn to show that all solid lines have slope less than 1. (c) Wannier function $w_{3,10}$ is shown localized near $k = 10 \times 2\pi$. (d) Wannier function $w_{3,10}$ is shown localized near $x = 3$.

j_k increases; $\Delta^{(i)}x_j$ appears to grow more slowly. Actually, it can be proved that the product of $\Delta x_j \Delta k_j$ diverges as j_k increases no matter what initial wave packets are chosen (see Appendix B). This divergent behavior of $\Delta x \Delta k$ is called strong uncertainty relation [36].

However, the divergence is not very severe. As shown in Fig. 1(b) where both axes are in logarithmic scales, all the growth slopes are much less than one. Therefore, all orders of the relative spreads $\Delta^{(i)}x_j/j_k$ and $\Delta^{(i)}k_j/2\pi j_k$ fall to zero quickly as j_k increases. This suggests that for the one-dimensional system, the requirement Eqs. (5) and (6) are satisfied in the sense

$$\lim_{\langle p \rangle_j / p_0 \rightarrow \infty} \frac{\Delta^{(i)}p_j}{\langle p \rangle_j} = \lim_{\langle p \rangle_j / p_0 \rightarrow \infty} \frac{p_0 \Delta^{(i)}q_j}{\langle p \rangle_j q_0} = 0, \quad (9)$$

where we have used $p = \hbar k$, $q = x$, and $\langle p \rangle_j \approx j_k p_0$.

B. Quantum energy shell

In classical phase space, there is an important concept of energy surface, where the dynamics of an isolated system is confined. Energy surface, which is of no width, is no longer valid in the quantum phase space, which consists of cells of finite size. However, a similar concept, energy shell of finite width, can be introduced. For this purpose, we need to first show that each of our Planck cells is localized in energy for most of the macroscopic systems of physical interest.

For an isolated system of fixed number of particles $N \gg 1$ with Hamiltonian $H(\mathbf{p}, \mathbf{r})$, where \mathbf{p} and \mathbf{r} are $3N$ -dimensional vectors, define p_C as the typical magnitude of momentum of any particle and r_C as the typical length scale on which H changes relatively significantly. For example, r_C can be the mean free path of a particle or the characteristic scale of the external potential. We define the index

$$I \equiv p_C r_C / \hbar. \quad (10)$$

In this work we focus on the cases where I is considerably large.

We expect that the quantum phase space is reduced to the classical phase space in the limit $I \rightarrow \infty$ in the sense that the relative size of a Planck cell and the relative spreads of the Wannier functions tend to zero. This is indeed the case. We construct Planck cells defined by $p_0 = p_C / \sqrt{I}$ and $r_0 = r_C / \sqrt{I}$. We immediately have $p_0 / p_C = r_0 / r_C = I^{-1/2} \rightarrow 0$ in the limit $I \rightarrow \infty$. Suppose that j_C is the momentum index such that $\langle p \rangle_{j_C} \approx p_C$. For a typical Planck cell j whose $|j_k| \lesssim j_C$, we have according to Eq. (9)

$$\frac{\Delta^{(i)}p_j}{p_C} \lesssim \frac{\Delta^{(i)}p_{j_C}}{p_C} \rightarrow 0, \quad (11)$$

and similarly,

$$\frac{\Delta^{(i)}r_j}{r_C} = \frac{p_0}{r_0} \frac{\Delta^{(i)}r_j}{p_C} \lesssim \frac{p_0}{r_0} \frac{\Delta^{(i)}r_{j_C}}{p_C} \rightarrow 0, \quad (12)$$

for $i = 2, 3, \dots$ in the limit $I \rightarrow \infty$. We obtain the desirable picture, the quantum phase space becoming the classical phase space as $I \rightarrow \infty$. We thus call $I \rightarrow \infty$ classical limit. We will continue to use this choice of p_0 and r_0 in the following discussion.

Now we are ready to show that indeed our Wannier functions are localized in energy. To avoid cumbersome partial derivatives and summations, we illustrate the point with single-particle one-dimensional potential $V(x)$; the case of kinetic energy and multiparticle systems should be essentially the same. For a typical Planck cell j , we expand V at $\langle x \rangle_j$ where $|w_j\rangle$ is localized and compute its relative spread

$$\frac{\Delta V^2}{V_0^2} \equiv \left\langle \frac{(V - V_0)^2}{V_0^2} \right\rangle_j = \sum_{i=2}^{\infty} a_{j,i} \left(\frac{\Delta^{(i)} x_j}{r_C} \right)^i, \quad (13)$$

where $V_0 \equiv V(\langle x \rangle_j)$. As V varies on the scale r_C , it is easy to see that $a_{j,i} = O(1)$. Therefore, the relative spread $\Delta V^2/V_0^2$ tends to zero in the classical limit $I \rightarrow \infty$.

As our Wannier functions are localized in energy, when we map an energy eigenstate $|\phi_\alpha\rangle$ with eigen-energy E_α to the quantum phase space, only the Planck cells with their energies $E_j \equiv \langle w_j | H | w_j \rangle \approx E_\alpha$ are significantly occupied. We say that energy eigenstate $|\phi_\alpha\rangle$ crosses Planck cell j when $\langle w_j | \phi_\alpha \rangle$ is significantly nonzero. As a result, we can define an energy shell a of energy interval $[E_a, E_a + \Delta E_a]$ as a set of phase cells w_j 's such that $\langle \phi_\alpha | \Delta_a | \phi_\alpha \rangle \approx 1$ when $E_\alpha \in [E_a, E_a + \Delta E_a]$. The projection operator $\Delta_a \equiv \sum_{j=1}^{N_a} |w_j\rangle \langle w_j|$, where $N_a \equiv \text{tr } \Delta_a$ is the number of Planck cells in energy shell a . Energy shell a is said to be significantly occupied by a quantum state $\psi(t)$ when $\langle \psi(t) | \Delta_a | \psi(t) \rangle$ is considerably larger than zero.

We draw the quantum phase space schematically in Fig. 1(a), where squares are for Planck cells and circles represent eigenenergies. Two energy shells are illustrated: outer one with blue Planck cells and the inner one with orange Planck cells. Each energy eigenstate may cross many Planck cells; at the same time, one Planck cell can be crossed by many energy eigenstates. The purple Planck cell 2 is in the inner orange energy shell while the gray cell 1 is in neither shell colored.

III. HIERARCHY OF ENERGY SCALES

In this section we examine the energy scales involved and establish a hierarchy among them. It will become clear later that these energy scales and their hierarchy play crucial roles in regulating the long-time dynamics of the system.

One energy scale is $\Delta_E E$, the typical difference between adjacent eigenenergies. The typical energy uncertainty $\Delta_Q E$ in a Planck cell is another energy scale. For a typical Planck cell j , we have

$$\Delta_Q E \approx \left[\sum_{\alpha} (E_\alpha - E_j)^2 |\langle w_j | \phi_\alpha \rangle|^2 \right]^{\frac{1}{2}}. \quad (14)$$

For a quantum system with a large number of particles $N \gg 1$, it should be expected that though w_j 's are localized in energy, eigenstates that cross every Planck cell are numerous. To see this, we note that the density of state $\rho(E)$ grows exponentially

while $\Delta_Q E$ increases polynomially as $N \rightarrow \infty$. Therefore, for a typical many-particle system, we have $\Delta_E E \ll \Delta_Q E$.

Consider a general quantum state $|\psi(t)\rangle = \sum_{\alpha} c_{\alpha}(t) |\phi_{\alpha}\rangle$, and denote $\wp_{\alpha} \equiv |c_{\alpha}(t)|^2$. For this quantum state, there exists an energy scale $\Delta_C E$ defined as

$$\Delta_C E \equiv \left[\sum_{j,\alpha} (E_{\alpha} - E_j)^2 \wp_{\alpha} |\langle w_j | \phi_{\alpha} \rangle|^2 \right]^{\frac{1}{2}}, \quad (15)$$

where $E_j \equiv \langle w_j | H | w_j \rangle$ is the average energy of Planck cell j . We call $\Delta_C E$ the correlation energy scale. As we will show later, only the Planck cells that are separated by energy less than $\Delta_C E$ are correlated. A comparison between Eqs. (14) and (15) indicates that we have $\Delta_Q E \approx \Delta_C E$ for a typical quantum state.

Many properties, in particular macroscopic properties of a system, are not sensitive to the details of a quantum state. Since $\Delta_E E \ll \Delta_Q E$, we define a smoothed function over energy scale $\Delta_Q E$ as follows:

$$\langle f_{\alpha} \rangle_s(E) \equiv \frac{\sum_{|E_{\alpha}-E|<\Delta_Q E} f_{\alpha}}{\sum_{|E_{\alpha}-E|<\Delta_Q E} 1}. \quad (16)$$

For example, $\langle \wp_{\alpha} \rangle_s(E)$ is the smoothed probabilities of the quantum state ψ at E . We can now introduce another energy scale $\Delta_{mc} E$ on which $\langle \wp_{\alpha} \rangle_s$ can be regarded as constant. This energy scale $\Delta_{mc} E$ indicates the width of the energy shell, which is significantly occupied by ψ . In this work we focus on the quantum state such that the following hierarchy of magnitudes is satisfied:

$$\Delta_E E \ll \Delta_Q E \approx \Delta_C E \ll \Delta_{mc} E \ll E, \quad (17)$$

where $E \equiv \langle \psi | H | \psi \rangle$. For a quantum state prepared in real experiments for a many-body system, both $\Delta_{mc} E$ and E are of macroscopic size while $\Delta_Q E$ and $\Delta_C E$ are microscopic. Therefore, the hierarchy in Eq. (17) are readily satisfied in real experiments.

In textbooks on quantum statistical mechanics [1], the microcanonical ensemble is established on an energy shell of width $\Delta_{mc} E \ll E$. Usually no lower bound is given for $\Delta_{mc} E$. Here we see that it should have a quantum lower bound of $\Delta_Q E$, which will be shown later to play a key role to guarantee the equilibration of the system.

Finally, we assume that the eigenstates are not highly concentrated in the highly occupied energy shell $[E, E + \Delta_{mc} E]$. Mathematically, this means that the density of states $\rho(E)$ satisfies

$$\int_{E_j - \Delta E}^{E_j + \Delta E} dE \rho(E) \ll \int_{E_j - \Delta_{mc} E}^{E_j + \Delta_{mc} E} dE \rho(E), \quad (18)$$

whenever $\Delta E \ll \Delta_{mc} E$. Despite a few exceptions (flat band etc.), this assumption is not strong and should be satisfied by most of the macroscopic systems in high-energy states.

IV. ENTROPY FOR PURE QUANTUM STATE AND AN INEQUALITY FOR ITS FLUCTUATIONS

As we can now map a wave function unitarily to the quantum phase space, we can use its probability distribution

in the phase space to define an entropy. For a pure quantum state $\psi(\mathbf{r})$, we define its entropy as

$$S_w(\psi) \equiv - \sum_j \langle \psi | \mathbf{W}_j | \psi \rangle \ln \langle \psi | \mathbf{W}_j | \psi \rangle, \quad (19)$$

where $\mathbf{W}_j \equiv |w_j\rangle\langle w_j|$ is the projection to Planck cell j characterized by Wannier function $w_j(\mathbf{r})$.

Consider an isolated quantum system described by ψ . As this state evolves with time according to the Schrödinger equation, its entropy $S_w(\psi)$ will evolve in time. Will the entropy increase and eventually approach a maximum in accordance with the second law of thermodynamics? The answer is yes for a large class of quantum systems in the sense established by von Neumann in 1929 [2]. In the 1929 paper, von Neumann introduced an entropy for pure quantum states; he then proved an inequality concerning the long-time dynamical behavior of this entropy. According to this inequality, if the system starts with a low-entropy state, the system will evolve into high-entropy states and stay there almost all the time with small fluctuations. Von Neumann called this inequality quantum H theorem. We will prove a similar inequality in this section.

As the system evolves, the probability in each Planck cell j will change with time ($\hbar = 1$)

$$\begin{aligned} \wp_j(t) &\equiv \langle \psi(t) | \mathbf{W}_j | \psi(t) \rangle \\ &= \sum_{\alpha, \beta} \langle \psi(0) | \phi_\alpha \rangle \langle \phi_\alpha | \mathbf{W}_j | \phi_\beta \rangle \langle \phi_\beta | \psi(0) \rangle e^{i(E_\alpha - E_\beta)t}. \end{aligned} \quad (20)$$

We define $\bar{\wp}_j$ as the long time averaging of $\wp_j(t)$ and introduce a corresponding entropy

$$S_E(\psi) \equiv - \sum_j \bar{\wp}_j \ln \bar{\wp}_j. \quad (21)$$

We call it ensemble entropy for pure state ψ . The ensemble entropy S_E does not change with time. We find that under some reasonable conditions, the entropy $S_w(\psi)$ will approach $S_E(\psi)$ and stay close to it almost all the time with small fluctuations. First we present a rather universal inequality concerning the long-time behavior of our entropy, which will imply the equilibration of our entropy under reasonable conditions. We leave details of the proof to Appendix C; the inequality is as follows.

Theorem. For a quantum system governed by a Hamiltonian whose eigenvalues satisfy the following conditions 1, 2, and 3, and for every j , $0 \leq \bar{\wp}_j \leq 1/e$, we have

$$\frac{\overline{[S_w(\psi(t)) - S_E]^2}}{S_E^2} \leq C + \frac{8}{S_E} + \frac{4}{S_E^2}, \quad (22)$$

where

$$C \equiv \sum_{j, j'} C_{jj'} (\bar{\wp}_j \ln \bar{\wp}_j) (\bar{\wp}_{j'} \ln \bar{\wp}_{j'}) / \left(\sum_j \bar{\wp}_j \ln \bar{\wp}_j \right)^2 \quad (23)$$

and $C_{jj'} \equiv \overline{[\wp_j(t) - \bar{\wp}_j][\wp_{j'}(t) - \bar{\wp}_{j'}]} / \bar{\wp}_j \bar{\wp}_{j'}$.

The three conditions are

- *Condition 1.* $E_\alpha = E_\beta \Rightarrow \alpha = \beta$;

- *Condition 2.* $E_\alpha - E_\beta = E_{\alpha'} - E_{\beta'}, \alpha \neq \beta \Rightarrow \alpha = \alpha', \beta = \beta'$;
- *Condition 3.* $E_\alpha + E_\chi - E_\beta - E_\gamma = E_{\alpha'} + E_{\chi'} - E_{\beta'} - E_{\gamma'}, \{\alpha, \chi\} \cap \{\beta, \gamma\} = \emptyset \Rightarrow \{\alpha, \chi\} = \{\alpha', \chi'\}$ and $\{\beta, \gamma\} = \{\beta', \gamma'\}$.

Conditions 1 and 2 are commonly used [2,16,37], representing no degeneracies of energies and energy gaps, respectively. Condition 3 implies differences between energy gaps are also distinct. From the random matrix theory [38], we believe condition 3 should be satisfied by most nonintegrable systems; as a result, the inequality should hold for a majority of quantum systems. These three conditions have a close connection with moments of $\wp_j(t)$ statistically, i.e., $\overline{\wp_j(t)}$, $\overline{\wp_j(t)^2}$, and $\overline{\wp_j(t)^4}$. For example, with condition 1, we have

$$\overline{\wp_j} = \sum_\alpha c_{\alpha j}^* c_{\alpha j}, \quad (24)$$

where $c_{\alpha j} \equiv \langle \psi(0) | \phi_\alpha \rangle \langle \phi_\alpha | w_j \rangle$. For the rest of details, please see Appendix C.

We now discuss the physical interpretation of C , $C_{jj'}$, and the inequality. Clearly, $0 \leq |C_{jj'}| \leq 1$ signifies the fluctuation correlation between Planck cells j and j' ; C can be regarded as some kind of averaging over $C_{jj'}$ with weight $-\bar{\wp} \ln \bar{\wp}$. Hence, C characterizes the averaged fluctuation correlation between cells. With such understanding, the inequality can be understood intuitively: when S_E is large, that is the probability distribution spreads over many Planck cells, the correlation of \wp between the majority of Planck cells are small; the total entropy S_w undergoes small fluctuations most of the time. In these situations, the inequality Eq. (22) implies a quantum H theorem similar to von Neumann's.

Indeed we can demonstrate that S_E is large and C is small under the following two conditions:

- The hierarchy Eq. (17) and the assumption Eq. (18) hold.
- For significantly occupied energy shells, the occupancy rate

$$R \equiv \langle \wp_\alpha \rangle_s^2 / \langle \wp_\alpha^2 \rangle_s \quad (25)$$

is high.

R signifies the fluctuation of \wp_α : if all eigenstates are equally occupied, $R = 1$; if only one of N_c consecutive eigenstates is occupied, $R = 1/N_c$.

(a) *Estimate of S_E .* We can show (see Appendix D)

$$S_E^{\max} - S_E \lesssim -\ln R, \quad (26)$$

where

$$S_E^{\max} \equiv - \int_{-\infty}^{\infty} dE \rho(E) \langle \wp_\alpha \rangle_s(E) \ln \langle \wp_\alpha \rangle_s(E). \quad (27)$$

By Jensen's inequality $S_E^{\max} \geq \ln d_{\text{eff}}$, where $d_{\text{eff}}^{-1} \equiv \sum_\alpha \wp_\alpha^2$ is the effective number of eigenstates occupied [32]. d_{eff} can certainly also be regarded as the microscopic states occupied in a macroscopic quantum state. For a quantum state prepared in real experiments, d_{eff} is a very large number [16,32]. When R is reasonably high, $R \approx 1$, we have $S_E \approx S_E^{\max} \geq \ln d_{\text{eff}}$. Therefore, S_E is indeed very large.

(b) *Estimate of C .* As our Wannier functions are localized in energy as discussed in Sec. II, Planck cells i and j far apart are not likely to share energy eigenfunctions (that is, for energy eigenstate ϕ_α , $\langle w_i | \phi_\alpha \rangle$ and $\langle w_j | \phi_\alpha \rangle$ are not significant

simultaneously); thus, with condition 1 and 2, \wp_i should not be considerably correlated with \wp_j . When hierarchy Eq. (17) holds, $\Delta_Q E \approx \Delta_C E \ll \Delta_{mc} E$, pairs of Planck cells not significantly correlated should be the majority in Eq. (23). As a result, C should be small. In fact we estimate (see Appendix D)

$$C \lesssim \Delta_C E / \Delta_{mc} E. \quad (28)$$

When S_E is maximized with $C \approx 0$, the inequality Eq. (22) shows that the relative fluctuation of S_w away from S_E is small when it is averaged over a long time. This means that when the system starts with a low-entropy state, it will relax dynamically to states whose entropies are very close to S_E . Otherwise, the inequality would be violated. Note that it is possible that the system can evolve into a state whose entropy is far away from S_E . When this happens, the system will relax dynamically back in a short time to states whose entropies are high and close to S_E . This reminds us of the Poincaré recurrence in classical dynamic systems. So, the morale is the same for both quantum and classical dynamics: due to the time reversal symmetry inherently possessed by both quantum and classical systems, it is impossible to rule out that the system evolves dynamically to a lower-entropy state. However, with the conditions above we can assert that the large deviation from the maximized entropy is possible only rarely in quantum dynamics.

As the quantum system equilibrates, not only its entropy reaches its maximum, other observables such as momentum or density distribution also settle. In our definition of entropy, it is clear when the entropy reaches its maximum, $\langle w_j | \psi \rangle$ can acquire distinct phase factors while not affecting the total entropy. When $\langle w_i | \mathbf{p} | w_j \rangle$ is small (relatively) for $i \neq j$, $\langle \psi | \mathbf{p} | \psi \rangle$ does not significantly depend on those phase factors, either. In macroscopic systems, if Planck cell i and j are close to each other (with $|p_i - p_j|$ much less than $p \equiv (p_i + p_j)/2$), \mathbf{p} can be regarded as a constant on the cells, thus $\langle w_i | \mathbf{p} | w_j \rangle \approx p \langle w_i | w_j \rangle = 0$ for $i \neq j$; if Planck cell i and j are far apart, their overlapping is small and, as a result, $\langle w_i | \mathbf{p} | w_j \rangle$ is relatively small. Similar argument applies to other observables (such as \mathbf{x}) as long as the observable varies on a scale much larger than Δp and Δx of Wannier functions. The inequality proved by Riemann for the fluctuations of observables [16,32] is also an indication that observables should equilibrate when the entropy approaches its maximum value.

As we are able to compute the Wannier functions w_j numerically, the entropy for quantum pure states and the relaxation of our entropy toward a maximum can now be illustrated with a concrete example. We are trying to answer whether a macroscopic many-body quantum system can equilibrate dynamically. However, as we have seen in this work and in many other works (see, e.g., Refs. [2,16]), the conclusion relies on only the structure of eigenenergies of the system (degeneracy, energy gaps, etc.), which are shared by both single-particle and many-body systems according to the random matrix theory [38]. This means that in many situations it is sufficient to use single-particle systems to illustrate entropy for pure states and the quantum H theorem.

We choose to use ripple billiard with which we are very familiar. The ripple billiard is an infinite potential well with $V = 0$ in the area enclosed by $y = \pm b$, $x = \pm b \pm a \cos(\pi y/b)$, and $V = \infty$ otherwise [39,40]. In our numerical computation, the initial state is a moving Gaussian wave packet and the

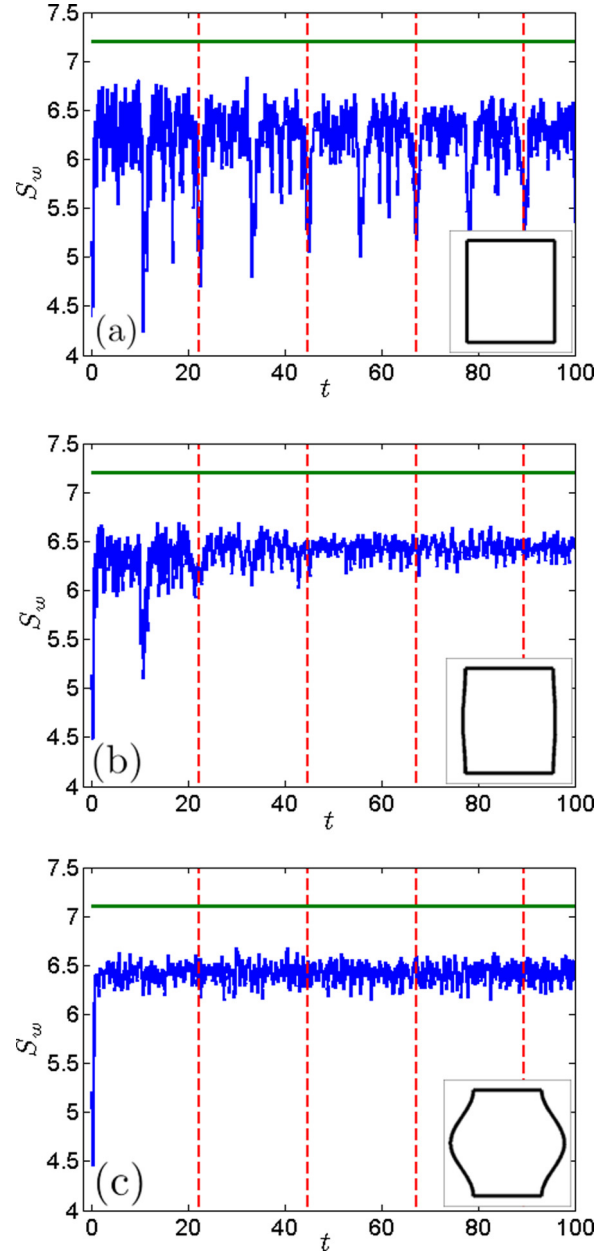


FIG. 2. (Color online) Time evolution of $S_w[\psi(t)]$ for three different ripple billiards. The initial state is a moving Gaussian wave packet. The vertical dashed red lines indicate the theoretical recurrence time for a square infinite potential well of size $2b \times 2b$. The horizontal green lines are the ensemble entropy S_E . The three ripple billiards shown in the insets are characterized by $\epsilon = a/b = 0.25\%$, 2.5% , 25% , respectively.

simulation is carried out on a 64×64 grid. The results for the entropy $S_w[\psi(t)]$ are plotted in Fig. 2 for ripple billiards with three different values of $\epsilon = a/b$. When ϵ is small, the system is nearly integrable and S_w is almost periodic but with a decaying oscillating amplitude [see Fig. 2(a)]. As ϵ becomes larger and the system gets far away from the integrable regime, the entropy S_w rises quickly to a maximum value and stays there with small fluctuations as discussed. The ensemble entropy S_E is also plotted and it deviates visibly from the long-time averaged value of S_w . The reason is that since this is

a single-particle system, S_w and S_E are not large. As a result, the right-hand side of the inequality Eq. (22) is not very small.

A few remarks are warranted before we conclude this section. There seems to be a hidden assumption in von Neumann's proof of his quantum H theorem besides two explicitly stated conditions (identical to conditions 1 and 2 here). This assumption is equivalent to eigenstate thermalization hypothesis [8,12] as pointed out in Ref. [25] and by an anonymous referee. In our opinion, this assumption is linked directly to Eq. (27) in von Neumann's proof [30], which is highly questionable. In contrast, we do not have any other assumption in our proof of the inequality Eq. (22) besides the three conditions. The conditions for C to be small, such as the hierarchy of energy scales, have also been explicitly expressed. Our effort here is to follow the line of von Neumann and Reimann to understand the microscopic origin of the second law of thermodynamics without any hypothesis. It is true that our inequality with $C \approx 0$ does not exclude the happening of large deviation from the maximized entropy. However, this kind of large deviation occurs rarely according to our analysis. More efforts are needed to find out exactly how rare these events are. The usual fluctuation theorem seems not applicable here as it depends on many concepts, such as temperature, heat bath, and entropy, whose quantum origins are not clear themselves.

V. GENERALIZATION TO MIXED STATES AND COMPARISON WITH VON NEUMANN'S ENTROPY

In quantum mechanics, we are all familiar with the von Neumann entropy that is defined as

$$S_v(\rho) \equiv -\text{tr } \rho \ln \rho, \quad (29)$$

where ρ is the density matrix for mixed states. This entropy S_v is zero for any pure state. This fact leads to a well-known dilemma: a large system in a pure state has zero entropy while any of its subsystems that interacts or entangles with the rest of the system has nonzero entropy S_v .

To compare our entropies to S_v , we need to generalize our entropy for mixed states. There is a straightforward way to accomplish the goal: for N -particle mixed states ρ^N , we define

$$S_w(\rho^N) \equiv \sum_{j_1 j_2 \dots j_N} s_w(\text{tr } \rho^N \mathbf{W}_{j_1} \otimes \mathbf{W}_{j_2} \otimes \dots \otimes \mathbf{W}_{j_N}), \quad (30)$$

where $s_w(\wp) = -\wp \ln \wp$.

Several basic properties that $S_w(\rho^N)$ shares with S_v [41] are listed below:

Invariance. $S_w(\rho^N)$ depends on $\{w_j\}$ but not on the choice of basis in the Hilbert space. This is a result of the invariance of the trace.

Positivity. $S_w \geq 0$ since $s_w(x) \geq 0$ for $0 \leq x \leq 1$.

Concavity. For $\lambda_1, \lambda_2 > 0$, $\lambda_1 + \lambda_2 = 1$,

$$S_w(\lambda_1 \rho_1^N + \lambda_2 \rho_2^N) \geq \lambda_1 S_w(\rho_1^N) + \lambda_2 S_w(\rho_2^N). \quad (31)$$

This originates from the concavity of $s_w(x)$.

Additivity.

$$S_w(\rho_1^M \otimes \rho_2^N) = S_w(\rho_1^M) + S_w(\rho_2^N) \quad (32)$$

The equality indicates that for two independent systems, the total entropy is the sum of the two. The property is also inherited from $s_w(x)$.

Proof of these properties is essentially the same as that in Ref. [41] and hence omitted here.

Despite these similarities, there is one crucial difference between our entropy and S_v . As we have mentioned, for S_v there is a well-known dilemma: for a large system on a pure state, $S_v = 0$ while its subsystem has nonzero entropy. In stark contrast, as we shall show, for our entropy S_w , a large system always has bigger entropy than its subsystem. To demonstrate this, we only need to prove that the entropy S_w decreases when one particle is traced out of an N -particle system.

Without loss of generality, we tend to trace out the N th particle and write

$$\rho^N = \sum_{i, i_N, i', i'_N} c_{i, i_N, i', i'_N} |\psi_i^{N-1}, \psi_{i_N}\rangle \langle \psi_{i'_N}^{N-1}, \psi_{i'_N}|. \quad (33)$$

Here ψ 's are general orthonormal basis, not energy eigenstates. With the use of the inequality $s_w(\wp_1 + \wp_2) \leq s_w(\wp_1) + s_w(\wp_2)$ for $\wp_1, \wp_2 \geq 0$, the proof is straightforward:

$$\begin{aligned} S_w(\rho^N) &= \sum_{j, j_N} s_w \left(\sum c \langle \psi_i^{N-1} | \mathbf{W}_j^{N-1} | \psi_i^{N-1} \rangle \langle \psi_{i'_N} | \mathbf{W}_{j_N} | \psi_{i'_N} \rangle \right) \\ &\geq \sum_j s_w \left(\sum_{j_N} \sum c \langle \psi_i^{N-1} | \mathbf{W}_j^{N-1} | \psi_i^{N-1} \rangle \langle \psi_{i'_N} | \mathbf{W}_{j_N} | \psi_{i'_N} \rangle \right) \\ &= \sum_j s_w \left(\sum c \langle \psi_i^{N-1} | \mathbf{W}_j^{N-1} | \psi_i^{N-1} \rangle \langle \psi_{i'_N} | \sum_{j_N} \mathbf{W}_{j_N} | \psi_{i'_N} \rangle \right) \\ &= \sum_j s_w \left(\sum c \langle \psi_i^{N-1} | \mathbf{W}_j^{N-1} | \psi_i^{N-1} \rangle \langle \psi_{i'_N} | \psi_{i'_N} \rangle \right) \\ &= S_w(\rho^{N-1}), \end{aligned} \quad (34)$$

where the subscripts i, i_N, i', i'_N are omitted for brevity without causing confusion.

We introduce a density matrix

$$\rho_{\text{mc}} \equiv \sum_{\alpha} |\langle \psi(0) | \phi_{\alpha} \rangle|^2 |\phi_{\alpha}\rangle \langle \phi_{\alpha}|. \quad (35)$$

This density matrix can be regarded as a microcanonical ensemble for two reasons: (1) It is easy to check that $S_E = S_w(\rho_{\text{mc}})$. This means that the system's entropy is essentially given by ρ_{mc} at equilibrium. (2) Reimann [16] has also shown that the expectation of all observables can also be computed with ρ_{mc} at equilibrium. This ensemble is clearly different from the conventional microcanonical ensemble in textbooks [1] as it depends on the initial condition. The ensemble in Eq. (35) is also different from von Neumann's [2] that involves certain coarse-graining of energy. However, both our ensemble and von Neumann's depend more or less on the choice of initial conditions. This can lead to very interesting new physics: we are at liberty to choose an initial condition

that composes of energy eigenstates from two very different energy shells, which can lead to an equilibrium state with two distinct temperatures [28].

VI. CONCLUSION

In summary, we have used Kohn's method to construct a complete set of Wannier functions that are localized at both given positions and momenta. We then established a quantum phase space, where each Planck cell is represented by one of these Wannier functions. By mapping unitarily a quantum pure state to this quantum phase space, we have defined an entropy for pure states. A hierarchy of energy scales is proposed and the properties of this entropy have been examined. In particular, we have shown that for our entropy, a system always has larger entropy than its subsystems.

The long-time dynamical behavior of our entropy has been examined and found to obey an inequality, which like the quantum H theorem proved by von Neumann [2], along with reasonable hypotheses, indicates that a majority of isolated quantum systems equilibrate dynamically: starting with reasonable initial states, the quantum system will evolve into a state with maximized entropy and stay there almost all the time with small fluctuations. Due to the time reversal symmetry, the system does sometimes undertake large fluctuations. However, the quantum H theorem demands that these large fluctuations happen rarely and are short-lived, which provides a quantum perspective of the second law of thermodynamics.

As already pointed out in the introduction, there have been renewed interests in the foundation of quantum statistical mechanics. These new efforts have not only led to better theoretical understanding of the issue but also to new physical predications and challenges that await for answers from experimentalists. For example, a quantum state that is at equilibrium but with multiple temperatures was predicted based on the microcanonical ensemble established by von Neumann [28]. And it was shown recently [29,42,43] that quantum systems can relax much faster than what has been observed in reality. Can this multiple temperature state be realized in experiments? Does a quantum state that can relax as fast as what the theorists have predicted really exist? The answers may ultimately lie in understanding the borderline between the microscopic and the macroscopic world.

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APPENDIX A: PROPOSITION FOR ORTHOGONALIZATION

We prove here a proposition based on which one can show the orthogonality of $\{w_j(x)\}$.

Proposition 1. Assume $f_j(k) \in L^2(\mathbb{R})$ ($j \in \mathbb{N}$) if for almost every $k \in [0, 2\pi)$, for all $j, j' \in \mathbb{N}$

$$\sum_{n \in \mathbb{Z}} f_j^*(k + 2n\pi) f_{j'}(k + 2n\pi) = \frac{1}{2\pi} \delta_{jj'}, \quad (\text{A1})$$

then we have

$$\int_{\mathbb{R}} f_j^*(k) f_{j'}(k) e^{-ij_x k} dk = \delta_{jj'} \delta_{0j_x}, \quad (\text{A2})$$

for all $j, j' \in \mathbb{N}$, and $j_x \in \mathbb{Z}$.

Proof.

$$\begin{aligned} & \int_{\mathbb{R}} f_j^*(k) f_{j'}(k) e^{-ij_x k} dk \\ &= \sum_{n \in \mathbb{Z}} \int_{2n\pi}^{2(n+1)\pi} f_j^*(k) f_{j'}(k) e^{-ij_x k} dk \\ &= \sum_{n \in \mathbb{Z}} \int_0^{2\pi} f_j^*(k + 2n\pi) f_{j'}(k + 2n\pi) e^{-ij_x(k+2n\pi)} dk \\ &= \int_0^{2\pi} \sum_{n \in \mathbb{Z}} f_j^*(k + 2n\pi) f_{j'}(k + 2n\pi) e^{-ij_x k} dk \\ &= \frac{\delta_{jj'}}{2\pi} \int_0^{2\pi} e^{-ij_x k} dk = \delta_{jj'} \delta_{0j_x}. \end{aligned}$$

The converse is also valid and the proof is omitted here. For the construction of localized orthonormal basis in the main text, $f_j(k) = \tilde{w}_{jk}(k)$. Noticing that

$$\int_{\mathbb{R}} \mathcal{F}\{f(x)\}^*(k) \mathcal{F}\{g(x)\}(k) dk = \int_{\mathbb{R}} f^*(x) g(x) dx \quad (\text{A3})$$

and $\mathcal{F}\{f(x - j_x)\} = \mathcal{F}\{f(x)\} e^{-ij_x k}$, where

$$\mathcal{F}\{f(x)\}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x) e^{-ikx} dx, \quad (\text{A4})$$

we have

$$\begin{aligned} & \int_{\mathbb{R}} w_{jk}^*(x) w_{j'_k}(x - j_x) dx \\ &= \int_{\mathbb{R}} \mathcal{F}\{w_{jk}(x)\}^*(k) \mathcal{F}\{w_{j'_k}(x - j_x)\}(k) dk \\ &= \int_{\mathbb{R}} \tilde{w}_{jk}^*(k) \tilde{w}_{j'_k}(k) e^{-ij_x k} dk = \delta_{jk j'_k} \delta_{0j_x}. \end{aligned} \quad (\text{A5})$$

APPENDIX B: STRONG UNCERTAINTY RELATION

The numerical results in main text with Gaussian wave packets as the initial nonorthogonal basis indicate that $\Delta x_j \Delta k_j$ diverge at large k . In fact, this divergence does not depend on the choice of initial wave packets; it is always the case as long as one uses Kohn's method to generate a complete set of basis that has translational symmetry. Here we offer the proof.

Let $\{w_{jk}(x - j_x)\}_{j_k, j_x \in \mathbb{Z}}$ be an orthonormal basis generated from initial wave packets \tilde{g}_{jk} as discussed in Sec. II. For convenience, we apply Schmidit orthogonalization process in order $j_k = 0, 1, -1, 2, -2, \dots$. First we show that $h(k) \equiv \lim_{j_k \rightarrow +\infty} \tilde{w}_{jk}(k + 2j_k\pi)$ exists. Since $\tilde{w}_{jk}(k + 2n\pi) \equiv v_{k, j_k}(n) / \sqrt{2\pi}$, it is sufficient to prove that for any fixed k , $v_k(n) \equiv \lim_{j_k \rightarrow +\infty} v_{k, j_k}(n + j_k)$ exists. Introduce a subspace of $l^2(\mathbb{Z})$,

$$H_{k,l} \equiv \text{span } v_{k, j_k}(n + l + 1), \quad (B1)$$

for $l \in \mathbb{N}$. Noticing v_{k,j_k} is the linear combination of u_{k,j'_k} ($|j'_k| \leq |j_k|$),

$$\begin{aligned} H_{k,l} &= \text{span}_{|j_k| \leq l} u_{k,j_k}(n+l+1) \\ &= \text{span}_{|j_k| \leq l} \tilde{g}_{j_k}[k+2(n+l+1)\pi] \\ &= \text{span}_{|j_k| \leq l} \tilde{g}_0[k+2(n+l-j_k+1)\pi] \\ &= \text{span}_{1 \leq j_k \leq 2l+1} \tilde{g}_0(k+2j_k\pi+2n\pi). \end{aligned} \quad (\text{B2})$$

From Schmidit orthogonalization process, we know that

$$\begin{aligned} v_{k,l+1}(n+l+1) &= \mathbf{N} \mathbf{P}_{H_{k,l}^\perp} u_{k,l+1}(n+l+1) \\ &= \mathbf{N} \mathbf{P}_{H_{k,l}^\perp} \tilde{g}_0(k+2n\pi), \end{aligned} \quad (\text{B3})$$

where \mathbf{N} is the normalization operator and \mathbf{P} is the projection operator. We have to prove that as $l \rightarrow +\infty$, the limit of Eq. (B3) exists. Since \mathbf{N} is continuous except at the origin, it is sufficient to show that

$$\lim_{l \rightarrow +\infty} \mathbf{P}_{H_{k,l}^\perp} \tilde{g}_0(k+2n\pi) \text{ exists and } \neq 0. \quad (\text{B4})$$

Denote $r_{k,l} \equiv \mathbf{P}_{H_{k,l}^\perp} \tilde{g}_0(k+2n\pi)$. Since $H_{k,l}^\perp$ is monotonically decreasing and \mathbf{P} is orthogonal projection, $\|r_l\|$ (subscript k omitted) is decreasing and $r_l - r_{l'} \perp r_{l'}$ for $l < l'$. Hence, $\|r_l - r_{l'}\|^2 = \|r_l\|^2 - \|r_{l'}\|^2 \rightarrow 0$ as $l \rightarrow +\infty$. $\{r_l\}$ converges. Note that

$$r_k \equiv \lim_{l \rightarrow +\infty} r_{k,l} \neq 0 \Leftrightarrow \tilde{g}_0(k+2n\pi) \notin H_k \equiv \overline{\bigcup_{l \in \mathbb{N}} H_{k,l}}. \quad (\text{B5})$$

For reasonable initial wave packets, this is always the case. For example, when \tilde{g}_0 is compactly supported, $\exists N$ such that $\tilde{g}_0(k+2N\pi) \neq 0$ and $\forall n > N$, $\tilde{g}_0(k+2n\pi) = 0$, hence $\tilde{g}_0 \notin H_k$.

From the proof above, we see $v_{k,l+1} \in H_{k,l}^\perp$, hence $v_{k,l+1} \perp v_{k,j_k}$ for all $|j_k| \leq l$. As a result of the limiting process, $r_k(n) \perp r_k(n+p)$ for all $p \neq 0$. The proof is valid for every k , hence $h(k)$ and its translations form a periodic orthonormal basis. Due to Balian's proof [36], for h , $\Delta x = \infty$ or $\Delta k = \infty$. Thus, no matter how the initial wave packet is chosen, by our orthogonalization approach, strong uncertainty relation holds, if space translational symmetry is required; i.e.,

$$\sup \Delta x_j \sup \Delta k_j = \infty.$$

APPENDIX C: PROOF OF THE INEQUALITY

Here we present the detailed proof of the inequality Eq. (22). First we provide two inequalities that will be useful later:

$$\overline{[\wp_j(t) - \overline{\wp_j}]^2} \leq \overline{\wp_j^2}, \quad (\text{C1})$$

and

$$\overline{[\wp_j(t) - \overline{\wp_j}]^4} \leq 9\overline{\wp_j^4}. \quad (\text{C2})$$

Derivation of inequality Eq. (C1) needs conditions 1 and 2, while for inequality Eq. (C2) all three conditions are necessary. The proof of the inequality Eq. (C1) is

as follows:

$$\overline{[\wp_j(t) - \overline{\wp_j}]^2} = \sum_{\alpha \neq \beta} c_{\alpha j} c_{\alpha j}^* c_{\beta j} c_{\beta j}^* = \overline{\wp_j^2} - \sum_{\alpha} |c_{\alpha j}|^4 \leq \overline{\wp_j^2}. \quad (\text{C3})$$

It is straightforward but more care is needed to prove Eq. (C2). Since in the proof only one Planck cell j is considered, we suppress the subscript j of $c_{\alpha j}$ for brevity. Before time averaging, we have

$$\begin{aligned} [\wp_j(t) - \overline{\wp_j}]^4 &= \left[\sum_{\alpha \neq \alpha'} c_{\alpha} c_{\alpha'}^* e^{i(E_{\alpha} - E_{\alpha'})t} \right]^4 \\ &= \sum_{\substack{\alpha \neq \alpha', \beta \neq \beta' \\ \chi \neq \chi', \gamma \neq \gamma'}} c_{\alpha} c_{\alpha'}^* c_{\beta} c_{\beta'}^* c_{\chi} c_{\chi'}^* c_{\gamma} c_{\gamma'}^* \\ &\quad \times e^{i(E_{\alpha} + E_{\beta} + E_{\chi} + E_{\gamma} - E_{\alpha'} - E_{\beta'} - E_{\chi'} - E_{\gamma'})t}. \end{aligned} \quad (\text{C4})$$

This yields

$$\overline{[\wp_j(t) - \overline{\wp_j}]^4} = \overline{\sum_{\alpha \neq \alpha', \beta \neq \beta', \chi \neq \chi', \gamma \neq \gamma'} c_{\alpha} c_{\alpha'}^* c_{\beta} c_{\beta'}^* c_{\chi} c_{\chi'}^* c_{\gamma} c_{\gamma'}^*}, \quad (\text{C5})$$

where the overlined summation is over only the terms that satisfy the energy relation

$$E_{\alpha'} + E_{\beta'} + E_{\chi} + E_{\gamma} = E_{\alpha} + E_{\beta} + E_{\chi'} + E_{\gamma'}. \quad (\text{C6})$$

This sum can be divided into four parts.

- $\alpha = \beta'$ and $\beta = \alpha'$.

In this case, the energy relation becomes $E_{\chi} + E_{\gamma} = E_{\chi'} + E_{\gamma'}$. According to condition 2, $\chi = \gamma'$ and $\gamma = \chi'$. The sum of relevant terms converts into

$$\sum_{\alpha \neq \beta, \chi \neq \gamma} c_{\alpha} c_{\beta}^* c_{\alpha}^* c_{\beta} c_{\chi} c_{\gamma}^* c_{\chi}^* c_{\gamma} \leq \overline{\wp_j^4}. \quad (\text{C7})$$

- $\alpha = \beta'$ and $\beta \neq \alpha'$.

The energy relation is now

$$E_{\chi} + E_{\gamma} - E_{\beta} = E_{\chi'} + E_{\gamma'} - E_{\alpha'}. \quad (\text{C8})$$

(i) When $\chi = \beta$, $E_{\gamma} - E_{\gamma'} = E_{\chi'} - E_{\alpha'}$. With condition 2, this implies that $\gamma = \chi'$ and $\gamma' = \alpha'$. We then have

$$\sum_{\substack{\beta \neq \gamma, \gamma \neq \alpha' \\ \alpha \neq \alpha', \beta \neq \alpha}} c_{\alpha} c_{\alpha'}^* c_{\beta} c_{\beta'}^* c_{\gamma} c_{\gamma'}^* c_{\alpha'} \leq \overline{\wp_j^4}. \quad (\text{C9})$$

(ii) When $\chi \neq \beta$, we have $\gamma = \beta$. This can be seen in the energy relation $E_{\chi} + E_{\gamma} - E_{\beta} - E_{\delta} = E_{\chi'} + E_{\gamma'} - E_{\alpha'} - E_{\delta}$ with E_{δ} being an arbitrary eigenenergy. If $\gamma \neq \beta$, choose δ such that $\{\chi, \gamma\} \cap \{\beta, \delta\} = \emptyset$; according to condition 3, it is required $\beta = \alpha'$, which is a contradiction. Since $\gamma = \beta$, the rest of the calculation is similar to that in (i).

Overall, this part of the summation is no more than $2\overline{\wp_j^4}$.

- $\alpha \neq \beta'$ and $\beta = \alpha'$.

Similarly, this part contributes $2\overline{\wp_j^4}$.

- $\{\alpha, \beta\} \cap \{\alpha', \beta'\} = \emptyset$.

In this case, condition 3 demands that $\{\alpha, \beta\} = \{\chi, \gamma\}$ and $\{\alpha', \beta'\} = \{\chi', \gamma'\}$. Among the four different combinations, we choose $\alpha = \chi, \beta = \gamma, \alpha' = \gamma', \beta' = \chi'$, which leads to

$$\sum_{\substack{\gamma \neq \alpha', \alpha \neq \beta' \\ \alpha \neq \alpha', \gamma \neq \beta'}} c_\alpha c_\alpha^* c_\gamma c_\gamma^* c_\alpha^* c_\beta^* c_\beta^* c_\gamma^* c_\alpha' \leq \bar{\wp}_j^4. \quad (\text{C10})$$

As the three other combinations are similar, the sum is less or equal to $4\bar{\wp}_j^4$.

Summing all these cases, we obtain the inequality Eq. (C2).

In the proof, we also use the following equality: for $\wp, \bar{\wp} > 0$, there exists $0 < \xi < 1$ such that

$$\wp \ln \wp = \bar{\wp} \ln \bar{\wp} + (1 + \ln \bar{\wp})(\wp - \bar{\wp}) + \frac{\xi(\wp - \bar{\wp})^2}{\bar{\wp}}. \quad (\text{C11})$$

We are now ready to present the full proof of the inequality Eq. (22). Assume for every $j, \bar{\wp}_j < 1/e$.

$$\begin{aligned} & \left\{ \sum_j [\wp_j(t) \ln \wp_j(t) - \bar{\wp}_j \ln \bar{\wp}_j] \right\}^2 \\ &= \left\{ \sum_j \left[(1 + \ln \bar{\wp}_j) [\wp_j(t) - \bar{\wp}_j] + \frac{\xi_j(t) [\wp_j(t) - \bar{\wp}_j]^2}{\bar{\wp}_j} \right] \right\}^2 \\ &= \sum_{j,j'} (1 + \ln \bar{\wp}_j)(1 + \ln \bar{\wp}_{j'}) [\wp_j(t) - \bar{\wp}_j] [\wp_{j'}(t) - \bar{\wp}_{j'}] + 2 \sum_{j,j'} \frac{1 + \ln \bar{\wp}_j}{\bar{\wp}_{j'}} [\wp_j(t) - \bar{\wp}_j] \xi_{j'}(t) [\wp_{j'}(t) - \bar{\wp}_{j'}]^2 \\ &\quad + \sum_{j,j'} \frac{1}{\bar{\wp}_j \bar{\wp}_{j'}} \xi_j(t) \xi_{j'}(t) [\wp_j(t) - \bar{\wp}_j]^2 [\wp_{j'}(t) - \bar{\wp}_{j'}]^2 \\ &\leq \sum_{j,j'} (1 + \ln \bar{\wp}_j)(1 + \ln \bar{\wp}_{j'}) \bar{\wp}_j \bar{\wp}_{j'} C_{jj'} - 2 \sum_{j,j'} \frac{1 + \ln \bar{\wp}_j}{\bar{\wp}_{j'}} \sqrt{[\wp_j(t) - \bar{\wp}_j]^2 [\wp_{j'}(t) - \bar{\wp}_{j'}]^2} \\ &\quad + \sum_{j,j'} \frac{1}{\bar{\wp}_j \bar{\wp}_{j'}} \sqrt{[\wp_j(t) - \bar{\wp}_j]^4 [\wp_{j'}(t) - \bar{\wp}_{j'}]^4} \\ &\leq \sum_{j,j'} (1 + \ln \bar{\wp}_j)(1 + \ln \bar{\wp}_{j'}) \bar{\wp}_j \bar{\wp}_{j'} C_{jj'} - 2 \sum_{j,j'} \frac{1 + \ln \bar{\wp}_j}{\bar{\wp}_{j'}} \bar{\wp}_j 3\bar{\wp}_{j'}^2 + \sum_{j,j'} \frac{9}{\bar{\wp}_j \bar{\wp}_{j'}} \bar{\wp}_j^2 \bar{\wp}_{j'}^2 \leq CS_E^2 + 8SE + 4. \end{aligned}$$

For the first inequality, “ \leq ”, we have used $\bar{\wp}_j < 1/e$; in the last step, we have used $|C_{jj'}| \leq 1$. For a typical wave function of a many-body quantum system, it spreads out over thousands of Planck cells in the phase space; therefore, $\bar{\wp}_j < 1/e$ is satisfied almost always.

APPENDIX D: ESTIMATE OF S_E AND C

Estimate of S_E . This is equivalent to showing Eq. (26).

Suppose that $J \equiv [E, E + \Delta E]$ ($\Delta_C E \ll \Delta E \lesssim \Delta_{mc} E$) is a macroscopic energy shell that is significantly occupied by the quantum state ψ . For brevity, we use $j \in J$ to represent $E_j \equiv \langle w_j | H | w_j \rangle \in [E, E + \Delta E]$, and $\alpha \in J$ for $E_\alpha \in [E, E + \Delta E]$.

As $\Delta_C E$ is the correlation energy scale, we have

$$\wp_\alpha |\langle w_j | \phi_\alpha \rangle|^2 \ll 1, \quad (\text{D1})$$

when $|E_j - E_\alpha| \gg \Delta_C E$. Since $\Delta E \gg \Delta_C E$, we have for a typical (energy away from end points of J) $j \in J$

$$\bar{\wp}_j \approx \sum_{\alpha \in J} \wp_\alpha |\langle w_j | \phi_\alpha \rangle|^2, \quad (\text{D2})$$

and for a typical $\alpha \in J$

$$\sum_{j \in J} |\langle w_j | \phi_\alpha \rangle|^2 \approx 1. \quad (\text{D3})$$

With Eqs. (17) and (18), these lead to

$$\sum_{j \in J} \bar{\wp}_j \approx \sum_{j \in J} \sum_{\alpha \in J} \wp_\alpha |\langle w_j | \phi_\alpha \rangle|^2 \approx \sum_{\alpha \in J} \wp_\alpha. \quad (\text{D4})$$

For matrix $A_{j\alpha} \equiv |\langle w_j | \phi_\alpha \rangle|^2$ ($j \in J, \alpha \in J$), the sum of every row of $A^T A$ is less than one. By the Perron-Frobenius theorem, the eigenvalue of $A^T A$ must be equal or less than one in module and we have

$$\sum_{j \in J} \bar{\wp}_j^2 \approx P^T A^T A P \leq P^T P = \sum_{\alpha \in J} \wp_\alpha^2, \quad (\text{D5})$$

where the column vector $(P)_\alpha \equiv \wp_\alpha$. We are now ready to estimate the entropy:

$$\begin{aligned} S_{E,J} &\equiv - \sum_{j \in J} \bar{\wp}_j \ln \bar{\wp}_j \geq - \sum_{j \in J} \bar{\wp}_j \ln \left(\frac{\sum_{j \in J} \bar{\wp}_j^2}{\sum_{j \in J} \bar{\wp}_j} \right) \\ &\gtrsim - \sum_{\alpha \in J} \wp_\alpha \ln \left(\frac{\sum_{\alpha \in J} \wp_\alpha^2}{\sum_{\alpha \in J} \wp_\alpha} \right) \\ &\approx - \sum_{\alpha \in J} \wp_\alpha \ln(\langle \wp_\alpha \rangle_s / R) \\ &\approx S_{E,J}^{\max} + \sum_{\alpha \in J} \wp_\alpha \ln R. \end{aligned} \quad (\text{D6})$$

In the first line of the above derivation, Jensen's inequality for function $-\ln x$ is applied. If J is the only energy shell significantly occupied by ψ , we already have Eq. (26). If we have more than one such energy shell, we sum Eq. (D6) for all J and obtain Eq. (26).

Estimate of C . Define $d_{\epsilon,j}$ as the minimal d such that

$$\sum_{|E_\alpha - E_j| < d} \wp_\alpha |\langle w_j | \phi_\alpha \rangle|^2 > (1 - \epsilon) \bar{\wp}_j, \quad (\text{D7})$$

where E_j is the average energy of w_j . We say that Planck cells j and j' overlap if $|E_j - E_{j'}| < d_{\epsilon,j} + d_{\epsilon,j'}$. We consider two cells j and j' that do not overlap. With conditions 1 and 2, we have

$$C_{jj'} \bar{\wp}_j \bar{\wp}_{j'} \leq \left| \sum_{\alpha} \wp_\alpha \langle w_j | \phi_\alpha \rangle \langle \phi_\alpha | w_{j'} \rangle \right|^2. \quad (\text{D8})$$

Without loss of generality, we assume $E_j < E_{j'}$ and split the above sum into two parts: one part close to j and the other

close to j' .

$$\begin{aligned} C_{jj'} \bar{\wp}_j \bar{\wp}_{j'} &\leq 2 \left| \sum_{E_\alpha < E'} \wp_\alpha \langle w_j | \phi_\alpha \rangle \langle \phi_\alpha | w_{j'} \rangle \right|^2 \\ &\quad + 2 \left| \sum_{E_\alpha \geq E'} \wp_\alpha \langle w_j | \phi_\alpha \rangle \langle \phi_\alpha | w_{j'} \rangle \right|^2, \end{aligned} \quad (\text{D9})$$

where $E' \equiv E_j + d_{\epsilon,j}$. The first term, by Cauchy-Schwartz inequality, is less or equal to

$$2 \sum_{E_\alpha < E'} \wp_\alpha |\langle w_j | \phi_\alpha \rangle|^2 \sum_{E_\alpha < E'} \wp_\alpha |\langle \phi_\alpha | w_{j'} \rangle|^2 < 2\epsilon \bar{\wp}_j \bar{\wp}_{j'}. \quad (\text{D10})$$

A similar argument applies to the second term and we have

$$C_{jj'} \leq 4\epsilon. \quad (\text{D11})$$

Next we need to establish that nonoverlapping Planck cells are the majority in the pair of cells involved. For this purpose, it is sufficient to show that for any significantly occupied Planck cell j , the sum S_j of entropies over cells overlapping with j is much less than S_E . This is indeed the case:

$$\begin{aligned} S_j &\lesssim - \int_{E_j - d_\epsilon}^{E_j + d_\epsilon} dE \rho(E) \langle \wp_\alpha \rangle_s(E) \ln \langle \wp_\alpha \rangle_s(E) \\ &\ll - \int_{E_j - \Delta_{mc} E}^{E_j + \Delta_{mc} E} dE \rho(E) \langle \wp_\alpha \rangle_s(E) \ln \langle \wp_\alpha \rangle_s(E) \\ &\leq S_E^{\max} \approx S_E. \end{aligned} \quad (\text{D12})$$

In the above derivation, we have used that $\langle \wp_\alpha \rangle$ are effectively constant on a range of $\Delta_{mc} E$, S_E is maximized, and assumption Eq. (18). This yields the inequality Eq. (28) if we set $\epsilon = \Delta_C E / \Delta_{mc} E$, and hence $\Delta_C E \ll d_\epsilon \lesssim \sqrt{\Delta_C E \Delta_{mc} E} \ll \Delta_{mc} E$ (estimated according to Eqs. (15) and (D7) for typical j).

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- [1] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).
[2] J. von Neumann, *Zeitschrift für Physik* **57**, 30 (1929).
[3] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, *Eur. Phys. J. H* **35**, 173 (2010).
[4] T. Kinoshita, T. Wenger, and D. S. Weiss, *Nature* **440**, 900 (2006).
[5] D. A. Smith, M. Gring, T. Langen, M. Kuhnert, B. Rauer, R. Geiger, T. Kitagawa, I. Mazets, E. Demler, and J. Schmiedmayer, *New J. Phys.* **15**, 075011 (2013).
[6] V. I. Yukalov, *Laser Phys. Lett.* **8**, 485 (2011).
[7] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics*, No. 657 in Lecture Notes in Physics (Springer-Verlag, Berlin, 2004).
[8] M. Srednicki, *Phys. Rev. E* **50**, 888 (1994).
[9] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, *Phys. Rev. Lett.* **96**, 050403 (2006).
[10] S. Popescu, A. J. Short, and A. Winter, *Nat. Phys.* **2**, 754 (2006).
[11] H. Dong, S. Yang, X. F. Liu, and C. P. Sun, *Phys. Rev. A* **76**, 044104 (2007).
[12] M. Rigol, V. Dunjko, and M. Olshanii, *Nature* **452**, 854 (2008).
[13] S. Goldstein, J. L. Lebowitz, C. Mastrodonato, R. Tumulka, and N. Zanghì, *Proc. R. Soc. A: Math. Phys. Eng. Sci.* **466**, 3203 (2010).
[14] N. Linden, S. Popescu, A. J. Short, and A. Winter, *Phys. Rev. E* **79**, 061103 (2009).
[15] P. Reimann, *Phys. Rev. Lett.* **99**, 160404 (2007).
[16] P. Reimann, *Phys. Rev. Lett.* **101**, 190403 (2008).
[17] P. Reimann and M. Kastner, *New J. Phys.* **14**, 043020 (2012).
[18] J. Cho and M. S. Kim, *Phys. Rev. Lett.* **104**, 170402 (2010).
[19] T. N. Ikeda, Y. Watanabe, and M. Ueda, *Phys. Rev. E* **84**, 021130 (2011).
[20] K. Ji and B. V. Fine, *Phys. Rev. Lett.* **107**, 050401 (2011).
[21] V. Yukalov, *Phys. Lett. A* **375**, 2797 (2011).
[22] S. Sugiura and A. Shimizu, *Phys. Rev. Lett.* **108**, 240401 (2012).
[23] D. Snoke, G. Liu, and S. Girvin, *Ann. Phys.* **327**, 1825 (2012).
[24] W.-g. Wang, *Phys. Rev. E* **86**, 011115 (2012).
[25] M. Rigol and M. Srednicki, *Phys. Rev. Lett.* **108**, 110601 (2012).

- [26] A. Riera, C. Gogolin, and J. Eisert, *Phys. Rev. Lett.* **108**, 080402 (2012).
- [27] C. Ududec, N. Wiebe, and J. Emerson, *Phys. Rev. Lett.* **111**, 080403 (2013).
- [28] Q. Zhuang and B. Wu, *Laser Phys. Lett.* **11**, 085501 (2014).
- [29] S. Goldstein, T. Hara, and H. Tasaki, *New J. Phys.* **17**, 045002 (2015).
- [30] J. Neumann, *Eur. Phys. J. H* **35**, 201 (2010).
- [31] S. Goldstein, J. L. Lebowitz, C. Mastrodonato, R. Tumulka, and N. Zanghi, *Phys. Rev. E* **81**, 011109 (2010).
- [32] A. J. Short, *New J. Phys.* **13**, 053009 (2011).
- [33] Q. Zhuang and B. Wu, *Phys. Rev. E* **88**, 062147 (2013).
- [34] W. Kohn, *Phys. Rev. B* **7**, 4388 (1973).
- [35] C. K. Zachos, D. B. Fairlie, and T. L. Curtright, eds., *Quantum Mechanics in Phase Space* (World Scientific, Singapore, 2005).
- [36] J. Bourgain, *J. Funct. Anal.* **79**, 136 (1988).
- [37] A. J. Short and T. C. Farrelly, *New J. Phys.* **14**, 013063 (2012).
- [38] H.-J. Stöckmann, *Quantum Chaos: An Introduction* (Cambridge University Press, Cambridge, 1999).
- [39] W. Li, L. E. Reichl, and B. Wu, *Phys. Rev. E* **65**, 056220 (2002).
- [40] H. Xiong and B. Wu, *Laser Phys. Lett.* **8**, 398 (2011).
- [41] A. Wehrl, *Rev. Mod. Phys.* **50**, 221 (1978).
- [42] T. Monnai, *J. Phys. Soc. Jpn.* **83**, 064001 (2014).
- [43] A. S. Malabarba, L. P. García-Pintos, N. Linden, T. C. Farrelly, and A. J. Short, *Phys. Rev. E* **90**, 012121 (2014).