Physical Distance Between Quantum States

Zhenduo Wang (王朕铎),¹ Yijie Wang (王一杰),¹ and Biao Wu (吴飙)¹,²,³

¹International Center for Quantum Materials, School of Physics, Peking University, 100871, Beijing, China
²Wilczek Quantum Center, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China
³Collaborative Innovation Center of Quantum Matter, Beijing 100871, China

(Dated: July 14, 2020)

We propose a physical distance between two quantum states. Qualitatively different from existing distances for quantum states, for example, the Fubini-Study distance, the physical distance between two orthogonal quantum states can be very small. This allows us to discuss the dynamical divergence of two quantum states that are initially very close by physical distance and define quantum Lyapunov exponent. We are also able to use physical distance to define quantum chaos measure, which can lead to quantum analogue of the classical Poincaré section. Three different systems, kicked rotor, three-site Bose-Hubbard model, and spin-1/2 XXZ model, are used to illustrate the physical distance.

I. INTRODUCTION

One of the most intuitive ways to understand the physical states is to compare. By different ways of comparison people can classify the physical states and reveal the hidden rules of the colorful world. A good comparison should not only tell us whether two states are the same or not but also tell us how much difference exists between them. Once we can represent the physical states as proper elements in mathematics, distance is a good comparison that tell us quantitatively how similar or different two states are. In classical mechanics, the physical states of a system are points in its phase space and the Euclidean distance between points measures quantitatively the difference between the states that they represent. Using this distance, one can define the Lyapunov exponent to characterize the dynamical sensitivity to initial conditions in a chaotic system [1].

Various different distances have also been introduced to measure the difference between quantum states. However, all of them are related to the inner product $\langle \psi_1 | \psi_2 \rangle$ between two quantum states $| \psi_1 \rangle$ and $| \psi_2 \rangle$. As a result, two mutually orthogonal quantum states always have the same distance. This is clearly inadequate in many situations. One example is shown in Fig. 1 where there are three well localized wave packets that are orthogonal to each other. It is intuitively evident that the the wave packet at $x_2$ is physically closer to the one at $x_3$ than the one at $x_1$. Another example is a one dimensional spin chain. Suppose that we have three states $| \phi_1 \rangle = |1, 1, 1, \cdots, 1 \rangle$, $| \phi_2 \rangle = | -1, 1, \cdots, 1 \rangle$, and $| \phi_3 \rangle = | -1, -1, \cdots, 1, 1, \cdots, 1 \rangle$, which are are orthogonal to each other. It is clear that $| \phi_1 \rangle$ and $| \phi_2 \rangle$ are very closely to each other physically as they have almost the same magnetization while $| \phi_3 \rangle$ is very different to each other physically. Hamming distance would be more appropriate.

In this work we propose a physical distance between quantum states based on the Wasserstein distance. Due to the use of the distance defined between basis vectors, our quantum distance is capable of quantifying the physical difference between quantum states. Consequently, our physical distance can be very small between a pair of mutually orthogonal quantum states. This is qualitatively different from existing distances defined between quantum states, for example, Fubini-Study distance [9]. With this physical distance, we are able to discuss the dynamical divergence between two quantum states which are initially very close by the physical distance. This leads us to define two parameters, quantum Lyapunov exponent and quantum chaos measure, which can be used to characterize the dynamical behavior of a quantum state. In particular, the quantum chaos measure can be used to construct the quantum analogue of the classical Poincaré section.

We will introduce our definition of quantum physical distance in Sec. III. The soundness and usefulness of our distance is then illustrated with examples in Sec. III

In Sec. IV with quantum physical distance, we define two parameters, quantum Lyapunov exponent and quantum chaos measure. The former characterizes the short-time dynamical behavior of a quantum state while the latter the long-time dynamical behavior of a quantum state. These concepts are numerically illustrated with three different quantum systems in Sec. V, which include the kicked rotor as the system which has a clear classical counterpart, a three-site Bose-Hubbard model whose classical counterpart is a mean field theory, and the spin-chain which does not have an obvious classical
counterpart. Finally we discuss and conclude.

II. PHYSICAL DISTANCE BETWEEN QUANTUM STATES

Our physical distance between quantum states is based on the Wasserstein distance, which is a distance function defined between probability distributions on a metric space. In computer science it is known as the earth mover’s distance and has been widely used in many fields [10, 11]. To define a Wasserstein distance, we need both a metric space and a distribution function. To have them, for a quantum system, we choose a complete set of orthonormal basis $B = \{ |\xi_1⟩, \ldots, |\xi_n⟩ \}$ and define a distance between the bases $d(ξ_i, ξ_j)$. This gives us a metric space. When a given quantum state $|ψ⟩$ is expanded in terms of this basis, we have a probability distribution on the set $B$

$$p_i(ψ) = |⟨ξ_i |ψ⟩|^2, \quad i = 1, \ldots, n.$$  

(1)

Our physical distance between two quantum states $|ψ_1⟩, |ψ_2⟩$ is the Wasserstein-$λ$ distance between distributions $p_i(ψ_1)$ and $p_j(ψ_2)$

$$D_λ(ψ_1, ψ_2) = \left[ \inf_\rho \sum_{i,j} P_{ij} d^λ(ξ_i, ξ_j) \right]^{1/λ}$$  

(2)

where $λ$ is a positive integer and $\inf_\rho$ means the minimum over all the distributions $P_{ij} \in [0, 1]$ that satisfy

$$\sum_i P_{ij} = p_j(ψ_2); \quad \sum_j P_{ij} = p_i(ψ_1).$$  

(3)

It is clear that the above definition still works even when $n$ is infinite. For most of the cases studied in this work, we choose $λ = 1$. This definition of physical distance can be generalized straightforwardly for mixed states. To do it, one only needs to specify the probability distribution as $p_i(\hat{ρ}) = Tr(ξ_i |\xi_i⟩ ⟨\xi_i | ξ) for a mixed state described by density matrix $\hat{ρ}$. In Ref. [12], a Wasserstein distance was defined between quantum states but the distribution is the Husimi function of a quantum state.

Two points warrant attention. (1) For a given quantum system, the choice of the orthonormal basis $B$ is not unique. It depends on the physical issue that people want to address. For example, for a spin-lattice system, if we are interested in the magnetization along a given direction, then the spin up and down states in that direction are a natural choice and the distance $d$ for the metric can be chosen as the Hamming distance. (2) Our physical distance $D_λ$ is not a distance on the Hilbert space $H$. There exists the states $|ψ_1⟩ \neq |ψ_2⟩$ for which $D_λ(ψ_1, ψ_2) = 0$, for example, $|ψ_1⟩ = (|ξ_1⟩ + |ξ_2⟩)/\sqrt{2}$ and $|ψ_2⟩ = (|ξ_1⟩ - |ξ_2⟩)/\sqrt{2}$. Therefore, our distance is a function of states and basis, i.e., quantum states and the way to extract physical information from them. More thorough discussion will be given with examples in the following sections.

III. EXAMPLES OF PHYSICAL DISTANCE

In this section, we use a few examples to illustrate the physical distance between quantum states. We will see that it can indeed capture quantitatively the physical difference between quantum states and is consistent with our physical intuition. There are various distances between quantum states based on the inner product of quantum states; for the sake of convenience, we compare our physical distance to one of them, Fubini-Study distance [9].

The first example is a one-dimensional spinless particle and we are interested in its position. In this case, the basis $B$ consists of infinite number of vectors $|x⟩$, which are delta functions. We define the distance $d$ between two basis vectors $|x⟩$ and $|x’⟩$ as $d(x, x’) = |x - x’|$. Consider two different quantum states, which are delta functions located at two different locations, $x_1$ and $x_2$, respectively. Then according to our definition, the physical distance between them is $D_2(x_1, x_2) = |x_1 - x_2|$. In contrast, the Fubini-Study distance between $|x_1⟩$ and $|x_2⟩$ is one as long as $x_1 \neq x_2$. Let us consider a Gaussian wave packet,

$$|x⟩|ψ_{x_0, p_0; σ⟩ = \frac{1}{(2πσ^2)\frac{1}{2}} \exp \left[ -\frac{(x - x_0)^2}{4σ^2} + \frac{ixp_0}{\hbar} \right].$$  

(4)

One can find that the physical distance between two different Gaussian states is [12]

$$D_2(|ψ_{x_1, p_1; σ_1⟩, |ψ_{x_2, p_2; σ_2⟩} = \sqrt{(x_1 - x_2)^2 + (σ_1 - σ_2)^2}.$$  

(5)

If the two Gaussian wave packets have the same width $σ_1 = σ_2$, we simply have $D_2 = |x_1 - x_2|$, which is just what our physical intuition expects. In contrast, the Fubini-Study distance between these two Gaussian packets is close to one as long as $|x_1 - x_2| \gg σ_1, 2$. It is interesting to note that $D_2$ is independent of the momentum. This is reasonable as we are currently interested in the particle’s position. If one is interested in the particle’s momentum, one can similarly define $d(p, p’) = |p - p’|$ and then find the physical distance in momentum between two Gaussian packets as

$$D_2(|ψ_{x_1, p_1; σ_1⟩, |ψ_{x_2, p_2; σ_2⟩} = \sqrt{(p_1 - p_2)^2 + (σ_1 - σ_2)^2},$$  

(6)

where $σ_{1, 2}$ are the widths of the wave packets in the momentum space.

The above simple example shows that the physical distance depends on what physics we want to explore. Mathematically, this is achieved by choosing an appropriate set of orthonormal basis $B$. In the above example, the basis vectors are chosen to either delta functions or plane waves. If we want to explore physics that is related explicitly to both position and momentum, we can choose $B$ to be a set of Wannier basis. As shown in Fig [2], the classical phase space is divided into Planck cells and each Planck cell is assigned a Wannier function $|w_j⟩$ [14-16]. These orthonormal Wannier functions $|w_j⟩$ form
First, it shares the same spirit with our physical distance, it is a Wasserstein-like metric for particle number distributions. Second, there is no exponential scaling between distance and particle number, which exists in the Fubini-Study distance.

We use a special case to illustrate the second point. Consider a system of \( N \) identical Bosons and its two quantum states. In one state \( |\Psi_1\rangle \), all the Bosons are in the mode \( |e_1\rangle \); in the other state \( |\Psi_2\rangle \), all the Bosons are in the state \( \alpha|e_1\rangle + \beta|e_2\rangle \). It can be shown that \( D_1(\Psi_1, \Psi_2) \propto N \). In contrast, the Fubini-Study distance is about \( 1 - |\alpha|^2 N \), which can be regarded as one when \( N \) is large even when \( \alpha \sim 1 \), reflecting the fact that the two many-body states \( |\Psi_1\rangle \) and \( |\Psi_2\rangle \) are almost orthogonal to each other when \( N \) is large no matter how close the single particle states \( |e_1\rangle \) and \( \alpha|e_1\rangle + \beta|e_2\rangle \) are to each other. So, our physical distance is more consistent with our intuition.

### IV. QUANTUM DYNAMICS AND PHYSICAL DISTANCE

As quantum dynamics is linear, it is often said that there is no true chaos, in the sense of the chaos seen in nonlinear classical dynamics [12]. The argument is as follows. Suppose that we have two quantum states \( |\psi_1\rangle \) and \( |\psi_2\rangle \). As quantum dynamics is linear, the inner product \( \langle \psi_1 | \psi_2 \rangle \) does not change with time. As a result, if these two states \( |\psi_1\rangle \) and \( |\psi_2\rangle \) are very close to each other, that is, \( \langle \psi_1 | \psi_2 \rangle \sim 1 \), they will always be close to each other. This implies no true chaos. However, many studies have shown that the dynamics in quantum chaotic systems is distinctively different from the one in quantum integrable systems. Physical distance defined above resolves this apparent dilemma.

We consider the case in Fig. 2. We use \( |w_1\rangle \) and \( |w_2\rangle \) to denote the two quantum states represented by the two Planck cells marked with 1 and 2. We let \( |w_1\rangle \) and \( |w_2\rangle \) to evolve, respectively, according to a given Schrödinger equation. As a result, at time \( t \), \( |w_1\rangle \) becomes \( |\phi_1(t)\rangle \) and \( |w_2\rangle \) evolves into \( |\phi_2(t)\rangle \). The Fubini-Study distance between these two states does not change with time as \( \langle \phi_1(t) | \phi_2(t) \rangle \) is small. When the dynamical evolution starts, the physical distance can grow. The linearity of quantum dynamics does not guarantee that the physical distance between \( |\phi_1(t)\rangle \) and \( |\phi_2(t)\rangle \) is small. The situation shown in Fig. 2 can happen: the physical distance grows with time in quantum dynamics while keeping \( \langle \phi_1(\phi_2) \rangle \) at zero. As we will show with our numerical calculation in the next section, this is indeed what happens in quantum chaotic systems.

So, in terms of physical distance, there is true chaos in quantum dynamics. In the following, using the concept of physical distance, we define two parameters to characterize the diverging and irregular quantum dynamics.
A. Quantum Lyapunov Exponent

Lyapunov exponent is one of the most important concepts in classical dynamics and it characterizes the rate of separation of infinitesimally close initial trajectories. Quantitatively, in a chaotic classical dynamics, the distance (usually \(L_2\) distance) between two points that are initially very close grows with time \(t\) as

\[
\|\delta Z(t)\| \approx e^{\lambda t}\|\delta Z(t = 0)\|
\]

where \(Z = (q,p)\) is the state in phase space. The parameter \(\lambda\) is the Lyapunov exponent. With the physical distance between two quantum states, the (maximum) Lyapunov exponent in quantum mechanics can be similarly defined as

\[
\lambda_Q = \lim_{t \to \infty} \lim_{\psi \to \psi'} \frac{1}{t} \log \frac{D(\psi(t), \psi'(t))}{D(\psi(0), \psi'(0))}
\]

This is very similar to the definition of Lyapunov component in classical mechanics, which can be obtained by replacing the physical distance between states \(D(\cdot, \cdot)\) with the distance in classical phase space. The symbol \(\psi' \to \psi\) means \(\psi, \psi'\) are close but different in the sense of physical distance.

For quantum systems where quantum phase spaces similar to Fig 2 can be constructed, we can always use physical distance similar to the one in Eq (3). In the semi-classical limit, \(\hbar \to 0\), the areas or volumes of the Planck cells approach zero and the quantum dynamics becomes classical. In this limit, we should have

\[
\lim_{\hbar \to 0} \lambda_Q = \lambda_C.
\]

Note that this relation holds only when the Lyapunov time (the inverse of Lyapunov exponent) is smaller than the Ehrenfest time \([18]\). So the limit \(t \to \infty\) is not a strict mathematical term and should be understood as a sufficiently long time before the wave packets become too wide spread.

B. Quantum Chaos Measure

Intuitively, chaos means disorder and irregularity in dynamics. In classical dynamics, this is indicated by the scattered points in Poincaré sections (see, e.g., Fig 4(a)), which are usually referred to as chaotic sea. How chaotic a classical dynamics is reflected by how much the chaotic seas occupy in the phase space. In the chaotic sea, there are regular motions, which are usually referred to as integrable island. When there is only “chaotic sea” in the Poincaré sections, the system becomes fully chaotic. In this case, we have ergodicity and/or mixing and the long-time average becomes identical to the microcanonical ensemble average \([19]\).

With physical distance, we can also compare the long-time average and the microcanonical ensemble average for quantum dynamics. In standard textbooks \([20]\), the microcanonical ensemble is regarded as a maximally mixed state and can be described by the density matrix \(\hat{I}/\text{Dim.} \). \(\hat{I}\) is the identity matrix and \(\text{Dim}\) is the dimension of the Hilbert space. This is usually a postulate in standard textbooks \([20]\). But it has been fully justified by many studies \([14, 19, 21, 23]\). We use the physical distance between the long-time-average of the density matrix and the density matrix \(\hat{I}/\text{Dim}\) to quantitatively measure the severity of quantum chaos. Mathematically, this difference is given by

\[
\Upsilon = D \left( \frac{1}{\text{Dim}}, \lim_{T \to \infty} \frac{1}{T} \int_0^T \hat{\rho}(t)dt \right)
\]

We call it quantum chaos measure. The measure \(\Upsilon\) depends on the initial quantum states. For some initial quantum states, \(\Upsilon\) is small and it means that the long-time-average density matrix is sufficiently close to the maximally mixed state. These quantum states belong to chaotic sea. For some initial states, \(\Upsilon\) is large and these states belong to integrable islands.

In the next section, our numerical results will show that we can use chaos measure to construct quantum Poincaré sections, which resemble classical Poincaré sections.

One can use other tools to quantify the degree of disorder in quantum dynamics, for example, quantum entropy of the form \(-\sum_i p_i \log p_i\). The core advantage of our chaos measure is its dependence on the choice of basis \(\mathcal{B}\). For example (see Appendix B for details), consider the following two probability distributions on set \(\{0, 1, 2, \cdots, 9\}\)

\[
p_A(x) = \begin{cases} 
1/5 & x < 5 \\
0 & x \geq 5
\end{cases}
\]

and

\[
p_B(x) = \begin{cases} 
1/5 & x \text{ is even} \\
0 & \text{otherwise}
\end{cases}
\]

The entropies of \(p_A\) and \(p_B\) are the same, but \(p_B\) appears much closer to the uniform distribution. This can be reflected by our chaos measure as we have \(\Upsilon_A = 5/2 ; \ Upsilon_B = 1/2\) with the metric \(d(x, y) = |x - y|\) on the base space. This difference means our measure \(\Upsilon\) can reveal finer property better than any other concepts that ignore the information of the base space. In Ref. [26], the length of a Planck cell was used to measure disorder in quantum dynamics; however, this concept is limited and can not be applied to spin systems.

V. NUMERICAL RESULTS

In this section, we will numerically study three different systems to illustrate the concept of physical distance. These three systems are quantum kicked rotor,
three-site Bose-Hubbard model, and spin-1/2 XXZ spin chain. The quantum kicked rotor has a natural classical counterpart. For the three-site Bose-Hubbard model, its classical counterpart is the mean-field theory and its effective Planck constant is the inverse of the particle number $1/N$. In contrast, the spin-1/2 XXZ spin chain has no obvious classical counterpart.

### A. Kicked Rotor

Kicked rotor is one of the systems which have been well studied both as a quantum and classical system. The Hamiltonian of a kicked rotor on a ring has the following dimensionless form \[24, 25\]

\[
H = \frac{1}{2} p^2 + K \cos q \sum_{n=-\infty}^{\infty} \delta(t - n)
\]

Its classical dynamics is equivalent to the following map

\[
\begin{align*}
p_{n+1} &= p_n + K \sin q_n \quad \text{mod} \ 2\pi \\
q_{n+1} &= q_n + p_{n+1} \quad \text{mod} \ 2\pi
\end{align*}
\]

where we have used the fact that the momentum $p$ and $p + 2n\pi$ are equivalent. $(q_n, p_n)$ is the position and momentum of the kicked rotor before the $n$-th kick. The kicking strength $K$ is the only control parameter; when it is bigger than $K_c = 0.971635$ the classical dynamics becomes chaotic.\[27\]

The quantum dynamics has one more parameter, the effective Planck constant $\hbar_{\text{eff}}$ \[24, 25\]. For simplicity, we choose $\hbar_{\text{eff}} = 2\pi/m^2$ with $m$ being an positive integer. In this case, we can divide the $2\pi \times 2\pi$ classical phase space into $m \times m$ Planck cells (similar to Fig. 2) and assign a Wanner function $\{X, P\}$ to each Planck cell \[24, 25\]. $X, P$ are the coordinates of a Planck cell. These Wanner functions $\{\{X, P\}\}$ form a complete set of orthonormal basis. We choose them as our choice of $B$ and define the distance between two basis vectors as $d(X, P; X', P') = \sqrt{(X' - X) \text{ mod } 2\pi)^2 + (P' - P) \text{ mod } 2\pi)^2}$.

In our numerical calculation, we choose the initial quantum states localized at $(4.7, 3)$ and $(4.7 + 2\pi/m, 3 + 2\pi/m)$. The dynamics near these two points becomes chaotic as $K$ increases as shown in Fig.4(a, c). The initial quantum states are the maximally localized Gaussian wave packets of the following form

\[
\langle x | \psi(x_0, p_0) \rangle = \frac{1}{(2\pi\hbar_{\text{eff}})^{1/4}} \exp \left[ -\frac{(x - x_0)^2}{2\hbar_{\text{eff}}} + \frac{ixp_0}{\hbar_{\text{eff}}} \right]
\]

As the two states evolve with time, we compute numerically the physical distance between them and see how they change with time. For comparison, we have also computed two other distances. One is the distance between the expectation values of $\hat{q}, \hat{p}$ for these two different quantum states. For convenience, we call it expectation distance. The other is the distance between two corresponding classical trajectories starting at $(4.7, 3)$ and $(4.7 + 2\pi/m, 3 + 2\pi/m)$. The results are plotted in Fig.3.

It is clear from Fig.3 that the physical distance agrees very well with the classical distance for the first several kicks. In contrast, during these kicks, the expectation distance can deviate largely from the classical distance. As the evolution goes on, both physical distance and expectation distance deviate far from the classical distance as expected because the wave packets get distorted. When $m$ is sufficiently large or, equivalently, $\hbar_{\text{eff}}$ is small enough, the Ehrenfest time would be longer than the Lyapunov time. In these cases, we should see that the physical distance agree with the classical distance for a much longer time; as a result, we would be able to estimate numerically the quantum Lyapunov exponent. Unfortunately, due to limited computation power that we have, we can not compute for very large $m$.

We have also computed quantum chaos measure for the kicked rotor. We use the maximally localized Gaussian wave packets as the initial states, scan the entire quantum phase space, and compute the measure for each Planck cell. The results are plotted in Figs. 4(b, d) and compared to the classical Poincaré sections in Figs. 4(a, c). The resemblance between them is unmistakable. Note that the chaos measure is the distance between long-time averaged density matrix and the maximally mixed state. In Figs. 4(b), the values of our measure are very large for many Planck cells. This means that the wave packets starting at these Planck cells do not spread out much and stay near the original Planck cells. When the kicking strength $K$ is large, the values of the measure become much smaller, indicating that the quantum dynamics become more chaotic and the wave packets began

\[\text{FIG. 3: The time evolution of three types of distances for the kicked rotor at different kick strengths } K. \text{ Blue lines are the distances between the points on classical trajectories, red lines are physical distance between wave packets in the quantum phase space, and black lines are the distance between the expectation values of operators } \hat{q}, \hat{p}. \text{ (a) } K = 0.3, m = 30; \text{ (b) } K = 0.9, m = 30; \text{ (c) } K = 1.5, m = 30. \text{ (d) has the same parameters } K = 1.5, m = 30 \text{ but with a longer time evolution.}\]
Hamiltonian is modeled, the quantumness is controlled by the particle number $N$ and the mean field Hamiltonian is its “classical counterpart”. As we will show, the physical distance is still applicable in this type of systems.

Since in the mean-field model each mode $a_j$ has a definite amplitude and phase, we choose a basis $B$ for the quantum model where each basis vector contains information for both amplitude (or particle number) and phase. For convenience, we take the total particle number $N = L^2 - 1$, where $L$ is an integer. The basis vector in $B$ is denoted as $|\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle$; its expectations for particles numbers are $\ell_{1,2} L + (L - 1)/2$ and for phases $2\pi \vartheta_{1,2}/L$. The details of this orthonormal basis $\{|\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle\}$ with $0 \leq \ell_{1,2}, \vartheta_{1,2} \leq L - 1$ can be found in Appendix A. This effectively creates a 4-dimensional quantum phase space with $L \times L \times L \times L$ Planck cells. Therefore, a natural choice for the basis metric is

$$d(\{\ell, \vartheta\}, \{\ell', \vartheta'\}) = \frac{1}{L} \sqrt{\sum_{i=1}^{2} (\Delta \ell_i^2 + \Delta \vartheta_i^2)} \quad (21)$$

where $\Delta \ell_i = |\ell_i - \ell'_i|$ and $\Delta \vartheta_i = \min(|\vartheta_i - \vartheta'_i|, L - |\vartheta_i - \vartheta'_i|)$ ($\vartheta_i$ is periodic). We can compute the physical distance between two quantum states or two classical points according to this metric just like what we did for the kicked rotor.

The classical motion of the system is nonintegrable for generic $c$. This is evident in the Poincaré section for $c/c_0 = 2$, $E = 0.8c_0$, $n_2 = 0.2475$, $\pi/2 > 0$ shown in Fig.6a, where we see both regular and chaotic motions. Note that $n_1, 2 = |a_{1,2}|^2$ and $\theta_{1,2} = \arg a_{1,2} = \arg a_{3}$. We choose the quantum initial state to be a coherent state $|\Psi\rangle = \frac{1}{\sqrt{N!}} \left(\sum_{i=1}^{3} a_i \hat{a}_i\right)^N |0\rangle$; its shape in our quantum phase space will be close to a Gaussian packet centered at the classical point $(a_1, a_2, a_3)^T$ with a width of order $1/\sqrt{N} \sim 1/L$.

We first choose a pair of initial conditions, $(n_1, \theta_1) = (0.220, 0.8\pi)$ and $(n_1, \theta_1) = (0.221, 0.8\pi)$, which are located in the integrable island of the Poincaré section in Fig.6a. The results are presented in Fig.5a. It can be seen that, when the dynamics is regular, the quantum physical distance coincides with the classical distance very well in a relatively long period of time. When the quantum resolution $L$ is increased from 6 to 9, the quantum physical distances have an obvious inclination to converge to the classical distance. This is quite surprising because the difference between two initial conditions is only of order $10^{-3}$ while for the highest quantum resolution $L = 9$ in our simulation the size of the Planck cell is of order $10^{-1}$. So, we expect that our physical distance match classical distance well even when the size of the Planck cell is significantly smaller than the classical distance between two initial conditions.

We choose a different pair of initial conditions, $(n_1, \theta_1) = (0.420, 0.8\pi)$ and $(n_1, \theta_1) = (0.421, 0.8\pi)$, which are located in the chaotic sea of Fig.6a. The numerical results are shown in Fig.5b. In this chaotic case, the total time that the quantum physical distances

![Image](image_url)

**FIG. 4:** (a)(c) Classical Poincaré sections and (b)(d) quantum chaos measures in the quantum phase space. The chaos measure for a Planck cell is computed by the evolution of a quantum state which is initially localized at the Planck cell. The figures are plotted by scanning the entire quantum phase space. Note that plotted in (b) is colored with logarithm scaling and the original values range is $[1.07, 82.3]$. In (d), the values of chaos measure range in $[0.03, 1.41]$.

B. Three-site Bose-Hubbard Model

We consider a different system, a three-site Bose-Hubbard model described by the following Hamiltonian [15]

$$H = -\frac{c_0}{2} \sum_{1 \leq i, j \leq 3, i \neq j} \hat{a}_i^\dagger \hat{a}_j + \frac{c}{2N} \sum_{j=1}^{3} \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j, \quad (19)$$

where $\hat{a}_j^\dagger$ and $\hat{a}_j$ are the Bosonic creation and annihilation operators for the mode $j$. $c$ is the scaled interaction strength and $N$ is the number of Bosons in the system. This system has a mean-field limit at $N \rightarrow \infty$, whose Hamiltonian is

$$H_{mf} = -\frac{c_0}{2} \sum_{1 \leq i, j \leq 3, i \neq j} a_i^* a_j + \frac{c}{2} \sum_{j=1}^{3} |a_j|^4, \quad (20)$$

where $|a_1|^2 + |a_2|^2 + |a_3|^2 = 1$. In this Bose-Hubbard model, the quantumness is controlled by the particle
and the classical distance coincide is much shorter. This can be explained with the Ehrenfest time, the time scale when the quantum-classical dynamics breakdown. For the chaotic dynamics, the Ehrenfest time is short and proportional to \( \ln N \) \( [15] \), while for the integrable dynamics this timescale is much longer and proportional to \( \sqrt{N} \) \( [15] \). So, for this chaotic dynamics, to see numerically exponential divergence of the quantum physical distance, we have to have \( N \) (or \( L \)) exponentially large. Unfortunately, for both integrable and chaotic cases, large \( N \) is beyond our numerical capacity.

We also computed quantum chaos measure for this Bose-Hubbard system, corresponding to the classical Poincaré section in Fig.6a with \( c/c_0 = 2 \). We divide the phase space with the quantum resolution \( L = 10 \), that is, the total particle number being \( N = 99 \). Our initial quantum states are coherent states \( |\Psi_i(t = 0)\rangle \), which are localized wavepackets occupying \( O(1) \) Planck cells. We calculate their long-time average density matrix \( \rho_\infty = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt |\Psi_c(t)\rangle \langle \Psi_c(t)| \), and project them onto the quantum phase space and obtain the distribution \( P_c(\ell_i, \vartheta_i) = \text{Tr} \{ \rho_\infty(\ell_i, \vartheta_i) \} \). The classical (or mean-field) dynamics is limited to a constant energy surface in the phase space. In contrast, the quantum dynamics is limited to an energy shell with certain thickness. To effectively reduce the computation burden, we only pick out Planck cells located within the Gaussian-broadening energy shell. To be specific, we Gaussian fit the smoothed envelope of the energy spectrums of these selected coherent states, with the fitting goodness \( R^2 = 0.994 \), and select out the phase cells with energy expectation values within \( \pm 3\sigma \) of the Gaussian. This method is able to capture \( 70\% \pm 7\% \) of the original coherent packets. We then set the energy shell with this Gaussian envelope to be the ergodic reference \( \rho_{\text{erg}} \) of the system following [28], in place of the classical microcanonical ensemble, and project it onto the space \( P_{\text{erg}}(\ell_i, \vartheta_i) = \text{Tr} \{ \rho_{\text{erg}}(\ell_i, \vartheta_i) \} \). Then we calculate the physical distance between \( P_{\text{erg}}(\ell_i, \vartheta_i) \) and each \( P_c(\ell_i, \vartheta_i) \) and obtain the chaos measure. The results are plotted in Fig.6b. We see that the classical Poincaré section in Fig.6a is very well recovered. The regular islands are distinguished by the coherent initial states that have a large physical distance from the ergodic envelope, while the chaotic sea is filled with initial states that are very close in physical distance to the ergodic envelope. Quite surprisingly, even the two small regular islands with size of only one single quantum phase cell are clearly seen. Therefore, we expect our chaos measure proposed here is able to distinguish regular island structures with size no
Note that this metric is different from the Hamming distance defined for the many-body states in Sec. III if we treat the states $|s_1, \ldots, s_N\rangle$ as Fock states for Fermions with $s_j$ particle in the single particle mode $|j\rangle$ and define the distance between corresponding single particle states $|j\rangle$’s as $d(|i\rangle,|j\rangle) = |i - j| : i, j = 1, \ldots, N$. For example, the most efficient way to transport $(1,1,0,0,0,0)$ to $(0,0,0,1,1,1)$ is to move each 1 in the first array to the position of corresponding 1s one by one in the second array.

In our numerical computation, we choose $N = 15$ and focus on the subspace with 5 spins up. The initial localized states are chosen to be states that have consecutive 1s in their boolean-valued arrays, such as $(1,1,1,1,0,\cdots,0)$ and $(0,1,1,1,1,1,\cdots)$.

To compute the quantum chaos measure, we choose the set of common eigenstates of all $\hat{s}^z_i$ as the basis $B$ and denote them as 01 valued vectors $\{|s_1, s_2, \ldots, s_N\rangle\}_{s_i \in \{0,1\}}$. The distance between them is defined as the $L_1$ measure between the arrays of positions of 1s. For example, the array for the positions of 1s in the state $|1,1,0,0,0\rangle$ is $(0,1,1,0,0)$, and the array for $|0,0,0,1,1\rangle$ is $(1,3,4)$. So, the distance between them is

$$d(|1,1,0,0,0\rangle,|0,0,0,1,1\rangle) = |3 - 0| + |4 - 1| = 6$$

Note that this metric is different from the Hamming distance, which is 4 between the states $|1,1,0,0,0\rangle$ and $|0,0,0,1,1\rangle$. In fact, this metric is the same as our distance defined for the many-body states in Sec. III if we treat the states $|s_1, \ldots, s_N\rangle$ as Fock states for Fermions with $s_j$ particle in the single particle mode $|j\rangle$ and define the distance between corresponding single particle states $|j\rangle$’s as $d(|i\rangle,|j\rangle) = |i - j| : i, j = 1, \ldots, N$. For example, the most efficient way to transport $(1,1,0,0,0,0)$ to $(0,0,0,1,1,1)$ is to move each 1 in the first array to the position of corresponding 1s one by one in the second array.

In our numerical computation, we choose $N = 15$ and focus on the subspace with 5 spins up. The initial localized states are chosen to be states that have consecutive 1s in their boolean-valued arrays, such as $(1,1,1,1,0,\cdots,0)$ and $(0,1,1,1,1,1,\cdots)$. There are in total ten of them, which are numbered according to the position of the first 1. The computed quantum chaos measure is shown in Fig. 8. It is clear from the figure that the chaos measure is much smaller for the chaotic case $\epsilon = 0.5$ than for the non-chaotic case $\epsilon = 0.01$. This is in agreement with the eigen-energy spacing statistics shown in Fig. 7.

**FIG. 7:** Eigen-energy spacing statistics for the XXZ spin chain that has 15 spins in the sub-Hilbert space with 5 spins up. The deflection is on the site $i^* = 2$ and the boundary condition is open with $J_1 = 1.0, J_2 = 0.5$. The red line is for $\epsilon = 0.5$ and is close to the Wigner-Dyson distribution (dashed line) while the blue line is for $\epsilon = 0.01$ and is close to Poisson distribution (dotted line).

**FIG. 8:** Quantum chaos measures for the 10 initially localized states in the XXZ spin chain model. The green line is for $\epsilon = 0.01$ and the red line for $\epsilon = 0.5$. The left side of the red line is large is caused by the deflection on the second site $i^* = 2$. The overall decrease of the chaos measure from $\epsilon = 0.01$ to $\epsilon = 0.5$ shows the spin chain becomes more chaotic as the deflection increases, which agrees the results of energy spacing statistics.

**C. Spin Chain**

We now study a system which does not have a clear classical counterpart. It is the spin-1/2 XXZ model with disorder described by the following Hamiltonian [29]

$$\hat{H} = \sum_{i=0}^{N-1} h_i \hat{s}^z_i + \sum_{i=0}^{N-2} \left\{ J_1 \left( \hat{s}^x_i \hat{s}^x_{i+1} + \hat{S}^y_i \hat{S}^y_{i+1} \right) + J_2 \hat{S}^z_i \hat{S}^z_{i+1} \right\},$$

where $\hat{s}^x, \hat{s}^y, \hat{s}^z$ are spin operators at the $i$th site and $h_i = \epsilon \delta_{i,i^*}$ is the magnetic field at a given random site denoted by $i^*$. In our model, $S^z = \sum_{i=1}^{N} \hat{s}^z_i$ is conserved and the Hilbert space can be divided into subspaces labelled by $S^z$. The spin system has different eigen-energy spacing statistics with different values of $\epsilon$ [29]. Two examples are shown in Fig. 7 which show that the case $\epsilon = 0.01$ is largely integrable while the case $\epsilon = 0.5$ is chaotic.

To compute the quantum chaos measure, we choose the set of common eigenstates of all $\hat{s}^z_i$ as the basis $B$ and denote them as 01 valued vectors $\{|s_1, s_2, \ldots, s_N\rangle\}_{s_i \in \{0,1\}}$. The distance between them is defined as the $L_1$ measure between the arrays of positions of 1s. For example, the array for the positions of 1s in the state $|1,1,0,0,0\rangle$ is $(0,1,1,0,0)$, and the array for $|0,0,0,1,1\rangle$ is $(1,3,4)$. So, the distance between them is

$$d(|1,1,0,0,0\rangle,|0,0,0,1,1\rangle) = |3 - 0| + |4 - 1| = 6$$

Note that this metric is different from the Hamming distance, which is 4 between the states $|1,1,0,0,0\rangle$ and $|0,0,0,1,1\rangle$. In fact, this metric is the same as our distance defined for the many-body states in Sec. III if we

**VI. DISCUSSION AND CONCLUSION**

In some cases the Wasserstein distance is not robust with respect to the distance matrix $d_{ij}$ defined for a pair of basis vector. For example, consider two distribution: $\delta(x)$ and $(1 - \eta)\delta(x) + \eta \delta(x - d)$ on a $1 - d$ Euclidean space. The Wasserstein distance between them is nothing but $\eta d$. That means no matter how small $\eta$ is, one can find a sufficient large $d$ so that the Wasserstein distance diverges. That is what we meant by that the distance is not robust with respect to $d_{ij}$. Fortunately, the distance matrix $d_{ij}$ in our numerical examples have upper bounds...
so that we do not need to worry about this.

Another challenge for our proposed physical distance is the complexity of computing the Wasserstein distance. In our numerical implement, we use python module named pyemd to compute the Wasserstein distance [30, 31]. Though the convex optimization problem for computing the distance is easy (it is a linear programing problem in discretized form [32]), we are facing an exponentially high dimensional Hilbert space in quantum mechanics and our code can not handle larger systems. But the core of this challenge is the dimension of the Hilbert space, which should also be a challenge to any other definitions with the similar concept. In this sense, our definition has an equivalent complexity to others.

In conclusion, we have proposed physical distance between two quantum states based on the Wasserstein distance between two probability distributions. This physical distance can be very small for two orthogonal quantum states. As a result, one can discuss the dynamical divergence of two quantum states, which are initially very close by physical distance, and directly define Lyapunov exponents for quantum states even though quantum dynamics is linear. The physical distance can also be used to define quantum chaos measure, which allows us to construct the quantum analogue of the classical Poincaré section. These concepts are illustrated with examples.

Acknowledgments

This work is supported by the the National Key R&D Program of China (Grants No. 2017YFA0303302, No. 2018YFA0305602), National Natural Science Foundation of China (Grant No. 11921005), and Shanghai Municipal Science and Technology Major Project (Grant No.2019SHZDZX01).

[1] V. I. Arnol'd, Mathematical methods of classical mechanics, vol. 60 (Springer Science & Business Media, 2013).
[2] N. Hadjisavvas, Annales de l’I.H.P. Physique théorique 4, 287 (1981).
[3] M. Hillery, Physical Review A 35, 725 (1987).
[4] S. Luo and Q. Zhang, Physical Review A 69, 032106 (2004).
[5] S. N. Filippov and V. I. Man’ko, Physica Scripta T140 (2010).
[6] S. Rana, P. Parashar, and M. Lewenstein, Physical Review A 93, 012110 (2016).
[7] W. K. Wootters, Physical Review D 23, 357 (1981), ISSN 05562821.
[8] S. L. Braunstein and C. M. Caves, Physical Review Letters 72, 3439 (1994).
[9] S. Kobayashi and K. Nomizu, Foundations of Differential Geometry (Wiley, New York, 1996).
[10] Y. Rubner, C. Tomasi, and L. J. Guibas, International Journal of Computer Vision 40, 99 (2000).
[11] D. Y. Orlova, N. Zimmerman, S. Meehan, C. Meehan, J. Waters, E. E. B. Ghosn, A. Filatenkov, G. A. Kolyagin, Y. Gernez, S. Tsuda, et al., PLOS ONE 11, 1 (2016).
[12] K. Zyczkowski and W. Słomczyński, Journal of Physics A: Mathematical and General 31, 9095 (1998).
[13] I. Olkin and F. Pukelsheim, Linear Algebra and Its Applications 48, 257 (1982).
[14] J. von Neumann, The European Physical Journal H 35, 201 (2010).
[15] X. Han and B. Wu, Physical Review A 93, 023621 (2016).
[16] Y. Fang, F. Wu, and B. Wu, Journal of Statistical Mechanics: Theory and Experiment 2018, 023113 (2018).
[17] M. Berry, Physica Scripta 40, 335 (1988).
[18] Y. Zhao and B. Wu, Science China Physics, Mechanics & Astronomy 62 (2019), ISSN 1674-1056.
[19] D. Zhang, H. T. Quan, and B. Wu, Physical Review E 94, 022150 (2016).
[20] K. Huang, Statistical Mechanics (Wiley, New York, 1987).
[21] J. v. Neumann, Zeitschrift für Physik 57, 30 (1929).
Appendix A: Quantum phase space for the three-site Bose-Hubbard model

1. Construction of the quantum phase space

The total particle number \( N \) is conserved in the three-site Bose-Hubbard Hamiltonian (Eq. 10). As a result, in the Fock states \( |N_1, N_2, N_3\rangle \), there are only two free parameters \( N_1, 2 \) and \( N_3 = N - N_1 - N_2 \). We consider a Hilbert space spanned by Fock states \( |N_1, N_2\rangle \) with \( 0 \leq N_1, 2 \leq N \), which contains the Hilbert space of the three-site Bose-Hubbard system. We further take \( N = L^2 - 1 \). For this \( L^2 \)-dimensional Hilbert space, we define a set of orthonormal basis

\[
|\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle = \frac{1}{L} \sum_{N_1=0}^{L-1} \sum_{N_2=0}^{L-1} e^{i \frac{2 \pi}{L} (N_1 \vartheta_1 + N_2 \vartheta_2)} |N_1 + \ell_1 L, N_2 + \ell_2 L\rangle,
\]

where the four indices \( \ell_1, 2, \vartheta_1, 2 \) are \( 0, 1, \ldots, L - 1 \). As a result, the \( L^2 \)-dimensional Hilbert space is arranged into a 4-dimensional phase space which is divided into \( L \times L \times L \times L \) Planck cells. Each Planck cell is represented by \( |\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle \). For this 4-dimensional phase space, there are two pairs of conjugate observables, \( \tilde{N}_1, 2 \), the particle number operators, and \( \tilde{\vartheta}_1, 2 \), the relative phase operators. They can be defined as

\[
\tilde{N}_i = \sum_{N_1=0}^{L} \sum_{N_2=0}^{L} N_i |N_1, N_2\rangle \langle N_1, N_2|,
\]

\[
\tilde{\vartheta}_i = \sum_{N_1=0}^{L} \sum_{N_2=0}^{L} \theta_{M_i} |\theta_{M_1}, \theta_{M_2}\rangle \langle \theta_{M_1}, \theta_{M_2}|,
\]

where \( |\theta_{M_1}, \theta_{M_2}\rangle \) is the Fourier transformation of the Fock basis

\[
|\theta_{M_1}, \theta_{M_2}\rangle = \frac{1}{N+1} \sum_{N_1=0}^{L} \sum_{N_2=0}^{L} e^{i (N_1 \theta_{M_1} + N_2 \theta_{M_2})} |N_1, N_2\rangle
\]

with \( \theta_{M_i} = \theta_{i}^{(0)} + 2 \pi M_i/(N+1) \) and \( M_i = 0, 1, \ldots, N \). In light of this, we can recast Eq. (A1) into

\[
|\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle = \frac{1}{L^3} \sum_{M_i=0}^{L} \sum_{M_2=0}^{L} \left( 1 - e^{-iL(\theta_{M_1} - 2 \pi \vartheta_1)}/2 \right) \left( 1 - e^{-iL(\theta_{M_2} - 2 \pi \vartheta_2)/2} \right) \\
\times e^{-iL(\ell_1 \theta_{M_1} + \ell_2 \theta_{M_2})} |\theta_{M_1}, \theta_{M_2}\rangle
\]

where each fraction takes its limit value if its denominator is 0.

We will show in the follow that each \( |\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle \) state represents a Planck cell in the phase space in the sense that their positions are fixed by the four parameters \( \ell_i, \vartheta_i \), and that their shapes are localized.

2. The positions of the Planck cells

We will analytically verify that for a given Planck cell \( |\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle \), \( \ell_i \) is proportional to the expectation value of particle number at this cell and \( \vartheta_i \) is proportional to the expectation value of the phase, up to some correction terms. The expectations are

\[
\langle \tilde{N}_i \rangle_{\ell_i, \vartheta_i} = \ell_i L + \frac{L - 1}{2},
\]

\[
\langle \tilde{\vartheta}_i \rangle_{\ell_i, \vartheta_i} = \frac{2 \pi}{L} \vartheta_i + \frac{1}{L^3} \sum_{M_i=0}^{L} \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2}^2 \vartheta_{M_i} - M_i - \frac{2 \pi \vartheta_i}{L}
\]

where \( \langle \cdot \rangle_{\ell_i, \vartheta_i} \) denotes the expectation value of the state \( |\ell_1, \vartheta_1; \ell_2, \vartheta_2\rangle \), and \( \theta_{M_i} = \theta_{M_i} - 2 \pi \vartheta_i \). The normalization of Eq. (A5) has been used in deriving Eq. (A7).

We can further show that the correction terms can be regarded as constants independent of \( \vartheta_i \). In Eq. (A6), this is obvious. We only need to examine Eq. (A7). We notice that in Eq. (A7), with fixed \( \theta_{i}^{(0)} \), altering \( \vartheta_i \to \vartheta_i + 1 \) is equivalent to adding an additional term to \( \theta_{M_i} \to \theta_{M_i} - 2 \pi/L \), and keeping \( \vartheta_i \) unchanged,

\[
\frac{1}{L^3} \sum_{M_i=0}^{L} \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2}^2 \vartheta_{M_i} - M_i - \frac{2 \pi \vartheta_i}{L}
\]

\[
\to \frac{1}{L^3} \sum_{M_i=0}^{L} \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2} - 2 \pi/L \]

\[
= \frac{1}{L^3} \sum_{M_i=0}^{L} \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2} - L \]

\[
= \frac{1}{L^3} \left( \sum_{M_i=0}^{N-L} + \sum_{M_i=L}^{N} \right) \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2} - 2 \pi/L
\]

\[
= \frac{1}{L^3} \sum_{M_i=0}^{N-L} \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2} - 2 \pi/L
\]

We can see that there are special points \( \theta_{M_i} \equiv 0(\text{mod}2\pi) \) where \( \sin \frac{L \theta_{M_i}}{2} \sin \frac{L \theta_{M_i}}{2} \) is of order \( O(L^2) \). Otherwise, the alteration of the correction term induced by \( \vartheta_i \to \vartheta_i + 1 \) is of order \( O(L^{-2}) \), which is ignorable compared to the shift in the first term of Eq. (A7), \( 2 \pi/L \). Since \( \vartheta_i \) has a period of \( L \) and \( \sin \theta_{M_i}/2 = \sin (\theta_{M_i} - 2 \pi \vartheta_i)/2 \)
and different choice of \( \theta \) is illustrated in Fig. 9a. This point is shown in Fig. 10a. The values of the correction term in Eq. (A7) is approximately a constant. This point is illustrated in Fig. 10a.

FIG. 9: The values of the correction term in Eq. (A7), \( C_\theta = \frac{1}{L^2} \sum_{M_i=0}^{N} \frac{\sin L \theta_{M_i}}{\sin \theta_{M_i}} \). (a) \( \theta_{M_i}^{(0)} \) is fixed at \( -\pi/L \). (b) \( \theta_{M_i}^{(0)} \) is changed to keep all the \( \tilde{\theta}_{M_i} \) lie in the region of \( [-\pi, \pi] \). Two periods of \( \theta_i \) are plotted in these two figures.

We can understand this question from another point of view. Since expectation values of well 1 and 2 are independent of each other, we may ignore the degrees of freedom related to well 2 and consider a reduced double-well case. Note that \( \theta_1 \) is actually a periodic quantity, and we should actually plot the amplitude \( |\langle \theta_M | \ell_1, \theta_1 \rangle|^2 \) on a ring. Therefore, different choice of \( \theta_1^{(0)} \) turns out to represent cutting the ring at different positions, as illustrated by Fig. 10. Obviously Fig. 10a will have a slightly larger expectation value of \( \theta_1 \) than Fig. 10b, but as long as the cut is not in the peak, whose width scales as \( O(L^{-1}) \), the deviation will be small. This is the origin of the correction term in Eq. (A7).

FIG. 10: \( |\langle \theta_{M_i} | \ell_1, \theta_1 \rangle|^2 \) versus \( \tilde{\theta}_{M_i} \), with fixed \( \tilde{\theta}_1 = 0 \) and different choice of \( \theta_1^{(0)} \). (a) \( \theta_1^{(0)} = -\pi/L \). (b) \( \theta_1^{(0)} = -\pi \).

If we allow \( \theta_1^{(0)} \) to change with the shifting of \( \tilde{\theta}_1 \) and keep all the \( \tilde{\theta}_{M_i} = \theta_1^{(0)} + 2\pi M_i/L^2 - 2\pi \tilde{\theta}_1/L \) \( (M_i = 0, 1, ..., L^2 - 1) \) lie in the region of \( [-\pi, \pi] \), as in Fig. 10b, then the peak in \( |\langle \theta_{M_i} | \ell_1, \theta_1 \rangle|^2 \) will always be at the middle point of the region, hence the correction term will be exactly 0 for arbitrary \( \theta_1 \), as shown in Fig. 10a.

3. Localization of the Planck cells

Finally, we analyze the fluctuations of these expectation values, i.e. the localization of the shapes of these Planck cells. The fluctuations are

\[
\Delta n_{i} = \frac{\sqrt{\langle N_i^2 \rangle_{\ell_i, \theta_i} - \langle N_i \rangle_{\ell_i, \theta_i}^2}}{N} = \frac{1}{\sqrt{12N}} \sim \frac{1}{\sqrt{12L}}. \quad (A9)
\]

\[
\Delta \theta_{i} = \sqrt{\langle \theta_i^2 \rangle_{\ell_i, \theta_i} - \langle \theta_i \rangle_{\ell_i, \theta_i}^2} = \frac{1}{L^2} \sum_{M_i=0}^{N} \left| \frac{\sin \frac{L \theta_{M_i}}{2}}{\sin \frac{\theta_{M_i}}{2}} \right|^2 \tilde{\theta}_{M_i} - C_\theta^2. \quad (A10)
\]

As discussed above, we can choose \( C_\theta = 0 \) so that Eq. (A10) can be further estimated as

\[
\Delta \theta_{i} \sim \frac{1}{L^3} \int_{-\pi}^{\pi} dx \cdot L^2 \cdot \sin^2 \frac{Lx}{2} \cdot \frac{x^2}{\sin^2 \frac{x}{2}} \quad (A11)
\]

\[
\sim \frac{A}{L} \int_{-\pi}^{\pi} dx \cdot \sin^2 \frac{Lx}{2} \sim \sqrt{\frac{\pi A}{L}}
\]

where \( A \) is a constant of order \( O(1) \) introduced due to the fact that \( x/\sin(x/2) \sim O(1) \) over the entire region of \( [-\pi, \pi] \). Therefore, for both the particle number and the phase, the fluctuations of the expectation values converge to 0 as \( L \) goes to infinity. This establishes the localized ‘cell’ picture of each Planck cell.

Appendix B: Examples of computing the Wasserstein distance

We use two examples to compute the Wasserstein distance between distributions. We consider two distributions

\[
p_A(x) = \begin{cases} 
1/5 & x < 5 \\
0 & x \geq 5 
\end{cases} \quad (B1)
\]

and

\[
p_B(x) = \begin{cases} 
1/5 & x \text{ is even} \\
0 & \text{otherwise} 
\end{cases} \quad (B2)
\]

on the set \( B = \{0, 1, \cdots, 9\} \). We want to compute the Wasserstein distance between them and the uniform distribution. We choose the metric on \( B \) as \( d(x, y) = \sqrt{\frac{1}{3} \left| \frac{x}{9} - \frac{y}{9} \right|^2} \).
The Wasserstein distance for $\lambda = 1$ is the minimum value of
\[ \sum_{i,j \in B} P_{ij} d(i,j). \] (B4)

This shows that the Wasserstein distance is the most efficient way to transform one distribution to another. As both distributions $p_A$ and $p_B$ are simple, the most efficient ways are shown in Fig. 11. For the distribution $p_A$, the non zero optimal $P^*_{ij}$ are
\[ P^*_{i,i} = P^*_{i,i+5} = 1/10 ; \quad i = 0, 1, \cdots, 4 \] (B5)
which means the Wasserstein distance: \( D_1(p_A, p_E) = 5 \times |5 - 0| \times 1/10 = 2.5 \). Similarly, we have \( D_1(p_B, p_E) = 5 \times |1 - 0| \times 1/10 = 0.5 \).