Ergodicity and Mixing in Quantum Dynamics

Dongliang Zhang(张东良),[1] H. T. Quan (全海涛),[1,2] and Biao Wu(吴飙)[3,2,4,*]

[1] *School of Physics, Peking University, Beijing 100871, China*
[2] *Collaborative Innovation Center of Quantum Matter, Beijing 100871, China*
[3] *International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China*
[4] *Wilczek Quantum Center, College of Science, Zhejiang University of Technology, Hangzhou 310014, China*

After a brief historical review of ergodicity and mixing in dynamics, particularly in quantum dynamics, we introduce definitions of quantum ergodicity and mixing using the structure of the system's energy levels and spacings. Our definitions are consistent with usual understanding of ergodicity and mixing. Two parameters concerning the degeneracy in energy levels and spacings are introduced; their relations to quantum ergodicity and mixing are demonstrated with right triangular billiards. With this billiard system, we find that a system is ergodic in its quantum dynamics may not be ergodic in its classical dynamics. At the end, we argue that, besides ergodicity and mixing, there may exist a third class of quantum dynamics which is characterized by a maximized entropy.

I. INTRODUCTION

Ergodicity and mixing are of fundamental importance in statistical mechanics. Ergodicity justifies the use of microcanonical ensemble and mixing ensures that a system approach equilibrium dynamically [1]. However, it is difficult to prove with mathematical rigor that a classical dynamical system is ergodic or mixing. As a result, the microcanonical ensemble in textbooks is still established with postulates [2]. More importantly, the concept of ergodicity and mixing is now obsolete in the following sense: they are defined for classical dynamics while the dynamics of microscopic particles are fundamentally quantum. To establish statistical mechanics with quantum dynamics, we need to define ergodicity and mixing in quantum dynamics. So far, a clear definition of ergodicity and mixing in quantum dynamics is still lacking.

In this work we define quantum ergodicity and mixing using the structure of the system's energy levels and spacings. With the early results by von Neumann [3] and Reimann [4], it can be shown that our definitions, which appear very mathematical, do lead to the usual understanding of ergodicity and mixing. We establish the conditions under which a quantum system is either ergodic or mixing by introducing two parameters characterizing the degeneracy in energy levels and spacings, respectively. We find that most of non-integrable finite quantum systems are both ergodic and mixing. Our general results are illustrated with right triangular billiards, whose classical dynamical properties have been studied in great detail [5, 6]. Besides a few special cases, the right triangular billiard is both ergodic and mixing in its quantum dynamics. It is clear from this example that a system whose quantum dynamics is ergodic may not be ergodic in the corresponding classical dynamics.

We draw a parallel between our paper and Peres's two papers [7, 8]. Peres introduced his definitions for quantum ergodicity and mixing in the first paper [7] then illustrated with examples these two concepts with his coauthors in the second paper [8]. In our paper we do both: we first introduce our definitions for quantum ergodicity and mixing and then illustrate them with examples.

II. QUANTUM ERGODICITY AND MIXING

A. History

Ergodicity was introduced by Boltzmann in 1871 as a hypothesis to understand thermodynamics microscopically [1]. Mixing was first discussed by Gibbs [9] and its mathematical definition was introduced by von Neumann in 1932 [10]. Both concepts concern the long time behavior of dynamical systems and are of fundamental importance to statistical mechanics. They are now the focus of a fully-developed branch of mathematics called ergodic theory[11, 12]. However, ergodicity and mixing are becoming less interesting to physicists for two reasons: (1) After decades of research with many meaningful results[11, 12], it is still not rigorously proved that many of the physical systems existing in nature are either ergodic or mixing. (2) Both ergodicity and mixing are only defined for classical systems while the microscopic particles are fundamentally quantum. Therefore, it is imperative to define both ergodicity and mixing to quantum systems.

The first physicist who discussed quantum ergodicity was von Neumann. In 1929, von Neumann proved two inequalities, which he named quantum ergodic theorem and quantum H-theorem [3], respectively. His ergodic theorem ensures that not only the long time average of a macroscopic observable equals to its microcanonical ensemble average but also has small fluctuations. In other words, the observable deviates considerably from its averaged value only rarely. So, by ergodicity von Neumann meant actually both ergodicity and mixing. Interestingly, mixing as defined for classical dynamics was only introduced three years later in 1932 by von Neumann [10]. In

*Electronic address: wubiao@pku.edu.cn

addition, according to von Neumann's H-theorem, once the quantum system dynamically relaxes to its equilibrium state, where macroscopic observables have small fluctuations, this state also has a maximized entropy.

Von Neumann's results had been criticized by many [7, 13]. We share the view by Goldstein *et al.* [13] that the criticism was mostly misguided; von Neumann had captured the essence of quantum ergodicity and mixing and his results are inspirational. Nevertheless, there do exit some issues with von Neumann's results. Most of the variables involved in the two theorems are not computable in principle [14]. The reason is as follows. To prove his theorems, von Neumann introduced a coarse-graining, which groups the Planck cells in quantum phase space into some big cells. All the microscopic states in one group of Planck cells correspond to a single macroscopic state. This kind of coarse-graining is certainly reasonable. However, no one knows how to technically establish such many-to-one mapping between macroscopic state and microscopic state. This makes many of von Neumann's variables in Ref. [3] uncomputable.

More recent definitions of ergodicity and mixing in quantum mechanics were given by Peres [7]. Peres recalled the behavior of dynamical variables in classical ergodic and mixing systems and expected that there should be analogous behavior in quantum ergodic and mixing systems. In accordance with von Neumann's results, Peres defined ergodicity as the time average of any quantum operator equal to its microcanonical ensemble average and mixing as any quantum operator having small fluctuations. However, Peres's definitions were based on his own definition of quantum chaos [7], which is a subject of debate itself. To define quantum chaos, Peres used an ambiguous concept of pseudorandom matrix. These two steps that are not mathematically very rigorous , along with other reasonable but ambiguous assumptions, render Peres's definitions not satisfactory.

In literature quantum ergodicity has been studied from a different perspective, where the concept "quantum ergodicity" is regarded as a branch of quantum chaos [15–22]. This group of researchers mainly focused on how the eigenfunctions of a Hamiltonian converges to equidistribution in classical phase space in the semi-classical limit or high energy limit with little discussion on dynamical behavior of a quantum system. Their definitions of quantum ergodicity and mixing rely on the corresponding classical cases and thus are not genuinely quantum mechanical.

In the following subsection we define quantum ergodicity and mixing using the energy structure of the system, that is, eigen-energies and energy spacings. Our definitions are mathematically precise. Furthermore, by following von Neumann [3] and Reimann [4], we can show that our definitions lead to the usual physical understanding of ergodicity and mixing. Our definitions are based on quantum dynamics and expressed in the language of pure quantum mechanics without referring to classical mechanics. Near the end of this paper, based on a recent work [14], we argue that we may be able to expand our definitions to include a third class of quantum dynamics, which is charactering by a maximized entropy.

B. Definitions

Consider a quantum system with discrete eigen-energies $\{E_n\}$ and corresponding energy eigenstates $\{|\phi_n\rangle\}$.

Ergodicity. A quantum system is ergodic if its eigen-energies satisfy

$$\delta_{E_m,E_n} = \delta_{mn}\,. \tag{I}$$

Mixing. A quantum system is mixing if its eigen-energies satisfy both the above condition (I) and the following condition

$$\delta_{E_k-E_l,E_m-E_n} = \delta_{km}\delta_{ln}\,, \quad \text{for } k \neq l, m \neq n\,. \tag{II}$$

Condition (I) indicates that there is no degenerate eigenstate. Condition (II) implies that there is no degeneracy in energy gaps between any pair of eigen-energies. It is clear that a quantum system that is mixing must be ergodic, similar to classical dynamics. As we shall show in the following, condition (I) can lead to the usual intuitive understanding of ergodicity: the long time average equals to the ensemble average. With both conditions (I) and (II), one can show that the so-defined mixing indeed means a small time fluctuation for an observable.

Suppose that the quantum system is in an initial state $|\psi(0)\rangle = \sum_n c_n|\phi_n\rangle$. After evolving for a period of time t, the quantum system is in a state described by $|\psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|\phi_n\rangle$. For an observable $\hat{A}$, its expectation value at time t is given by

$$\langle\hat{A}(t)\rangle \equiv \langle\psi(t)|\hat{A}|\psi(t)\rangle = \mathrm{tr}\hat{A}\hat{\rho}(t), \tag{1}$$

where $\hat{\rho}(t) \equiv |\psi(t)\rangle\langle\psi(t)|$ is the density matrix at time t. Its long time average is

$$\langle\hat{A}\rangle_T \equiv \lim_{T\to\infty}\frac{1}{T}\int_0^T \langle\hat{A}(\tau)\rangle d\tau\,. \tag{2}$$

We now introduce a density matrix

$$\hat{\rho}_{\mathrm{mc}} \equiv \sum_n |c_n|^2|\phi_n\rangle\langle\phi_n|\,. \tag{3}$$

This density matrix does not change with time and it can be regarded as describing a micro-canonical ensemble [3, 4, 14]. This allows us to define the ensemble average as

$$\langle\hat{A}\rangle_E \equiv \mathrm{tr}\hat{A}\hat{\rho}_{\mathrm{mc}}\,. \tag{4}$$

For a quantum system satisfying condition (I), it is easy to check [3, 7] that

$$\langle\hat{A}\rangle_E = \langle\hat{A}\rangle_T\,, \tag{5}$$

that is, the long time average of $\hat{A}$ equals to its micro-canonical ensemble average.

For a quantum system satisfying both conditions (I) and (II), one can prove [4, 23] that the long-time averaged fluctuation $\langle F_A^2\rangle_T$ satisfies

$$\langle F_A^2\rangle_T \equiv \frac{\left\langle \left| \langle \hat{A}(t)\rangle - \langle \hat{A}\rangle_E \right|^2 \right\rangle_T}{\|\hat{A}\|^2} \leq \mathrm{tr}\hat{\rho}_{\mathrm{mc}}^2, \qquad (6)$$

where $\|\hat{A}\|^2 = \sup \langle\psi|\hat{A}^\dagger\hat{A}|\psi\rangle$ is the upper limit of the expectation value of $\hat{A}$ in the Hilbert space. This demonstrates that a mixing quantum system indeed has small time fluctuations.

A few remarks are warranted here to put our definitions in perspective.

Remark 1. Our definitions of ergodicity and mixing for quantum systems are mathematically very precise . They do not involve any concepts and assumptions, which are mathematically ambiguous. Peres made many assumptions in his definitions [7], which are reasonable but ambiguous mathematically. In particular, we do not need to define quantum chaos first as Peres did [7].

Remark 2. Although our definitions appear very mathematical, as we have shown, they are consistent with the familiar physical pictures that we have had with ergodicity and mixing in classical dynamics: ergodicity means that long time average equals to ensemble average; mixing implies small time fluctuations. Moreover, similar to the classical case, a quantum mixing system is ergodic but not vice versa.

Remark 3. Our definitions have their roots in the 1929 paper, where von Neumann proved a quantum ergodic theorem [3]. However, von Neumann in 1929 did not distinguish between ergodicity and mixing. His view of ergodicity at that time is closer to the current view of mixing. In other words, his quantum ergodic theorem may be better called quantum mixing theorem.

It is worthwhile to note two interesting points: (i) von Neumann used both condition (I) and (II) to prove his quantum ergodic theorem; (ii) mixing in classical dynamics was introduced three years later in 1932 by von Neumann himself [10].

Remark 4. The density matrix $\hat{\rho}_{\mathrm{mc}}$ is used as the micro-canonical ensemble in the above discussion. It is not the standard micro-canonical ensemble found in textbooks [2],

$$\hat{\rho}_{\mathrm{tb}} = \frac{1}{N} \sum_{E_n\in[E,E+\delta E]} |\phi_n\rangle\langle\phi_n|\,, \qquad (7)$$

where N is the number of energy-eigenstates in energy interval $[E, E+\delta E]$. However, we can certainly choose an initial state such that $|c_n| = 1/N$ for $E_n \in [E, E+\delta E]$ and $|c_n| = 0$ otherwise. In this way, we recover the textbook micro-canonical ensemble $\hat{\rho}_{\mathrm{tb}}$. That is, $\hat{\rho}_{\mathrm{tb}}$ is just a special case of $\hat{\rho}_{\mathrm{mc}}$.

Remark 5. Our definitions of ergodicity and mixing for quantum systems are independent of initial conditions. Nevertheless, to thoroughly understand them, we do need to consider initial conditions as the density matrix $\hat{\rho}_{\mathrm{mc}}$ depends on initial conditions. If we choose an initial state where only a few eigenstates are occupied, not only $\hat{\rho}_{\mathrm{mc}}$ is no longer sensible to be regarded as a micro-canonical ensemble but also the fluctuation $\langle F_A^2\rangle_T$ in Eq.(6) is not small. However, this kind of initial conditions are hard to realize in experiment or to be found in nature for a many-body quantum system. Physically, when a many-body quantum system is excited by a practical means, it usually enters into a quantum state where a large number of eigenstates are occupied. This is also the reason that the standard micro-canonical ensemble $\hat{\rho}_{\mathrm{tb}}$, which looks quite artificial, works well as long as N is large.

This aspect is quite similar to classical systems. In an ergodic or mixing classical system there always exist solutions which are not ergodic or mixing, for example, the periodic orbits. However, these non-ergodic or non-mixing solutions are rare or have measure zero in rigorous mathematical language so that the overall properties of the system are not affected.

Remark 6. Although classical ergodicity and mixing are of fundamental importance in statistical mechanics, their definitions can be applied to single-particle systems. Similarly, our definitions can be applied to single-particle quantum systems.

C. Degeneracy parameters

We have used conditions (I) and (II) to define quantum ergodicity and mixing, respectively. However, when there are infrequent exceptions to these two conditions, a quantum system should still be ergodic or mixing in a practical sense. For instance, if a quantum system has a relatively small number of degeneracies, then almost all its states contain either no degenerate eigenstates or only a few. For the former, Eq.(5) still holds; for the latter, the left hand side in Eq.(6) differs the right hand side only slightly. So, in a practical sense, this quantum system is ergodic. The situation is similar for mixing: infrequent degeneracy in energy gap is not important. Von Neumann had a similar point of view [3]. Short and Farrelly showed quantitatively how infrequent degeneracy are not important [24].

It is therefore interesting to quantitatively measure the extent of the violation of these two conditions, and to see what will happen as the extent of the violation grows. To this end, we introduce two parameters ζ and ξ, which describe the average degeneracy in energy levels and average degeneracy in energy level spacings, respectively, for a given finite set of energy levels. The parameter ζ is defined as

$$\zeta = \frac{1}{N}\sum_{m,n} \left(\delta_{E_m,E_n} - \delta_{mn}\right), \qquad (8)$$

where N is the number of energy levels in the set. The other parameter ξ is defined as

$$\xi = \frac{1}{N(N-1)} \sum_{k\neq l, m\neq n} (\delta_{E_k - E_l, E_m - E_n} - \delta_{km}\delta_{ln}) \,. \quad (9)$$

Furthermore, it is useful to define two distribution functions, $f(\epsilon)$ and $g(\Delta)$. $f(\epsilon)$ is the probability of the eigen-energies having value ϵ; $g(\Delta)$ is the probability of the energy level spacings at Δ. With the aid of these distribution functions, we can reformulate the definitions of ζ and ξ, respectively, as

$$\zeta = N \sum_{\epsilon} f^2(\epsilon) - 1 \,, \quad (10)$$

$$\xi = N(N-1) \sum_{\Delta} g^2(\Delta) - 1 \,. \quad (11)$$

These two functions are clearly related; their explicit relation is

$$\begin{aligned} g(\Delta) = & \sum_{\epsilon} f(\epsilon) \frac{N f(\epsilon + \Delta) - \delta_{\Delta 0}}{N-1} \\ = & \frac{N}{N-1} \sum_{\epsilon} f(\epsilon) f(\epsilon + \Delta) - \frac{\delta_{\Delta 0}}{N-1}. \end{aligned} \quad (12)$$

We clarify that in our definition Δ can be negative. In other words, for two arbitrary energy levels E_m and E_n with $m \neq n$, $E_m - E_n$ and $E_n - E_m$ give rise to two energy level spacings rather than one. We also emphasize that our definitions of ζ and ξ are for a given set of energy levels not for all the energy levels in the system. The reason is that only a finite set of energy levels are involved in any meaningful physical process.

According to these definitions, the two conditions (I) and (II) are equivalent to $\zeta \equiv 0$ and $\xi \equiv 0$, respectively. The larger ζ(or ξ) is the stronger the non-degenerate-energy condition (I) (or the non-degenerate-gap condition (II)) is violated. We anticipate that for small ζ and ξ quantum systems can still be regarded as ergodic or mixing. For systems where ζ and ξ are strictly equal to zero, we say that they are *ideal* ergodic systems or *ideal* mixing systems.

III. MODEL

In this section we use an example to illustrate our concepts of quantum ergodicity and mixing. We consider the motion of one particle with mass m in a right triangular billiard, as is shown in Fig.1. Mathematically, this billiard is described by the following potential

$$V(x,y) = \begin{cases} 0 & 0 < x < l, 0 < y < \alpha x \\ \infty & \text{otherwise} \end{cases} . \quad (13)$$

Without loss of generality, we restrict ourselves to $\alpha \geq 1$ or $0 < \theta \leq \pi/4$ ($\alpha = \cot\theta$). It is interesting to note that this billiard system is equivalent to the system of two hard-core particles moving in one-dimensional square potential with infinite walls [6].

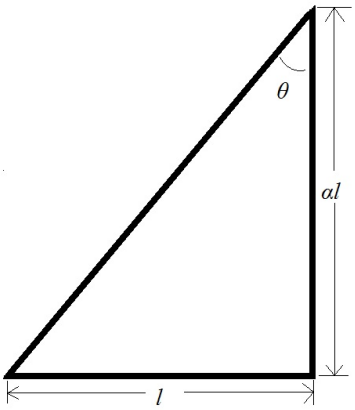

FIG. 1: A right triangle billiard. Without loss of generality, we take $\alpha \geq 1$ or, equivalently, $0 < \theta \leq \pi/4$.

We choose this simple model for two reasons. (1) We can study both the integrable cases and chaotic cases by adjusting α. (2) Many meaningful results on classical ergodicity and mixing in this model have been obtained previously [5, 6], and we can compare them to our quantum results.

The classical integrability of this model is well known. The system is integrable only when $\theta = \pi/4$ or $\theta = \pi/6$ (equivalently, $\alpha = 1$ or $\alpha = \sqrt{3}$). When $\theta = \pi M/N$, where M and N are two coprime integers and $(M,N) \neq (1,4), (1,6)$, the system has two independent invariants. However, it is regarded as pseudointegrable[25–27] because the invariant surface of classical motion in phase space has a genus $2 \leq g < \infty$ (it is integrable only when the genus $g = 1$). For all other values of θ, the triangle system has only one invariant and is generally regarded as chaotic.

To study the quantum dynamics of this model, we need to calculate the eigenenergies and eigenstates. This can be done only numerically for an arbitrary value of parameter α. We use the exact diagonalization method (see Appendix A for details). In our calculation, we choose $h = m = l = 1$. In addition, to avoid confusion, we use the single parameter α (instead of θ) to represent the shape of the triangle billiard in following discussion.

IV. DISTRIBUTIONS OF ENERGY LEVELS

In Section II we have defined quantum ergodicity and mixing with two conditions (I) and (II) that regard the distribution of the system's energy levels. In this section, we shall examine to what extent these two conditions are satisfied by the triangle billiard and how they are related

to the integrability of this model via parameters ζ and ξ. In the next section, we shall show that the quantum dynamics of the triangle billiard are dictated by these two conditions.

The study of quantum chaos has revealed that the structure of quantum energy levels of a system is closely related to the classical integrability of the system [7, 28]. One often uses the nearest spacing distribution(NSD) $p(s)$ of a system to describe its structure of quantum energy levels, where $s > 0$ is the spacing between two nearest energy levels. The following feature of NSD is well known. For a system whose classical dynamics is integrable, its NSD is Poisson-like with a peak distribution at $s = 0$. For a system whose classical dynamics is chaotic, the NSD of its quantum energy levels is Wigner-like: an almost zero probability density at $s = 0$ and a peak density at $s = s_m \neq 0$. This feature indicates that condition (I) is always satisfied by a quantum chaotic system. There is no clear conclusion for condition (II) as the peak at nonzero s in the Wigner distribution seems to suggest that condition (II) is not satisfied by a quantum chaotic system. However, our following numerical results show that condition (II) is also largely satisfied by a quantum chaotic system.

The Hamiltonian matrix of the triangle billiard is diagonalized numerically for a set of α. Its NSDs for the first 1000 energy levels are shown in Fig.2 for four typical values of α. As expected, two integrable cases $\alpha = 1$ and $\alpha = \sqrt{3}$ have lots of degenerate energy levels while the pseudointegrable and chaotic cases have few.

With the obtained eigen-energies we can compute ζ and ξ, the two parameters that we introduced to describe quantitatively how well the two conditions (I) and (II) for ergodicity and mixing are satisfied in a given system. We first construct the two distribution functions $f(\epsilon)$ and $g(\Delta)$ and then compute ζ and ξ using Eq.(10) and Eq.(11). The distribution function $f(\epsilon)$ together with $g(\Delta)$ is constructed by binning the energy levels with a width $\delta\epsilon = \hbar/T$, where T is the total time of a dynamical evolution. For a dynamical evolution of time T, energy levels or spacings separated by $\delta\epsilon = \hbar/T$ can be regarded as the same. In our calculation, we use $T = 40$ in accordance with our numerical study of quantum dynamics in the next section.

The results are shown in Table.I, where we see clearly the values of ζ and ξ are strongly correlated to the classical integrability of the system. For integrable systems, both ζ and ξ are large. As α changes and the system becomes more chaotic, ζ decreases almost to zero while ξ is reduced by about two orders of magnitude. These numerical results strongly suggest that conditions (I) and (II) are largely satisfied by chaotic systems.

The pseudointegrable systems are subtle. As one may have already noticed in Fig.2(c) and Table I, the pseudointegrable case $\alpha = \cot\pi/5$ behaves very much like a chaotic system. However, not all pseudointegrable systems has a chaotic NSD. Some pseudointegrable triangle billiards, such as the triangle with angles $(\pi/5, 2\pi/5, 2\pi/5)$, have Possion-like NSDs [29]. Apparently, these triangle billiards should have large ζ and ξ, and they are not ergodic and mixing. This difference shows that the relation between quantum ergodicity and mixing and classical integrability is very subtle in the case of pseudointegrable systems.

α	ζ	ξ
1^*	0.588	300.89
1.007846	0.032	14.39
1.015675	0	8.86
1.077744	0	8.65
1.154062	0	9.25
1.376382	0	11.04
1.461725	0	11.72
1.662013	0.002	13.33
1.700000	0.004	13.89
1.718079	0.010	18.84
1.725067	0.084	40.85
1.732051^*	0.414	167.03

TABLE I: Degeneracy parameters ζ and ξ for different values of α. The first 1000 energy levels are used in the calculation. Integrable cases are marked by superscript $*$. Clearly, integrable cases have much larger ζ and ξ.

V. QUANTUM DYNAMICAL BEHAVIOR

In this section we shall study the quantum dynamics of the triangle billiard for a set of typical values of α to see whether it exhibits ergodic or mixing behavior as described by Eq.(5) or Eq.(6), respectively, and how these dynamical behaviors are dictated by conditions (I) and (II) via parameters ζ and ξ.

To study the quantum dynamical behavior, we need to calculate the time evolution of a wave function. We use the method of eigenstate expansion. For an arbitrary initial wave function $\psi(x, y, 0)$, we expand it in terms of the energy eigenstates of the Hamiltonian $\phi_k(x, y)$

$$\psi(x, y, 0) = \sum_k c_k \phi_k(x, y)\,. \tag{14}$$

According to the Schördinger equation, the time evolution of this initial wave function is given by

$$\psi(x, y, t) = \sum_k c_k e^{\frac{-iE_k t}{\hbar}} \phi_k(x, y)\,. \tag{15}$$

As the expansion coefficients can be calculated easily as

$$c_k = \iint_{\Omega_1} \psi(x, y, 0)\phi_k^*(x, y)\mathrm{d}x\mathrm{d}y\,, \tag{16}$$

once we have obtained the expansion coefficients c_k, we can generate the wave function at any time. In our study, we choose a Gaussian wave packet as an initial state

$$\psi(x, y) = \frac{1}{\sqrt{4\pi\sigma^2}} e^{-\frac{1}{4\sigma^2}[(x-x_0)^2+(y-y_0)^2]} e^{-i2\pi(p_x x+p_y y)}\,, \tag{17}$$

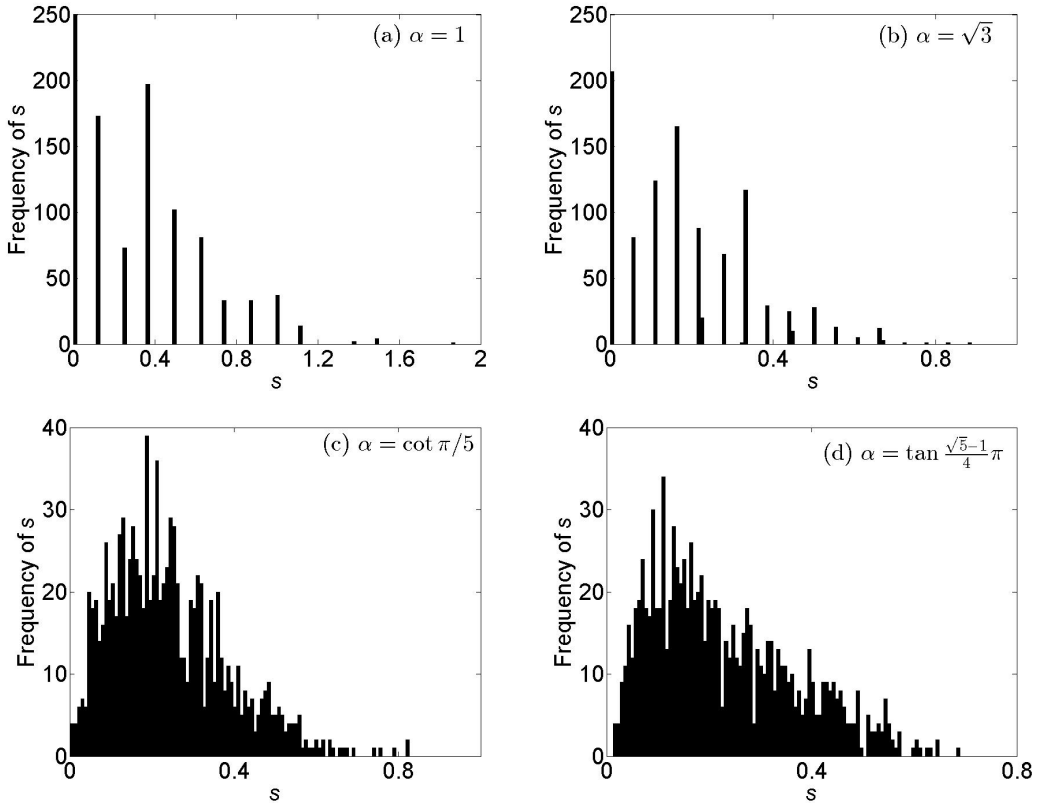

FIG. 2: Nearest spacing distribution of eigenenergies. (a)$\alpha = 1$ and (b)$\alpha = \sqrt{3}$ are two integrable cases. (c) $\alpha = \cot(\pi/5)$ is pseudointegrable. (d) is chaotic. Calculations are done in first 1000 energy levels.

where $x_0 = 0.5, y_0 = 0.3, p_x = 5\cos(e\pi), p_y = 5\sin(e\pi)$, and $\sigma = 0.02$. This initial state mainly occupies the first 1000 energy eigenstates.

It is sufficient to focus on the momentum of the system. For the initial condition in Eq.(17) we have exactly $\langle \vec{p} \rangle_E = 0$. The quantum dynamical evolutions of $\vec{p}$ are shown in Fig.3 for four typical values of α: $\alpha = 1$, $\alpha = \sqrt{3}$, $\alpha = \cot \pi/5$, and $\alpha = \tan \frac{\sqrt{5}-1}{4}\pi$. It is clear that the evolution of $\vec{p}$ varies greatly with different α. Before we discuss it in detail, let us first recall the classical dynamics for these four cases. The cases with $\alpha = 1$ and $\alpha = \sqrt{3}$ are integrable; $\alpha = \cot \pi/5$ is pseudointegrable and has only finite directions of $\vec{p}$ in classical dynamics which means nonergodicity. The case with $\alpha = \tan \frac{\sqrt{5}-1}{4}\pi$ is nonintegrable but classically nonergodic [6].

Let us come back to the quantum dynamics in Fig.3. For the two integrable cases, the long-time average is apparently not equal to its microcanonical ensemble average, and the fluctuation is large as well. For other cases, the momentum quickly relaxes to its microcanonical ensemble average and has only small fluctuations. The relaxation time is very short and is about $\sim 10^{-1}$ for these cases. Up to $t = 40$, we do not observe a revival or large deviation from the equilibrium value. These results demonstrate that the quantum dynamics for $\alpha = \cot \pi/5$ (the pseudointegrable regime) and $\alpha = \tan \frac{\sqrt{5}-1}{4}\pi$ are not only ergodic but also mixing. This is in stark contrast with their classical dynamics which are not even ergodic. This suggests that it is easier to have quantum ergodicity and mixing than their classical counterparts.

In order to check quantitatively whether a quantum system is mixing, we need to calculate the time-averaged relative fluctuation. The averaged deviation of the momentum operator $\vec{p}$ in a given evolution time T is

$$\langle \sigma^2_{\vec{p}} \rangle_T = \frac{1}{T}\int_0^T \left| \langle \psi(t)|\vec{p}|\psi(t)\rangle - \sum_k |c_k^2| \langle \phi_k|\vec{p}|\phi_k\rangle \right|^2 \mathrm{d}t. \tag{18}$$

Considering $E = \frac{\vec{p}^2}{2}$, the relative fluctuation of $\vec{p}$ is

$$\langle F^2 \rangle_T = \frac{\langle \sigma^2_{\vec{p}} \rangle_T}{|\vec{p}|^2} = \frac{\langle \sigma^2_{\vec{p}} \rangle_T}{2E} \tag{19}$$

As the relaxation time scale is $\sim 10^{-1}$ and the oscillating period for integrable systems is $\sim 10^1$, we choose $T = 40$ considering the balance between the accuracy of the result and computing cost.

The results of relative fluctuation for different α are shown in Fig.4. The dashed line is $\mathrm{tr}\rho^2_{\mathrm{mc}}$, the upper bound in Eq.(6). It can be clearly seen that for α away from 1 or $\sqrt{3}$, the averaged fluctuation is small, and the

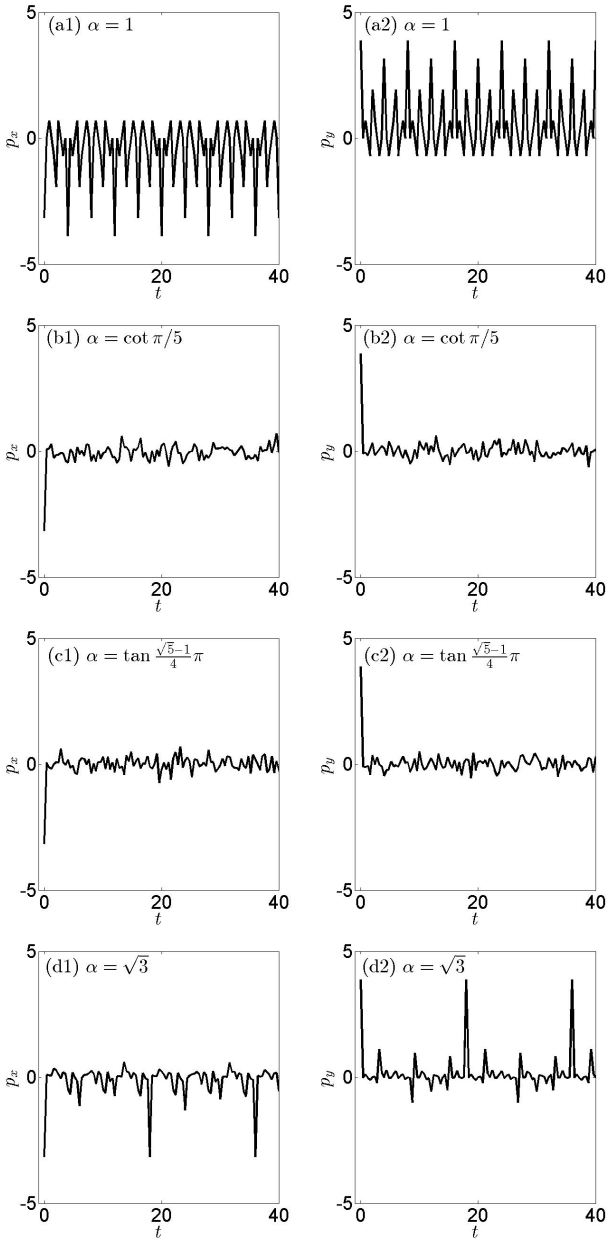

FIG. 3: Evolution of the momentum for different α. $\alpha = 1$ and $\alpha = \sqrt{3}$ are two integrable cases. $\alpha = \tan \frac{\sqrt{5}-1}{4}\pi$ is chaotic but nonergodic in classical mechanics [6]. $\alpha = \cot \pi/5$ is pseudointegrable.

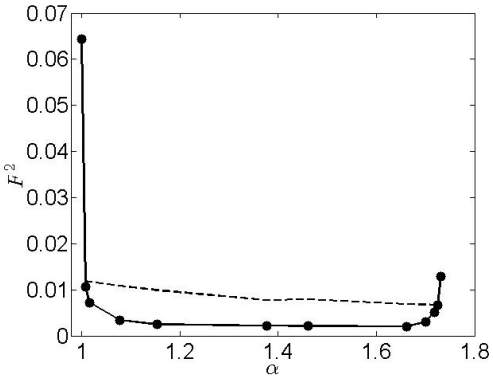

FIG. 4: Averaged relative fluctuations of the momentum via α. The solid points are the numerical results; the solid line is just a guidance; the dashed line is the upper bound $\mathrm{tr}\rho^2_{\mathrm{mc}}$ in Eq.(6).

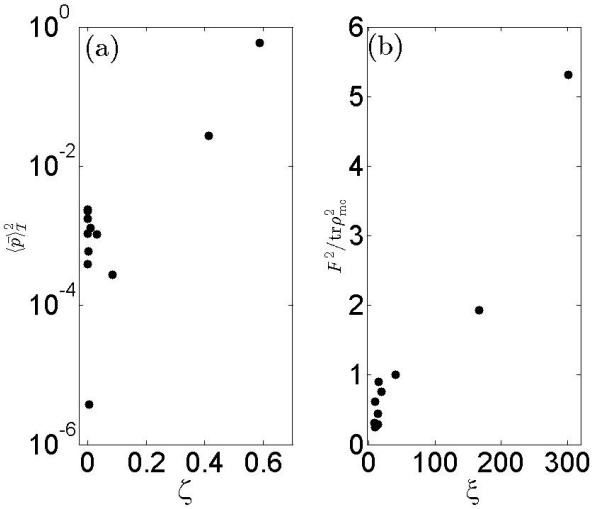

FIG. 5: (a)The square of time-averaged $\vec{p}$ at $T = 40$ with different ζ. The vertical axis is in log scale. Note that $\langle \vec{p} \rangle_E = 0$. (b)Averaged relative fluctuation vs. ξ. No mixing when $\langle F^2 \rangle_T / \mathrm{tr}\rho^2_{\mathrm{mc}} > 1$.

inequality Eq.(6) is satisfied. This confirms the intuitive picture in Fig. 3 that the quantum dynamics is mixing. When α approaches the two integrable cases, $\alpha = 1$ and $\alpha = \sqrt{3}$, the averaged fluctuation becomes much larger, and the inequality Eq.(6) is violated. In fact, at these two integrable cases, the averaged fluctuation reaches two local maxima. There is a rather rapid transition from mixing to nonmixing while the system is tuned from nonintegrable to integrable.

The quantum dynamic behavior shown in Fig. 3 are dictated by conditions (I) and (II). This can be seen clearly in Fig.5, where the square of time averaged momentum $\langle \vec{p} \rangle_T^2$ and its relative fluctuations are plotted against the two degeneracy parameters ζ and ξ, respectively. It is clear from the figure that for systems with significantly non-zero ζ, the time average of the momentum significantly deviates from the microcanonical ensemble value. We can see a strong positive correlation between the relative fluctuation $F^2/\mathrm{tr}\rho^2_{\mathrm{mc}}$ and ξ as well. These results illustrate that systems with small ζ and ξ have ergodic and mixing quantum dynamics, respectively. Our definitions of quantum ergodicity and mixing with conditions (I) and (II) are legitimate.

VI. DISCUSSION AND CONCLUSION

Let us summarize what we have done. We have given our own definitions of ergodicity and mixing for quantum systems with conditions (I) and (II). It can be rigorously proved that these two conditions lead to quantum dynamical behaviors which are described by Eq.(5) and Eq.(6) and are reminiscent of classical ergodic and mixing dynamics, respectively. Through an example, the triangle billiard, we have further shown that although both conditions (I) and (II), which are characterized by ζ and ξ, are related to classical integrability, there are differences. The most important is that a system whose classical dynamics is neither ergodic nor mixing can be both ergodic and mixing in its quantum dynamics.

Classical dynamics has an ergodic hierarchy [11, 12], which is

$$\text{Bernoulli} \subset \text{Kolmogorov} \subset \text{Mixing} \subset \text{Ergodic}\,. \tag{20}$$

Now mixing and ergodicity have their quantum counterparts. In particular, we have similar relation: quantum mixing systems are a subset of quantum ergodic systems. It is possible to expand this quantum ergodic hierarchy to three. We define a quantum system is *equilibrable* if the system satisfies

$$\begin{aligned} &E_m + E_n - E_k - E_l = E_{m'} + E_{n'} - E_{k'} - E_{l'} \text{ and} \\ &\{m,n\} \cap \{k,l\} = \emptyset \Rightarrow \{m,n\} = \{m',n'\}\{k,l\} = \{k',l'\}\,. \end{aligned} \tag{III}$$

This condition implies that there is no degeneracy in the gaps of energy gaps. One can find the full implication of this condition in Ref.[14]. Here we briefly summarize. The entropy for a quantum pure state $\hat{\rho} \equiv |\psi\rangle\langle\psi|$ is defined as [14]

$$\begin{aligned} S_w &\equiv -\sum_{\boldsymbol{q}_i,\boldsymbol{p}_j} \langle\psi|\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}|\psi\rangle \ln\langle\psi|\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}|\psi\rangle \\ &\equiv -\sum_{\boldsymbol{q}_i,\boldsymbol{p}_j} \mathrm{tr}(\hat{\rho}\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}) \ln \mathrm{tr}(\hat{\rho}\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}) \end{aligned} \tag{21}$$

where $\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j} \equiv |w_{\boldsymbol{q}_i,\boldsymbol{p}_j}\rangle\langle w_{\boldsymbol{q}_i,\boldsymbol{p}_j}|$ is the projection onto Planck cells in quantum phase space at position $\boldsymbol{q}_i$ and momentum $\boldsymbol{p}_j$ and $\{|w_{\boldsymbol{q}_i,\boldsymbol{p}_j}\rangle\}$ is a complete set of Wannier functions. This entropy S_w will change with time. An inequality regarding the relative fluctuation of entropy S_w, similar to Eq.(6), was proved in Ref.[14] with condition (III). This inequality means that a quantum system with small entropy S_w will relax dynamically to a state whose entropy S_w is maximized and stay at this maximized value with small fluctuations. This is illustrated with the triangle billiard in Fig.6. In this figure we see that the entropy S_w of the integrable cases, for which condition (III) is not satisfied, fluctuates periodically with large amplitude and does not stay at the maximum value. For cases with $\alpha = \tan\frac{\sqrt{5}-1}{4}\pi$ and $\alpha = \cot\pi/5$, where condition (III) is largely satisfied, the entropy quickly relaxes to the maximum value and stays there with small fluctuations. These results demonstrate that a quantum system that satisfies condition (III) is capable of equilibrating to a state where not only its observables fluctuate around its equilibrium value with small amplitude but also its entropy is maximized. This is the reason that we call such a quantum system *equilibrable*. In this way we have a quantum ergodic hierarchy

$$\textit{Equilibrable} \subset \text{Mixing} \subset \text{Ergodic}\,. \tag{22}$$

We do not call it quantum Kolmogorov as we do not see an apparent connection to the classical Kolmogorov mixing system at this moment.

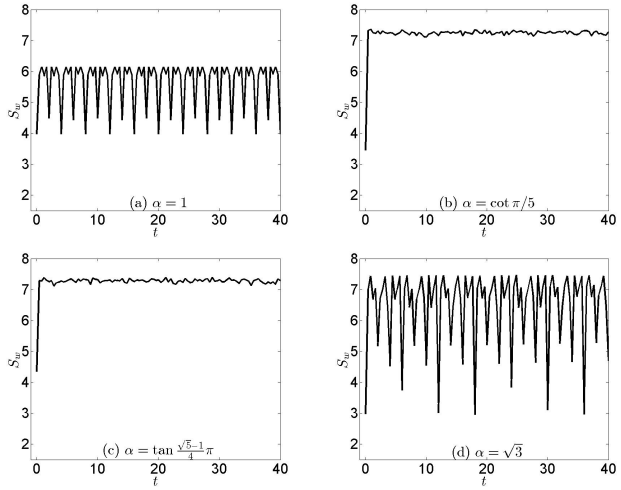

FIG. 6: Evolution of the entropy S_w for different α.

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Appendix A: The calculation of eigenenergies and eigenstates

As mentioned above, we use the exact diagonalization method to calculate the eigenenergies and eigenstates. We first choose an appropriate basis, then calculate the Hamiltonian matrix in the basis. Finally after diagonalization we can obtain the eigenenergies and eigenstates.

In order to minimize the numerical error within an acceptable range, the key is to choose the appropriate basis. Casually chosen basis may lead to larger errors.

Here we choose the basis as follows

$$|m,n\rangle = \frac{2}{l\sqrt{\alpha}}(\sin\frac{m\pi x}{l}\sin\frac{n\pi y}{\alpha l} - \sin\frac{n\pi x}{l}\sin\frac{m\pi y}{\alpha l}), \tag{A1}$$

This choice is similar to that in Ref.[29]. This basis is complete and orthogonal and it is easy to check that all these base functions $|m,n\rangle$ are zero on the boundary of the triangle. The elements of the Hamiltonian matrix can be computed analytically

$$\langle m_1,n_1|\hat{H}|m_2,n_2\rangle = \frac{h^2}{2ml^2}\left[\left(m_2^2+\frac{n_2^2}{\alpha^2}\right)(I(m_1,n_1,m_2,n_2)-I(n_1,m_1,m_2,n_2)) - \left(n_2^2+\frac{m_2^2}{\alpha^2}\right)(I(m_1,n_1,n_2,m_2)-I(n_1,m_1,n_2,m_2))\right] \tag{A2}$$

where

$$I(m,n,p,q) = \int_0^1 \mathrm{d}x\int_0^x \mathrm{d}y \sin m\pi x \sin n\pi y \sin p\pi x \sin q\pi y$$

$$= \begin{cases} \frac{1}{8}, & \text{if } m=p \ \&\ n=q \\ \frac{1}{8\pi^2}(1-(-1)^{m+n+p+q})\left[-\frac{\{p-m+n+q\}^{-1}+\{q+n-p+m\}^{-1}-\{p+m+n+q\}^{-1}-\{n+q-p-m\}^{-1}}{q+n}\right. & \\ \left. +\frac{2}{(m+p)^2}-\frac{2}{(m-p)^2}\right], & \text{if } m\neq p \ \&\ n=q \\ \frac{1}{8\pi^2}(1-(-1)^{m+n+p+q})\left[-\frac{\{p-m+n+q\}^{-1}+\{q+n-p+m\}^{-1}-\{p+m+n+q\}^{-1}-\{n+q-p-m\}^{-1}}{q+n}\right. & \\ \left. +\frac{\{p-m+q-n\}^{-1}+\{q-n-p+m\}^{-1}-\{m+p+q-n\}^{-1}-\{q-m-n-p\}^{-1}}{q-n}\right], & \text{if } m\neq p \ \&\ n\neq q \end{cases} \tag{A3}$$

with the curly braces $\{\cdot\}^{-1}$ representing

$$\{z\}^{-1} = \begin{cases} 0, & \text{if } z=0 \\ \frac{1}{z}, & \text{if } z\neq 0 \end{cases} \tag{A4}$$

This mark is only used in Eq.(A3) to simplify the expression.

After the above derivation, we take a cutoff in n_1,n_2,m_1,m_2 and choose $h=m=l=1$ to calculate the elements of Hamiltonian matrix. The eigenenergies and eigenstates can be obtained after diagonalization of the Hamiltonian matrix. As the elements of Hamiltonian matrix are explicit, the error of the eigenenergies and eigenstates mainly arises from the cutoff of n_1,n_2,m_1,m_2.

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