Equilibration of quantum chaotic systems

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Quantum ergordic theorem for a large class of quantum systems was proved by von Neumann [Z. Phys. 57, 30 (1929)] and again by Reimann [Phys. Rev. Lett. 101, 190403 (2008)] in a more practical and well-defined form. However, it is not clear whether the theorem applies to quantum chaotic systems. With the rigorous proof still elusive, we illustrate and verify this theorem for quantum chaotic systems with examples. Our numerical results show that a quantum chaotic system with an initial low-entropy state will dynamically relax to a high-entropy state and reach equilibrium. The quantum equilibrium state reached after dynamical relaxation bears a remarkable resemblance to the classical micro-canonical ensemble. However, the fluctuations around equilibrium are distinct: the quantum fluctuations are exponential while the classical fluctuations are Gaussian.

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I. INTRODUCTION

Boltzmann pondered on how to understand thermodynamics with the Newton’s equations: his answer to this question along with Gibbs’ theory have become the foundation of classical statistical mechanics [1, 2]. After quantum mechanics been fully formulated, many giants in physics discussed a similar issue: how to understand thermodynamics with the Schrödinger equation [3, 4]. In a 1929 paper, von Neumann provided an answer to this question by proving two inequalities “in full rigor and without disorder assumptions” [5]. These two inequalities, which he called the quantum ergodic theorem and the quantum H-theorem, respectively, laid down a foundation for quantum statistical mechanics. However, this work has been largely forgotten and apparently have never been mentioned in any modern textbook on quantum statistical mechanics [1, 2]. There are discussions on why this work had almost been forgotten [6]. In our opinion, one of the likely reasons is that von Neumann introduced a rather unfamiliar concept, macroscopic operators, to prove his theorems. It appears very hard to compute these commuting macroscopic operators, and related variables such as an entropy defined for a pure quantum state [1].

Recently there have been renewed interests on the foundation of quantum statistical mechanics [6-41] perhaps due to the remarkable progress in experimental realization of coherent quantum systems [12-47]. An important result achieved is an inequality proved by Reimann [6, 7] and later modified by Short et al. [8, 9]. This inequality can be regarded as a different version of von Neumann’s quantum ergodic theorem. The advantage of this new inequality is that every variable involved is well known and can be computed. For this reason, when we discuss quantum ergodic theorem, we refer to the inequality proved by Reimann unless stated otherwise.

According to the quantum ergodic theorem, an isolated quantum system starting with a far-from-equilibrium state will relax dynamically to an equilibrium state and stay there with very small fluctuations for almost all the time. To be more specific, for an isolated quantum system described by the wave function $|\psi(t)\rangle$, it will relax to the following equilibrium state

$$\rho_\infty = \sum_k |c_k|^2 |E_k\rangle \langle E_k| ,$$

where $|E_k\rangle$ is the energy eigenstate of the system and $c_k$’s are the expansion coefficients of $|\psi(t)\rangle$ in term of these eigenstates. The density matrix $\rho_\infty$ is regarded as the micro-canonical ensemble by von Neumann [3]. It is different from the usual micro-canonical ensemble found in textbooks [1, 2], where the coefficients $c_k$’s take an identical value within a narrow energy shell. As $|c_k|^2$’s do not change with time, the micro-canonical density matrix $\rho_\infty$ is completely determined by the initial condition. By utilizing this fact and the supposition principle, we were able to predict a new quantum state which is at equilibrium with multiple temperatures, challenging the conventional wisdom that an equilibrium state has only one temperature [10].

The quantum ergodic theorem holds only for quantum systems with no degenerate energy gaps. Mathematically, this condition is expressed as [4, 6, 7]

$$E_k - E_l = E_m - E_n \Rightarrow \begin{cases} E_k = E_l \text{ and } E_m = E_n \text{ or} \\ E_k = E_m \text{ and } E_l = E_n \end{cases} .$$

However, it is not clear at all how this condition of non-degenerate energy gap is related to the familiar classification of quantum systems by their integrability. For a general integrable system, this condition is not satisfied as quantum integrable systems have the Poisson...
distribution of energy level spacing \[48\], which imply the existence of many degenerate eigen-energies. However, there are plenty of examples of integrable systems, which have no energy degeneracy at all. In fact, there are already reports of dynamical relaxation in integrable systems \[49\].

The case for quantum chaotic systems is more complicated. As is well known, quantum chaotic systems have the Wigner distribution of energy level spacing \[48\]. The Wigner distribution has two prominent features: zero probability at zero energy level spacing and a peak at a finite energy level spacing. The former feature means that there is little degeneracy, which is favorite for the condition \(\mathbb{2}\) being satisfied. The latter implies that there are large number of energy level spacings around the peak value, which is clearly unfavorable for the condition \(\mathbb{2}\) being satisfied. As a result, it is not clear at all in the sense of mathematical rigor whether the quantum ergodic theorem and H-theorem hold for quantum chaotic systems or not. We led by intuition tend to believe that the quantum ergodic theorem and H-theorem should hold for quantum chaotic systems. Von Neumann believed that his theorems should hold when the condition \(\mathbb{2}\) is violated by “infrequent exceptions” \[4\]. This belief is now confirmed by Short and Farrelly \[9\]. Despite this progress, it is still not clear how these mathematical conditions are related to the integrability of a system. The main purpose of this paper is to demonstrate that the quantum ergodic theorem applies to quantum chaotic systems numerically with examples.

In this paper we study two quantum chaotic systems, the ripple billiard \[11, 53\] and the Henon-Heiles system \[10, 54\]. Our numerical simulation shows that both systems will indeed dynamically relax to an equilibrium state where the overall features of the wave function no longer change. For the ripple billiard system, where the successive energy-eigenstates can be computed, the quantum ergodic inequality can be verified directly. In addition, we define entropies for pure quantum states in the spirit of von Neumann as it is not clear how to compute the entropy defined for a pure quantum state by him. We find that these entropies will approach maximized values, offering another indication that the system is indeed equilibrating dynamically.

We have also analyzed the properties of the equilibrium state reached after the dynamical relaxation in quantum chaotic systems. We find an interesting correspondence between the quantum equilibrium state and the classical micro-canonical ensemble. We discuss the underlying mechanism with the correspondence between the quantum and the classical Liouville equations. At the end, we consider the statistical properties of fluctuations in quantum chaotic systems and find a distinction between the distributions of quantum fluctuations and the classical fluctuations.

This paper is organized as follows. In Section II we introduce the two quantum chaotic systems, ripple billiard and Henon-Heiles system. In Section III we study the dynamical equilibration of quantum chaotic systems. In Section IV we numerically verify the quantum ergodic theorem in the ripple billiard system. In Section V we discuss the quantum-classical correspondence for the equilibrium states in detail. In Section VI we discuss the fluctuation properties of the quantum systems and their corresponding classical systems. Finally in Section VII we discuss the implications for many-body cases and summarize our results.

II. MODELS

We focus on single particle quantum chaotic systems. There are two main reasons for this choice. First, single particle quantum systems are much less challenging numerically and easier to analyze. Second, according to random matrix theory, the statistics of energy level spacings of quantum chaotic systems only depends on the type of matrix of the system when its Hamiltonian is expressed in an orthonormal basis \[48\]. This property has nothing to do with whether the system is single particle or many body. According to the condition \(\mathbb{2}\), the property of the eigen-energy spectrum is the most important factor determining whether the quantum system will equilibrate or not. There are properties that exist only in many-body systems, for example, the correlations \[51\]. So far, no one has shown that the correlation plays any essential role in the equilibration process. We also emphasize that we here consider isolated quantum systems and do not consider the dynamics of quantum systems under external driving \[52\]. It is well known that a classical system will behave very differently under different driving. This feature seems to be shared by quantum systems \[52\].

A single particle in a two-dimensional chaotic potential is described by the Hamiltonian

\[
H = p^2 / 2m + V(x, y). \tag{3}
\]

We choose the Henon-Heiles potential \[54\] and the rip-
ple billiard as a two examples for our study. The Henon-Heiles potential is given by \( V(x, y) = \frac{1}{2}(x^2 + y^2) + \lambda(x^2 y - \frac{y^3}{3}) \). The energy contour of Henon-Heiles potential is shown in Fig. 1(a) it has four special points: one stable point \( O(0,0) \), three saddle points \( A(0,r_c), B(-\frac{\sqrt{3}}{2}r_c, -\frac{1}{2}r_c) \), \( C(\frac{\sqrt{3}}{2}r_c, -\frac{1}{2}r_c) \), where \( r_c \equiv 4 \). The classical orbits in the Henon-Heiles potential are chaotic when the energy is above \( V_c/2 \) and approach fully chaotic when the energy is close to \( V_c \) with \( V_c \equiv \frac{1}{6}\lambda \). For later use, we set \( p_0 = \sqrt{2mV_c} \).

Billiard systems are a two dimensional area surrounded by infinite potential walls at the edges. For the ripple billiard, as shown in Fig. 1(b) the left and right edges are described by functions \( x = \mp|b - a\cos(\pi y/b)| \) and the up and down edges are two straight lines at \( y = 2b \) and \( y = 0 \). The two geometrical parameters \( a, b \) control the shape of the billiard. When \( a = 0 \) the ripple billiard is a square with width \( 2b \). As \( a \) increases from zero, it changes from an integrable system to a mixed, then to a fully chaotic system. It becomes mixed again when \( a \) becomes very large. We have chosen for our computation \( a = 6, b = 15 \), which corresponds to a fully chaotic case.

The two systems are chosen because each of them has its own advantages. For the ripple billiard system, its successive eigenstates from the ground state up to the 3000th excited state can be computed numerically with great precision. To the best of our knowledge, for all other studied quantum chaotic systems, the high-energy eigenstates can only be computed selectively. The famous Henon-Heiles system is chosen to bring our study beyond what is considered by von Neumann and others as a pure quantum state and proved that this entropy will increase at a very slow rate.

### III. DYNAMICAL EQUILIBRATIONAL

We numerically study the wave packet dynamics with the Schrödinger equation for these two systems. In our numerical simulation we set \( m = \frac{1}{2}, \hbar = 1 \). The initial states are highly localized moving Gaussian wave packet for both systems,

\[
\psi(\vec{r}, t = 0) = \frac{\alpha}{\sqrt{\pi}} \exp(-\frac{1}{2}r_0^2(\vec{r} - \vec{r}_i)^2) \exp(i\vec{p}_0 \cdot \vec{r}/\hbar) \tag{4}
\]

with \( 1/\alpha = 3r_c/40, \vec{r}_i = (0,3,0)r_c, \) and \( \vec{p}_0 = \sqrt{3r_0}(\cos 10^\circ, \sin 10^\circ) p_0 \) for the Henon-Heiles system; \( 1/\alpha = a/6, \vec{r}_i = (0,0), \) and \( \vec{p}_i = (5,0) \) for the ripple billiard system. In both systems, a classical particle with the above initial position \( \vec{r}_i \) and momentum \( \vec{p}_i \) has a fully chaotic orbit, which we confirmed by computing the Poincare section.

The subsequent dynamical evolutions of these two Gaussian wave packets are computed. For the ripple billiard, the dynamical evolution can be found in Ref. 11; for the Henon-Heiles system, the evolution is illustrated in Ref. 11. Both evolutions are very similar to each other. Here is a brief description: the smooth Gaussian wave packet starts to spread out and gets diffracted by the potentials; the interference between diffracted waves begins to make the wave packet appear more and more irregular; eventually the wave packet spreads out over the classically allowed region rather uniformly with small speckles. This overall feature will no longer change, signaling that the system has dynamically equilibrated.

To illustrate this dynamical equilibration process, we compute how the expectation of momentum changes with time for the ripple billiard system. The results for both \( p_x \) and \( p_y \) are shown in Fig. 2, where the momenta are seen to relax to equilibrium values after a short period of large fluctuations.

Equilibration should be accompanied by a maximizing entropy. Von Neumann was able to define an entropy for a pure quantum state and proved that this entropy will stay very close to its ensemble entropy almost all the time (the quantum H-theorem) 11. However, there appears no viable procedure which one can use to compute this version of von Neumann entropy. As an alternative, we define an entropy in the spirit of von Neumann,

\[
S_r = - \int \frac{|\psi(x,y,t)|^2}{|\psi(x,y)|^2} \ln \frac{|\psi(x,y,t)|^2}{|\psi(x,y)|^2} dx dy, \tag{5}
\]

where \( |\psi(x,y)|^2 \) is the long time average of
FIG. 3: Time evolutions of entropy in (a) Henon-Heiles system; (b) ripple billiard.

\[ |\psi(x, y, t)|^2 \leq 10. \] As shown in Fig. 3, the entropy will increase with time with small fluctuations and eventually saturate to a maximized value. The increasing entropies in Fig. 3 can be regarded as a “spiritual” illustration of von Neumann’s quantum H-theorem.

In summary, we have observed numerically that dynamical equilibration indeed occurs in both the Henon-Heiles system and the ripple billiard: an initially localized Gaussian wave packet with low entropy will dynamically evolve into a quantum state with a maximized entropy, where the wave packet spreads out and looks irregular with speckles. This is clearly consistent with both the quantum ergodic theorem and quantum H-theorem. It is reasonable to expect that this kind of dynamical equilibration occurs in any quantum chaotic system. Meanwhile we note that the equilibration process for the Henon-Heiles system deserves more detailed study in the future. As noted before, the Henon-Heiles system has no bound states. As a result, a Gaussian wave packet will eventually leak out and spread out in the whole space, not confined to just the triangle area, beyond the tunneling time. In our numerical simulation, the equilibration time is clearly much shorter than the tunneling time. It would be very interesting to investigate in which situations where the equilibration time becomes shorter than the tunneling time. It might also be worthwhile to formulate mathematically the ergodic theorem for this kind of systems.

IV. VERIFICATION OF QUANTUM ERGODIC THEOREM

The mathematical expression of the quantum ergodic theorem is an inequality. For an arbitrary operator \( A \), this inequality reads [6, 8, 9]

\[
\sigma_A^2 = \left\langle \langle A | \psi(t) \rangle \langle \psi(t) \rangle \right\rangle_t - \left\langle \langle A | \rho_\infty \rangle \right\rangle_t^2, \leq \frac{1}{d_{\text{eff}}}, \tag{6}
\]

where \( d_{\text{eff}} \equiv 1/\sum_k |a_k|^4 \) measures effectively how many energy eigenstates are occupied in the state \( |\psi\rangle \). The subscript \( t \) in \( \langle \cdot \rangle_t \) indicates a long time averaging. We emphasize that this inequality is much stronger than the following approximation

\[
\left\langle \langle \text{tr}(A | \psi(t) \rangle \langle \psi(t) \rangle) \right\rangle_t \approx \text{tr}(A \rho_\infty), \tag{7}
\]

which can be readily proved for any quantum systems with no energy degeneracy. The above approximation can still be true even when \( \text{tr}(A | \psi(t) \rangle \langle \psi(t) \rangle) \) fluctuate greatly from \( \text{tr}(A \rho_\infty) \) as long as the positive large fluctuations cancel out the negative large fluctuations. However, the fluctuations cannot cancel each other in the inequality [10]; this means that the inequality [6] dictates that the fluctuations are very small most of the time when \( d_{\text{eff}} \gg 1 \). So, the approximation relation [7] coupled with the inequality [6] shows that the long time averaging is equivalent to ensemble averaging, essence of ergodicity, in all quantum systems that satisfy the condition [6].

To test numerically the inequality [6], one needs to compute the energy eigenstates \( |E_k\rangle \) successively up to a high energy value and find the expansion coefficients \( c_k \). We are able to do it for the ripple billiard system. The expansion coefficients of the initial state Eq. 4 are computed and shown in Fig. 4, where \( c_k \)'s are grouped according the symmetry of the eigenstates. Both groups peak around 500th eigenstates and have a width around 300. With the computed \( c_k \)'s, we find that the effective dimension \( d_{\text{eff}} \) is around 300, satisfying the condition \( d_{\text{eff}} \gg 1 \).

Without loss of generality, we choose to compute the left hand side (l.h.s.) of the inequality Eq. 6 for momentum operator \( \vec{P} = (p_x, p_y) \). By using the symmetry of the eigenstates, one can readily show exactly that \( \text{tr}(\rho_\infty \hat{p}_x) = 0 \) and \( \text{tr}(\rho_\infty \hat{p}_y) = 0 \). The time evolution of momentum is already shown in Fig. 2. We calculate the long time average between \( T = 10 T_s \) and \( t = 14 T_s \). The time unit \( T_s \equiv \frac{2(a+b)}{|p_i|/m} \) is the period of the motion of a classical particle with the same initial momentum and position. We find that \( \text{tr}(\hat{p}_x | \psi(t) \rangle \langle \psi(t) | \hat{p}_x \rangle) \simeq 0.0021 \) and \( \text{tr}(\hat{p}_y | \psi(t) \rangle \langle \psi(t) | \hat{p}_y \rangle) \simeq -0.0033 \), very close to the ensemble average \( \text{tr}(\rho_\infty \hat{p}_x) = 0 \) and \( \text{tr}(\rho_\infty \hat{p}_y) = 0 \), respectively. At the same time, we find that

\[
\langle \text{tr}(\vec{P} | \psi(t) \rangle \langle \psi(t) | \vec{P} \rangle) \rangle_t \approx 0.0039. \tag{8}
\]

For operator \( \vec{P} \), the maximum value \( \langle \vec{P} \rangle^2 = \sup \{|\psi\rangle | P | \psi \rangle \} \). Since we have chosen \( m = 1/2 \) and the wave function is only none zero inside the billiard, we have \( \langle \vec{P} \rangle^2 = \sup \{|\psi\rangle | H | \psi \rangle \} \), that is, \( \langle \vec{P} \rangle^2 \) is effectively the largest energy in the occupied Hilbert space. According to Fig. 4 the occupied Hilbert space is roughly spanned by the eigenstates between the 100th even-even(odd-even) eigenstates and the 1000th even-even(odd-even) eigenstates. The upper bound can be estimated as the eigenvalue of the 1000th even-even(odd-even) eigenstates, i.e. \( \langle \vec{P} \rangle^2 \simeq 55.64 \). So, the relative...
fluctuation or the l.h.s. of Eq. (6) is $\sigma_p^2 \approx 7 \times 10^{-5}$. As $1/d_{\text{eff}} \approx 3 \times 10^{-3}$, we see that the inequality (6) is clearly satisfied. Moreover, our computation in fact shows that it is possible to improve the inequality, for example, replacing $C$ by $\frac{2}{\sigma_p^2}$.

Before we proceed further, we want to mention that the inequality for quantum ergodicity proved by von Neumann [4] has a different upper bound on the r.h.s. However, his theoretical formalism relies on the introduction of macroscopic operators (such as macroscopic position and momentum) that commute with each other. It appears not be a straightforward task to construct these macroscopic operators and compute them numerically. As a result, we did not compute von Neumann’s upper bound.

V. QUANTUM-CLASSICAL CORRESPONDENCE AT EQUILIBRIUM

According to the quantum ergodic theorem, the equilibrium state is described by the density matrix $\rho_\infty$, which can be regarded as the quantum micro-canonical ensemble. We analyze this quantum equilibrium state and find that it possesses many features that resemble the classical micro-canonical ensemble. This kind of quantum-classical correspondence has been studied and found in a spin system [59, 60]. To illustrate this quantum-classical correspondence, we compare $\rho_\infty$ in both the real space and the momentum space with the classical micro-canonical ensemble

$$\rho_c = \frac{1}{\Omega} \delta(H(\vec{p}, \vec{r}) - E)$$

where $\Omega$ is the normalization factor and $H(\vec{p}, \vec{r})$ is the corresponding classical Hamiltonian of the fully chaotic system. Here we choose the Henon-Heiles system to analyze because its probability distribution in phase space is more general than the billiard system where $|\vec{p}|$ is a constant of motion. For the quantum results, we calculate $n_\infty(\vec{r}) = \langle \vec{r} | \rho_\infty | \vec{r} \rangle$ and $n_\infty(\vec{p}) = \langle \vec{p} | \rho_\infty | \vec{p} \rangle$ by long-time averaging; For the classical results, we calculate the probability distribution in real space and momentum space $n_c(\vec{r})$ and $n_c(\vec{p})$ from the micro-canonical ensemble $\rho_c(\vec{r}, \vec{p})$ by integration over $\vec{p}$ and $\vec{r}$ separately.

For better comparison, we choose the following marginal distribution without loss of generality: for the real space, we integrate out the $y$ dimension to obtain the density distribution $P(x)$; for the momentum space, we integrate out the angle variable to find the momentum distribution $f(p)$. The results are shown in Fig. 5(a) where we see the quantum and classical distributions are consistent, except for some quantum tunneling effect indicated by the non-zero value of the quantum distribution in the classically forbidden region.

This correspondence also exists in phase space. In quantum mechanics, the uncertainty relation does not allow the construction of a phase space in principle. However, a kind of quasi-quantum distribution in phase space can be constructed with the Husimi function $H_{\vec{r}, \vec{p}}$. This is to calculate the projection of the density operator on a Gaussian wave packet $\langle \vec{r}' | \vec{r}, \vec{p} \rangle = C \exp\left(-\frac{(\vec{r}' - \vec{r})^2}{2\sigma^2} + \frac{i\vec{p} \cdot (\vec{r}' - \vec{r})}{\hbar}\right)$ centered around position $\vec{r}'$ and momentum $\vec{p}$

$$H_{\vec{r}, \vec{p}} \equiv \langle \vec{r}', \vec{p} | \rho | \vec{r}, \vec{p} \rangle .$$

The Husimi function can be understood as coarse grained phase space density with parameter $\sigma$ controlling the coarse graining. We have computed the Husimi function $H_{\vec{r}, \vec{p}}$ for a density matrix $\rho \equiv |\psi\rangle \langle \psi|$ at $t = 0.2126$ (which is after equilibration) and compared it to the classical ensemble $\rho_c$. For easy illustration, we use a 2-dimensional section in the 4-dimensional phase space of the Henon-Heiles system. Without loss of generality, we choose the section at $y = 0, p_y = 0$ and the results are plotted in Fig. 5(b). We can see that the Husimi function centers around the phase space where the classical density is non-zero, indicating the quantum-classical correspondence. Note that the quantum fluctuations in the phase space are much larger than the ones seen in Fig. 5(a). The reason is that the results in Fig. 5(a) are obtained after being averaged over time and integrated over a given dimension.

One possible understanding for this correspondence is through the quantum and classical Liouville equations. Intuitively, one can think of the quantum wave-packet as an ensemble of particles with equivalent classical probability density in the phase space [61, 62]. The time evolution of quantum density matrix operator $\rho(t)$ is governed by the quantum Liouville equation, $\partial_t \rho(t) = \frac{i}{\hbar} [H, \rho(t)]$; the time evolution of the classical probability density $\rho_c(t)$ is governed by the classical Liouville equation, $\partial_t \rho_c(t) = \{H, \rho_c(t)\}_{PB}$. These two time evolution equations have an identical algebraic structure, implying a
possible quantum-classical correspondence in the equilibrium states. Moreover, there are numerical evidences for this correspondence in the studying of the time evolution of the ensemble average and quantum expectation value [61, 62]. Note that this quantum-classical correspondence is not implied in the quantum ergodic theorem [4, 6–9].

We emphasize here that the quantum-classical correspondence discussed so far needs to be understood in the sense of typicality [19–21, 24, 63]. As dictated by the quantum ergodic theorem, the equilibrium state is completely determined by the initial expansion coefficient \(|dy| c_k|^2\). For a typical initial state, \(|dy| c_k|^2\) should have a distribution similar to what is shown in Fig. 4 with a large effective dimension \(d_{\text{eff}}\). For these states, we expect that the quantum-classical correspondence hold. However, for many atypical states, this quantum-classical correspondence may not hold. For example, the ergodic inequality [8] holds for an energy eigenstate; but energy eigenstate does not belong to the typicality class. Here we use the ripple billiard to illustrate this point as the energy eigenstates in this system can be computed successively [11, 63]. We study the position space marginal distribution \(f(y) = \int \frac{d^2r}{2\pi} |\langle r| \rho | r\rangle|^2 dx\), and compare it with the classical result \((b - a \cos(2\pi y/L))/bL\). We compute \(f(y)\) first for the equilibrium state \(\rho(t \gg T_\text{c})\). We see in Fig. 6(a) that the quantum result (black line) are in good agreement with the classical result (red line). For completeness, we also show the density \(\langle \vec{r} | \rho | \vec{r}\rangle\) in Fig. 6(b).

For eigenstates, we choose to study the eigenstates that have relatively large expansion coefficients \(|dy| c_k|^2\) in the initial wave packet [4]. We find that the results for them are similar. Without loss of generality, we choose the 493rd even-even eigenstate with coefficient \(|dy| c_k|^2 = 0.0086\).

FIG. 5: (a) Comparison between quantum and classical equilibrium distributions in the Henon-Heiles system. \(P(x)\) is for the real space and \(f(p)\) for momentum space. The unit for \(x\) is \(r_c\) and the unit for \(p\) is \(p_0\). (b) Section of the Husimi function \(H_{r,p} \equiv \langle \vec{r}, \vec{p}|\rho(t)|\vec{r}, \vec{p}\rangle\) in the Henon-Heiles system at \(t = 0.2126\). The red circle is the section of the classical phase space density \(\rho_c(\vec{r}, \vec{p})\). The section is at \(y = 0, p_y = 0\). The unit for \(x\) is \(r_c\) and the unit for \(p_x\) is \(p_0\). The coarse-graining parameter for the Husimi function \(\sigma \simeq 0.11r_c\).

FIG. 6: (a) Marginal distributions \(f(y) \int n(\vec{r}) dx\) for the equilibrium state in the ripple billiard system. The black line is for the quantum result while the red line is for the classical result. (b) The density distribution \(n(\vec{r})\) of the equilibration state in the ripple billiard system. (c) Marginal distribution \(f(y)\) for the 493rd even-even eigenstate in ripple billiard system. (d) Density distribution \(n(x, y)\) of the 493rd even-even eigenstate. For this eigenstate, the expansion coefficient \(|dy| c_k|^2 = 0.0086\) in the initial Gaussian wave packet [4].

the example. The marginal distribution \(f(y)\) for this eigenstate is shown in Fig. 6(c). Compared with the result for the equilibrium state in Fig. 6(a) we see a clear
where the probability density and phases behave like the potential wall bring the wave function to a state strictly with the Schrödinger equation, the scattering by tem. Though the system is deterministic and evolves domness of wave function in a quantum chaotic sys-

VI. FLUCTUATION PROPERTY

While the equilibrium density operator \( \rho_\infty \) shares a good correspondence with the classical microcanonical ensemble \( \rho_c \), the operator \( \rho(t) \) does fluctuate around the equilibrium density operator, as shown in Fig. 6(b). This fluctuation has been shown to obey the exponential distribution in the ripple billiard system [11]. Here we focus on the Henon-Heiles system to bring this exponential distribution beyond billiard systems. To quantitatively show the fluctuation, we compare the probability density in both the real space and the momentum space, i.e. we compare \( n(\xi) \equiv \langle \xi|\rho(t)|\xi \rangle \) with \( n_\infty(\xi) \), \( \xi = \vec{r}, \vec{p} \).

Numerically this is realized by calculating the density \( n(\xi_i) \) and \( n_\infty(\xi_i)(i = 1, \ldots, N) \) of \( N \) small discrete region and calculate the distribution of the relative fluctuation \( n(\xi_i)/n_\infty(\xi_i) \). Due to limited numerical precision, we choose different \( N \) in the real space and momentum space and the results are shown in Fig. 7(a, b). Both distributions are found to be well fitted by exponential distribution. Due to the different \( N \), the coefficients of the fitted exponential distributions are different in the real space and the momentum space.

This exponential distribution results from the randomness of wave function in a quantum chaotic system. Though the system is deterministic and evolves strictly with the Schrödinger equation, the scattering by the potential wall bring the wave function to a state where the probability density and phases behave like random numbers. Here we demonstrate the randomness by computing the phase of the wave function and the normalized probability density correlation function \( C(r) = \frac{1}{\Delta \tau} \langle (n(0) - \bar{n})(n(r) - \bar{n}) \rangle \) in the real space after equilibrium in the Henon-Heiles system. The results are shown in Fig. 7(c, d). We see that the phases vary rapidly in real space and the spatial correlation in real space decreases exponentially to zero within small distance compared to the characteristic length scale \( r_c \). These features indicate certain randomness in the behavior of wave function in quantum chaotic systems. With this established randomness, the proof in Ref. [11] with
slight modification, can explain this exponential distribution (see also the Appendix). Note that this randomness of wave function in quantum chaotic system is consistent with the idea of typicality \cite{21}. It also supports, though not directly, the assumption we made in Eq. (2) and Eq. (3) in our previously work \cite{10}.

This exponential fluctuation is a pure quantum phenomenon. To show the quantum nature we consider the classical correspondence of an ensemble of particles obeying the same initial Gaussian distribution of position and momentum and calculate their time evolution.

The exponential distribution only exists for a complex particle quantum chaotic systems. We have re-derived these two distributions within the same mathematical framework in the Appendix.

VII. DISCUSSION AND SUMMARY

In summary, we have studied equilibration of quantum chaotic systems in the framework suggested by von Neumann in 1929. Our study has examined various aspects of this issue, such as dynamical equilibration, quantum-classical correspondence between quantum equilibrium density operator $\rho_\infty$ and classical microcanonical ensemble $\rho_c$, and the relative fluctuations around the equilibrium state. All the results are illustrated with two single particle quantum chaotic systems. We expect most of the results to hold in many-body quantum chaotic systems.

The dynamical equilibration should hold in many-body quantum chaotic systems because it is completely determined by the energy gap statistics, which is universal for all quantum chaotic systems. The quantum-classical correspondence should also hold as it apparently originates from the similarity between quantum and classical Liouville equations.

However, the fluctuation properties in a many-body system will generally have Gaussian form, different from the single-particle case. The only except might be a Bose-Einstein condensate or a superconductor where the many-body system can be described by a single-variable wave function. In all other cases, the probability density at a given point $\xi = \vec{r}, \vec{p}$ can be expressed by

$$ n(\xi) = \int d\xi_2 \cdots d\xi_N \ n(\xi_1, \xi_2 \cdots, \xi_N), \hspace{1cm} (11) $$

where $N$ is the number of particles in this system. The fluctuation in $n(\xi_1, \xi_2 \cdots, \xi_N)$ should have the exponential distribution due to the quantum chaotic nature of the many-body system. The integration over $N - 1$ variables will produce a Gaussian distribution due to the central limit theorem.

We note that one has to use many-body systems to discuss the canonical statistics for a subsystem of the large isolated system. However, one can use the correspondence between $\rho_\infty$ and $\rho_c$ illustrated here with single-particle systems to show that a subsystem of the many-body system will behave in canonical ensemble statistics. The derivation is similar to the work by Srednicki \cite{16} and here we do not discuss further.

Although von Neumann has laid down the basic theoretical framework for the dynamical equilibration in quantum systems in 1929 \cite{4}, we believe that the study of this fundamental issue has just started and many basic questions are still wait to be answered. Our study here and other related studies \cite{19, 50} have indicated that the quantum ergodic theorem hold for a class of quantum systems larger than what is specified by the condition \cite{2}. It is imperative to know how to relax the condition \cite{2} mathematically. We are also not clear about the properties of the entropy defined for a pure state by von Neumann. We believe that these studies will not only lead to a better perspective on the foundation of quantum statistical mechanics but also produce new physics such as the quantum multi-temperature equilibrium state predicted in Ref. \cite{10} by us.

Acknowledgments

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[1] K. Huang, *Statistical Mechanics*, page 176. John Wiley & Sons, Inc., 2 edition (1987).

[2] L. D. Landau and E. M. Lifshitz, *Statistical Mechanics*
metry requirements. This assumption follows naturally from our numerical observations(Fig. (c), (d)) and the spirit of random matrix theory, and was used by Berry in his study of eigen-wave functions in chaotic systems It is important to note the difference between equilibrium wave functions and eigenstates wave functions is that equilibrium wave functions are generally complex and eigenstates wave functions are real up to an overall phase for systems with time reversal symmetry. This key difference leads to the different distributions. For simplicity we restrict our derivation for real space wave functions in chaotic billiards. Extension to other systems and momentum space can be achieved (however, without strict mathematical rigorousness) by renormalizing densities with averaged values.

For a wave function \( \psi \), we discretize the system area into \( N \) equal infinitesimal pieces with their centers located at \( r_i, i = 1, \cdots, N \) and denote \( \alpha_i = \psi(r_i) \sqrt{A/N} \), where \( A \) is the total area of the system. It follows from normalization that \( \sum_{i=1}^{N} |\alpha_i|^2 = 1 \). The notation here is the same with Ref. \[1\]. For a complex wave function in dynamical evolution \( \alpha_0 \) is complex; for an eigenfunction \( \alpha_i \) is real. In the following we derive the distribution of \( |\alpha_j|^2 \) for both cases.

Note that the following proof is given without consideration of the discrete symmetries: (1) reflection symmetry initial state(Eqn. \[1\]) in ripple billiard system; (2) reflection symmetries in eigenstates of ripple billiard system, and (3) the reflection symmetries in eigenstates of Henon-Heiles system. This is because these symmetries can be treated by simply assuming full randomness of a wave function in a smaller area while changing the normalization, respectively, by 1/2(Eq. \[1\]), 1/4 (ripple billiard), or 1/6(Henon-Heiles).

1. Proof of exponential distribution of equilibrium wave function \[1\]

Consider \( N \) complex numbers \( \alpha_i \) that satisfies normalization condition \( \sum_{i=1}^{N} |\alpha_i|^2 = 1 \) and each complex number is equivalent to another. Suppose the \( N \) complex numbers are fully random subject to the normalization condition. This implies that each state \( \{\alpha_1, \alpha_2, \cdots, \alpha_N\} \) is of equal possibility on the hypersphere \( \sum_{i=1}^{N} |\alpha_i|^2 = 1 \). So the distribution of the amplitude of one complex number \( \alpha_j \) at \( |\alpha_j|^2 = \gamma \) is

\[
P(\gamma) = \frac{d^2\alpha_1 \cdots d^2\alpha_N \delta(\gamma - |\alpha_j|^2) \delta(1 - \sum_{i=1}^{N} |\alpha_i|^2)}{d^2\alpha_1 \cdots d^2\alpha_N \delta(1 - \sum_{i=1}^{N} |\alpha_i|^2)} \tag{A.1}
\]

Let \( x = |\alpha_j|^2 \). The denominator equals the surface area of \( 2N \)-dimensional hypersphere. The numerator includes a factor of a \( (2N - 2) \)-dimensional hypersphere with radius \( \sqrt{1-x} \). Recall the \( 2N \)-dimensional hypersphere of radius \( R \) has an area of \( S_{2N}(R) = \frac{2\pi^N}{N!} R^{2N-1} \). We have

\[
P(\gamma) = \frac{\int_0^\infty \pi dx \delta(x - \gamma) \frac{2\pi^{N-1}}{N!} (1-x)^{2N-3}}{2\pi^N \Gamma(N)} = (N-1)(1-\gamma)^{N-3/2} \tag{A.2}
\]

Let \( \gamma = \frac{4}{N} n(\vec{r}) \), where \( n(\vec{r}) = |\psi(\vec{r})|^2 \) is the probability density at \( \vec{r} \). We find that

\[
p(n(\vec{r}))dn(\vec{r}) = \lim_{N \to \infty} \frac{A}{N} P(\gamma)dn \lim_{N \to \infty} \frac{A}{N} (N-1)[1 - \frac{A}{N} n(\vec{r})]^N (1 - \frac{A}{N} n(\vec{r}))^{-3/2}dn(\vec{r}) = Ae^{-An(\vec{r})}dn(\vec{r}) \tag{A.3}
\]

We have thus shown that the distribution is exponential. For a billiard system, the averaged density \( n_0 = 1/A \). Therefore, we have

\[
p(n) = e^{-n/n_0}/n_0 \tag{A.4}
\]

2. Proof of Porter-Thomas distribution of eigenstate wave function

For an eigenstate wave function, everything is the same except that all the \( \alpha_i \) are real rather than complex. So, we have \( \sum_{i=1}^{N} \alpha_i^2 = 1 \), and similarly the distribution becomes

\[
P(\gamma) = \frac{\int d\alpha_1 \cdots d\alpha_N \delta(\gamma - \alpha^2) \delta(1 - \sum_{i=1}^{N} \alpha_i^2)}{d\alpha_1 \cdots d\alpha_N \delta(1 - \sum_{i=1}^{N} \alpha_i^2)} \tag{A.5}
\]

Let \( \alpha_i^2 = x \). The denominator equals the area of the \( N \)-dimensional hypersphere with unit radius. The numerator includes a factor of a \( (N-1) \)-dimensional hypersphere with radius \( \sqrt{1-x} \). This leads to

\[
P(\gamma) = \frac{\int_0^\infty dx x^{-1/2} \delta(\gamma - x) \frac{\pi^{(N-1)/2}}{\Gamma((N-1)/2)} (1-x)^{-N-2}}{2\pi^{N/2} \Gamma(N/2)} = \sqrt{\frac{\Gamma(1-\gamma)^{N-2}}{\Gamma((N-1)/2)}} \tag{A.6}
\]

With \( \gamma = \frac{4}{N} n(\vec{r}) \), we arrive at the Porter-Thomas distribution in the limit of large \( N \),

\[
p(n) = \sqrt{\frac{A}{2\pi n}} e^{-\frac{4n}{2\pi}} \tag{A.7}
\]
where we have used \( \lim_{N \to \infty} \frac{\Gamma(N/2)}{\Gamma((N-1)/2) \sqrt{N}} = \frac{1}{\sqrt{2}} \).