

Equilibration of quantum chaotic systems

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(Received 20 August 2013; revised manuscript received 13 November 2013; published 27 December 2013)

The quantum ergodic 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 a 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 microcanonical ensemble. However, the fluctuations around equilibrium are distinct: The quantum fluctuations are exponential while the classical fluctuations are Gaussian.

DOI: [10.1103/PhysRevE.88.062147](https://doi.org/10.1103/PhysRevE.88.062147)

PACS number(s): 05.30.-d, 05.45.Mt, 03.65.-w

I. INTRODUCTION

Boltzmann pondered on how to understand thermodynamics with 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 was 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" [4]. 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 has never been mentioned in any modern textbook on quantum statistical mechanics [1,2]. There are discussions on why this work has almost been forgotten [5]. 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 [4].

Recently, there has been renewed interest in the foundation of quantum statistical mechanics [6–41], perhaps due to the remarkable progress in experimental realization of coherent quantum systems [42–47]. 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 of the time. To be more specific, for an isolated quantum system described by the wave function $|\psi(t)\rangle$, it will relax to an equilibrium state

$$\rho_\infty = \sum_k |c_k|^2 |E_k\rangle \langle E_k|, \quad (1)$$

where $|E_k\rangle$ is the energy eigenstate of the system and c_k 's are the expansion coefficients of $|\psi(t)\rangle$ in terms of these eigenstates. The density matrix ρ_∞ is regarded as the microcanonical ensemble by von Neumann [4]. It is different from the usual microcanonical ensemble found in textbooks [1,2], where the coefficients c_k 's take an identical value within a narrow energy shell. As $|c_k|$'s do not change with time, the microcanonical density matrix ρ_∞ 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]

$$E_k - E_l = E_m - E_n \Rightarrow \begin{cases} E_k = E_l & \text{and} & E_m = E_n, \\ & \text{or} & \\ E_k = E_m & \text{and} & E_l = E_n. \end{cases} \quad (2)$$

However, it is not clear at all how this condition of nondegenerate 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 [49,50].

The case for quantum chaotic systems is more complicated. As is well known, quantum chaotic systems have the Wigner

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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 the favorite for condition (2) being satisfied. The latter implies that there are a large number of energy level spacings around the peak value, which is clearly not the favorite for condition (2) being satisfied. As a result, it is not clear at all, in the sense of mathematical rigor, whether the quantum ergodic theorem and the H theorem hold for quantum chaotic systems or not. We led by intuition tend to believe that the quantum ergodic theorem and the H theorem should hold for quantum chaotic systems. Von Neumann believed that his theorems should hold when condition (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 system [11,51] and the Henon-Heiles system [10,52]. 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 microcanonical 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 Sec. II we introduce the two quantum chaotic systems, ripple billiard and Henon-Heiles. In Sec. III we study the dynamical equilibration of quantum chaotic systems. In Sec. IV we numerically verify the quantum ergodic theorem in the ripple billiard system. In Sec. V we discuss the quantum-classical correspondence for the equilibrium states in detail. In Sec. VI we discuss the fluctuation properties of the quantum systems and their corresponding classical systems. Finally, in Sec. 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,

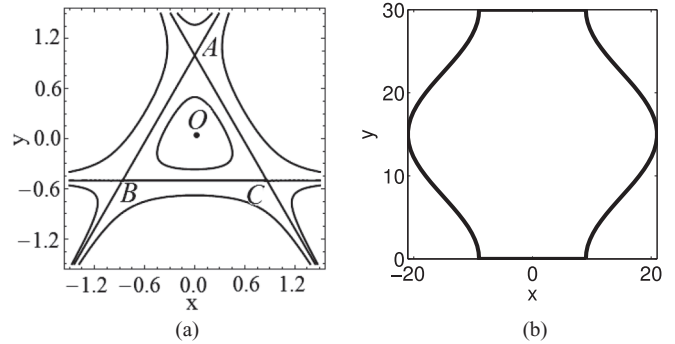


FIG. 1. (a) Energy contours of the Henon-Heiles potential $V(x,y)$. The thick solid lines are the contours for $V/V_c = 1/2, 1, 2$, from inside to outside. The unit of axis is r_c . A, B, and C are three saddle points and O is the stable point. (b) The shape of a ripple billiard system.

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 condition (2), the property of the eigenenergy 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 [53]. 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 [54]. It is well known that a classical system will behave very differently under different drivings. This feature seems to be shared by quantum systems [54].

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 [52] and the ripple billiard system [51] as two examples for our study. The Henon-Heiles potential is given by $V(x,y) = \frac{U}{2}(x^2 + y^2) + \lambda(x^2y - \frac{y^3}{3})$. The energy contour of Henon-Heiles potential is shown in Fig. 1(a); it has four special points: one stable point O (0,0) and 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 $r_c \equiv \frac{U}{\lambda}$. 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 $V_c \equiv \frac{U^3}{6\lambda^2}$. For later use, we set $p_0 = \sqrt{2mV_c}$.

Billiard systems are a two-dimensional areas surrounded by infinite potential walls at the edges. For the ripple billiard system [51], 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 system 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 [51]. To the best of our knowledge, for all other studied quantum chaotic systems, the high-energy eigenstates can only be computed selectively [55]. The famous Henon-Heiles system is chosen to bring our study beyond billiards where $|p|$ is a constant of motion, allowing us to gain more insights into general systems. In addition, we note that the Henon-Heiles system is beyond what is considered by von Neumann and others as it has no bound eigenstates mathematically. However, its resonant states can be regarded as bound states in our numerical studies, where the dynamical evolution lasts for a finite time and hard-wall boundaries are imposed at a distance [56].

III. DYNAMICAL EQUILIBRATION

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,

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

with $1/\alpha = 3r_c/40$, $\vec{r}_i = (0.3, 0)r_c$, and $\vec{p}_i = \sqrt{7/10}(\cos 10^\circ, \sin 10^\circ)p_0$ 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 system, the dynamical evolution can be found in Ref. [11]; for the Henon-Heiles system, the evolution is illustrated in Ref. [10]. Both evolutions are very similar to each other. Following 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) [4]. However, there appears to be 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

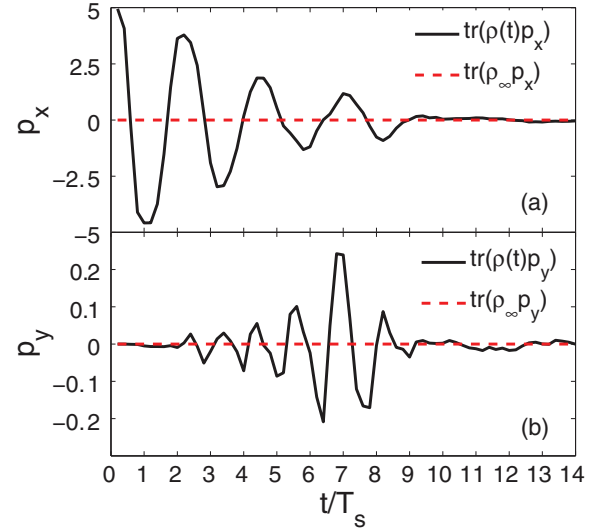


FIG. 2. (Color online) Time evolution of (a) $\langle \psi | P_x | \psi \rangle$ and (b) $\langle \psi | P_y | \psi \rangle$ in the ripple billiard system. The red lines are $\text{tr}(\rho_\infty P_x)$ and $\text{tr}(\rho_\infty P_y)$. The initial condition of \vec{P} is $(5, 0)$. $T_s \equiv \frac{2(a+b)}{|p_i|/m}$.

von Neumann,

$$S_r = - \int \frac{|\psi(x, y, t)|^2}{|\psi_\infty(x, y)|^2} \ln \frac{|\psi(x, y, t)|^2}{|\psi_\infty(x, y)|^2} dx dy, \quad (5)$$

where $|\psi_\infty(x, y)|$ is the long-time average of $|\psi(x, y, t)|^2$ [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 heuristic 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 system: 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 the 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

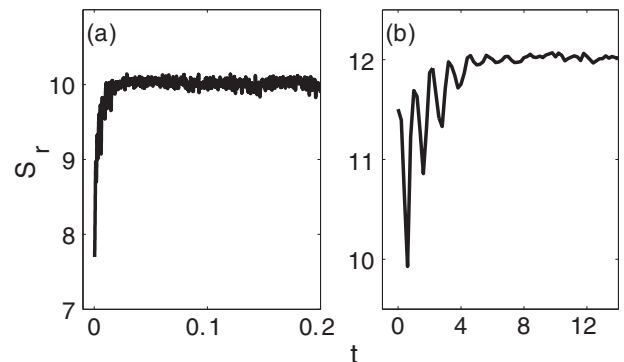


FIG. 3. Time evolutions of entropy in (a) the Henon-Heiles system and (b) the ripple billiard system.

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 these 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]

$$\sigma_A^2 \equiv \frac{\langle |\text{tr}\{A |\psi(t)\rangle \langle \psi(t)|\} - \text{tr}(A\rho_\infty)|^2 \rangle_t}{\|A\|^2} \leq \frac{1}{d_{\text{eff}}}, \quad (6)$$

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 approximation

$$\langle \text{tr}\{A |\psi(t)\rangle \langle \psi(t)|\} \rangle_t \approx \text{tr}(A\rho_\infty), \quad (7)$$

which can be readily proved for any quantum systems with no energy degeneracy. The above approximation can still be true even when $\text{tr}\{A |\psi(t)\rangle \langle \psi(t)|\}$ fluctuates 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 (6); 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, the essence of ergodicity, in all quantum systems that satisfy condition (2).

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 eigenstate and have a width of

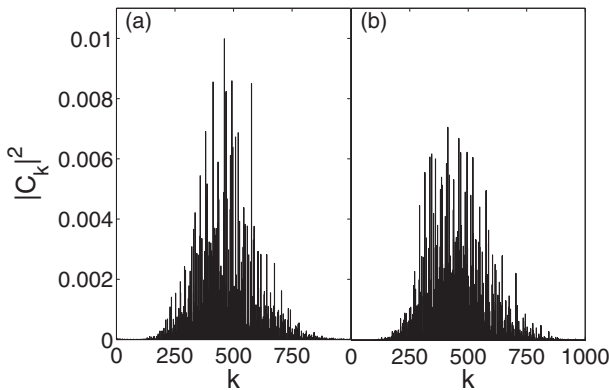


FIG. 4. The distribution of expansion coefficients c_k in the ripple billiard system for (a) even-even eigenstates and (b) odd-even eigenstates.

around 300. With the computed c_k 's, we find that the effective dimension d_{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 $\text{tr}(\rho_\infty p_x) = 0$ and $\text{tr}(\rho_\infty p_y) = 0$. The time evolution of momentum is shown in Fig. 2. We calculate the long-time average between $t = 10T_s$ and $t = 14T_s$. The time unit $T_s \equiv \frac{2(a+b)}{|p_x|/m}$ is the period of the motion of a classical particle with the same initial momentum and position. We find that $\langle \text{tr}\{|\psi(t)\rangle \langle \psi(t)| p_x\} \rangle_t \simeq 0.0021$ and $\langle \text{tr}\{|\psi(t)\rangle \langle \psi(t)| p_y\} \rangle_t \simeq -0.0033$, very close to the ensemble average $\text{tr}(\rho_\infty p_x) = 0$ and $\text{tr}(\rho_\infty p_y) = 0$, respectively. At the same time, we find that

$$\begin{aligned} & \langle |\text{tr}\{\vec{P} |\psi(t)\rangle \langle \psi(t)|\} - \text{tr}(\vec{P}\rho_\infty)|^2 \rangle_t \\ &= \langle |\text{tr}\{\vec{P} |\psi(t)\rangle \langle \psi(t)|\}|^2 \rangle_t \simeq 0.0039. \end{aligned} \quad (8)$$

For operator \vec{P} , the maximum value $\|\vec{P}\|^2 = \sup\{\langle \psi | P^\dagger P | \psi \rangle\}$. Since we have chosen $m = 1/2$ and the wave function is only nonzero inside the billiard, we have $\|\vec{P}\|^2 = \sup\{\langle \psi | H | \psi \rangle\}$; that is, $\|\vec{P}\|^2$ 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., $\|\vec{P}\|^2 \simeq 55.64$. So, the relative fluctuation or the l.h.s. of Eq. (6) is $\sigma_P^2 \simeq 7 \times 10^{-5}$. As $1/d_{\text{eff}} \simeq 3 \times 10^{-3}$, we see that the inequality (6) is clearly satisfied. Moreover, our computation, in fact, shows that the right hand side (r.h.s.) of the inequality is about 30 times larger than the l.h.s. This indicates that it is possible to improve the inequality, for example, replacing $\|A\|^2$ with the averaged value.

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 ρ_∞ , which can be regarded as the quantum microcanonical ensemble. We analyze this quantum equilibrium state and find that it possesses many features that resemble the classical microcanonical ensemble. This kind of quantum-classical correspondence has been studied and found in a spin system [57,58]. To illustrate this quantum-classical correspondence, we compare ρ_∞ in both the real space and the momentum space with the classical microcanonical ensemble

$$\rho_c = \frac{1}{\Omega} \delta[H(\vec{p}, \vec{r}) - E], \quad (9)$$

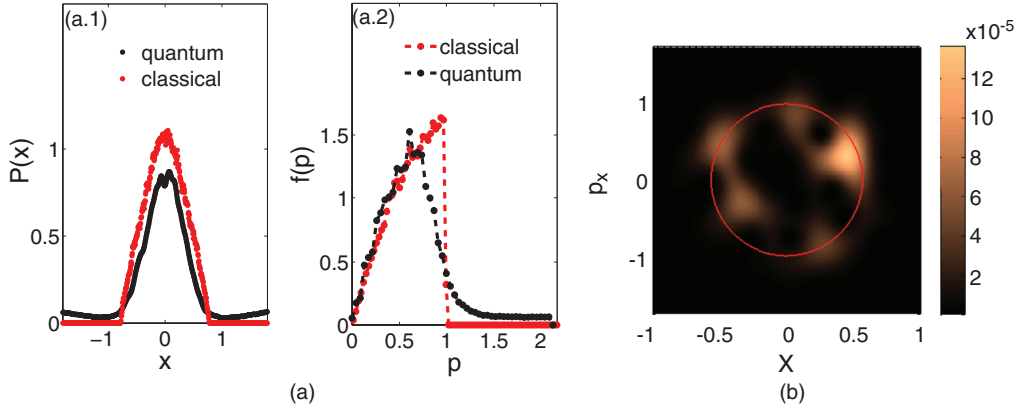


FIG. 5. (Color online) (a) Comparison between quantum and classical equilibrium distributions in the Henon-Heiles system. $P(x)$ is for the real space and $f(p)$ for momentum space. The unit for x is r_c and the unit for p is p_0 . (b) Section of the Husimi function $H_{r,p} \equiv \langle \vec{r}, \vec{p} | \hat{\rho}(t) | \vec{r}, \vec{p} \rangle$ 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 $\sigma \simeq 0.11r_c$.

where Ω 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 microcanonical ensemble $\rho_c(r, p)$ 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 that the quantum and classical distributions are consistent, except for some quantum tunneling effect indicated by the nonzero 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 quasiquantum distribution in phase space can be constructed with the Husimi function $H_{r,p}$ [59,60]. This is to calculate the projection of the density operator on a Gaussian wave packet $\langle \vec{r}' | \vec{r}, \vec{p} \rangle = C \exp[-\frac{(\vec{r}' - \vec{r})^2}{2\sigma^2} + \frac{i\vec{p} \cdot (\vec{r}' - \vec{r})}{\hbar}]$ centered around position \vec{r} and momentum \vec{p} ,

$$H_{r,p} \equiv \langle \vec{r}, \vec{p} | \rho | \vec{r}, \vec{p} \rangle. \quad (10)$$

The Husimi function can be understood as coarse-grained phase space density with parameter σ controlling the coarse graining. We have computed the Husimi function $H_{r,p}$ 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 ρ_c . For easy illustration, we use a two-dimensional section in the four-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 nonzero, 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, $\partial_t \rho(t) = \frac{1}{i\hbar} [H, \rho(t)]$; the time evolution of the classical probability density $\rho_c(t)$ is governed by the classical Liouville equation, $\partial_t \rho_c(t) = [H, \rho_c(t)]_{\text{PB}}$. 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 $|c_k|^2$. For a typical initial state, $|c_k|^2$ should have a distribution similar to what is shown in Fig. 4 with a large effective dimension d_{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 (6) holds for an energy eigenstate; but energy eigenstate does not belong to the typicality class. Here we use the ripple billiard system to illustrate this point as the energy eigenstates in this system can be computed successively [11,51]. We study the position space marginal distribution $f(y) = \int \langle \vec{r} | \rho | \vec{r} \rangle dx$, and compare it with the classical result $[b - a \cos(2\pi y/L)]/bL$. We compute $f(y)$ first for the equilibrium state $\rho(t \gg T_s)$. We see in Fig. 6(a) that the quantum result (black line) is in good agreement with the classical result (red line).

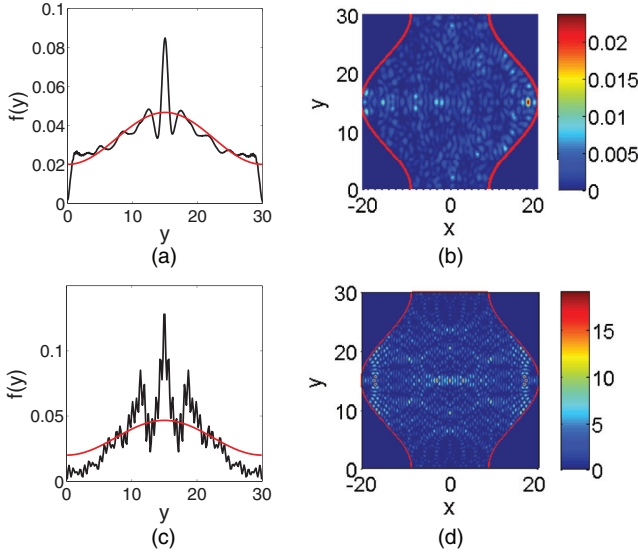


FIG. 6. (Color online) (a) Marginal distributions $f(y) \int n(\vec{r}) dx$ for the equilibrium state in the ripple billiard system. The black line is for the quantum result while the red line is for the classical result. (b) The density distribution $n(r)$ of the equilibration state in the ripple billiard 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 $|c_k|^2 = 0.0086$ in the initial Gaussian wave packet (4).

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 $|c_k|^2$ 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 eigenstates with coefficient $|c_k|^2 = 0.0086$ as the example. The marginal distribution $f(y)$ for this eigenstate is shown in Fig. 6(a). Compared with the result for the equilibrium state in Fig. 6(a), we see a clear distinction: the eigenstate has larger fluctuations and bigger deviation from the classical distribution. In fact, this distinction is also seen in the density plot. As seen in Fig. 6(d), the density distribution for the eigenstate has certain uneven patterns, similar to what have been found in “scar” states [64]; these patterns are absent in the distribution of the equilibrium state [Fig. 6(b)]. Although eigenstates appear to be too special, their difference from a typical quantum state does indicate that not all quantum states that satisfy the inequality (6) can relax to an equilibrium state which has the quantum-classical correspondence. In other words, all quantum states in a chaotic system may be classified into two groups: one has the quantum-classical correspondence and the other does not. It is not yet clear whether there are simple ways to separate them other than using direct computation as we did. In Ref. [58], a remarkable correspondence between eigenstates and their classical counterparts is found for the shape of eigenfunctions and the local spectral density of states. This seems to indicate that when the properties not related to the complexity of a wave function are considered, the quantum-classical correspondence can still be found for eigenstates.

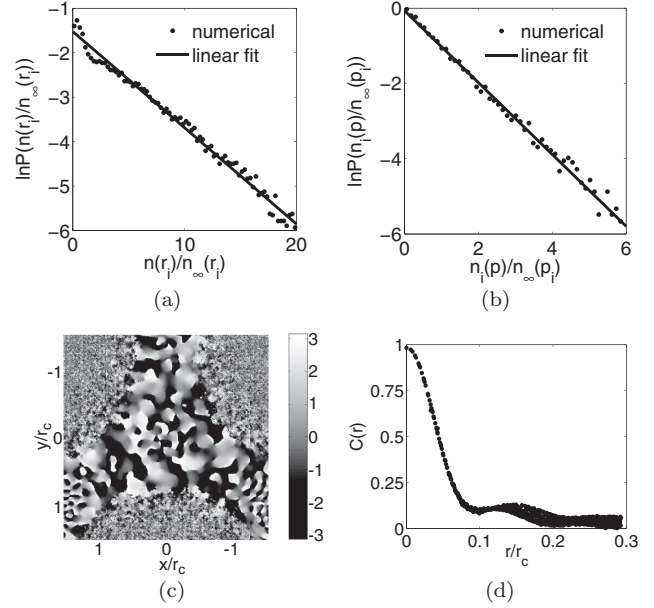


FIG. 7. (a) Log plot of the distribution function $P[n(r_i)/n_\infty(r_i)]$ of the relative quantum fluctuation $n(r_i)/n_\infty(r_i)$. (b) Log plot of the distribution function $P[n(p_i)/n_\infty(p_i)]$ of the relative quantum fluctuation $n(p_i)/n_\infty(p_i)$. (c) The phase of the equilibrated wave function in the real space for the Henon-Heiles system. (d) The normalized spatial correlation function $C(r) = \frac{1}{\langle \Delta n^2 \rangle} \langle [n(0) - \bar{n}][n(r) - \bar{n}] \rangle$ of density in the real space at equilibrium for the Henon-Heiles system.

VI. FLUCTUATION PROPERTY

While the equilibrium density operator ρ_∞ shares a good correspondence with the classical microcanonical ensemble ρ_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 $n_\infty(\xi_i)$ ($i = 1, \dots, N$) of N small discrete region and calculating 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 Figs. 7(a) and 7(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 brings 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

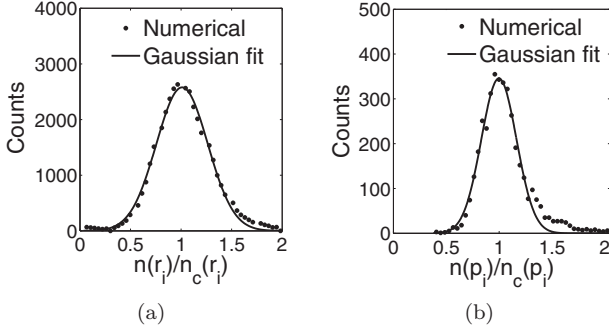


FIG. 8. (a) The distribution function $P[n(r_i)/n_\infty(r_i)]$ of the relative classical fluctuation $n(r_i)/n_\infty(r_i)$. (b) The distribution function $P[n(p_i)/n_\infty(p_i)]$ of the relative classical fluctuation $n(p_i)/n_\infty(p_i)$.

$C(r) = \frac{1}{\langle \Delta n^2 \rangle} \langle [n(0) - \bar{n}][n(r) - \bar{n}] \rangle$ in the real space after equilibrium in the Henon-Heiles system. The results are shown in Figs. 7(c) and 7(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 [21]. It also supports, though not directly, the assumption we made in Eqs. (2) and (3) in our previous work [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. Their phase space distribution $\rho_c(t)$ approaches the microcanonical distribution ρ_c due to the ergodicity in the Henon-Heiles system with certain fluctuation. Following the quantum case, we calculate the relative fluctuations $n_c(\xi, t)/n_c(\xi)$, $\xi = \vec{r}, \vec{p}$ and study their distributions. The classical relative fluctuations is Gaussian as indicated in Fig. 8. This shows that the exponential distribution of relative fluctuations is of quantum nature and absent in the classical system.

Besides the difference from classical case, we note that this exponential distribution is also different from the Porter-Thomas distribution in eigenstates [65] and the result is now known as the Berry's conjecture [66]. These results are only for eigenstates, which are real up to an overall phase for systems with time reversal symmetry. The exponential distribution only exists for a complex wave function, For a generic quantum system, even if all of its energy-eigenstates are real, its dynamical wave function is, in general, complex. This distinction again shows that the general equilibrium statistical properties cannot be understood simply by properties of single eigenstates. The superposition of numerous eigenstates is crucial. We feel it very helpful to compare directly the exponential distribution and the the Port-Thomas distribution [65]. We have rederived 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 ρ_∞ and classical microcanonical ensemble ρ_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 exception 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

$$n(\xi_1) = \int d\xi_2 \cdots d\xi_N n(\xi_1, \xi_2, \dots, \xi_N), \quad (11)$$

where N is the number of particles in this system. The fluctuation in $n(\xi_1, \xi_2, \dots, \xi_N)$ 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 ρ_∞ and ρ_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 [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 [4], we believe that the study of this fundamental issue has just started and many basic questions still wait to be answered. Our study here and other related studies [49,50] have indicated that the quantum ergodic theorem hold for a class of quantum systems larger than what is specified by condition (2). It is imperative to know how to relax condition (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 multitemperature equilibrium state predicted in Ref. [10] by us.

ACKNOWLEDGMENTS

This work is supported by the NBRP of China (Grant No. 2012CB921300, 2013CB921900) and the NSF of China

(Grant No. 11274024,11334001) and the RFDP of China (Grant No. 20110001110091).

APPENDIX: DERIVATION OF EXPONENTIAL DISTRIBUTION AND PORT-THOMAS DISTRIBUTION

Here we give detailed derivations for the exponential distribution of equilibrium wave function [11] and the Port-Thomas distribution of eigenstate wave function [65] with the assumption that wave function in quantum chaotic systems achieve the maximum randomness subject to the restriction of normalization and other symmetry requirements. This assumption follows naturally from our numerical observations [Figs. 7(c) and 7(d)] and the spirit of random matrix theory and was used by Berry in his study of eigenwave functions in chaotic systems [66]. It is important to note that the difference between equilibrium wave functions and eigenstates wave functions is that equilibrium wave functions are generally complex and eigenstate 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 rigorosity) by renormalizing densities with averaged values.

For a wave function ψ , we discretize the system area into N equal infinitesimal pieces with their centers located at $\vec{r}_i, i = 1, \dots, N$ and denote $\alpha_i = \psi(\vec{r}_i)\sqrt{\frac{A}{N}}$, 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. [11]. For a complex wave function in dynamical evolution, α_i is complex; for an eigenfunction, α_i is real. In the following we derive the distribution of $|\alpha_i|^2$ for both cases.

Note that the following proof is given without consideration of the discrete symmetries: (1) reflection symmetry initial state [Eq. (4)] in the ripple billiard system; (2) reflection symmetries in eigenstates of the ripple billiard system, and (3) the reflection symmetries in eigenstates of the 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. (4)], 1/4 (ripple billiard), or 1/6 (Henon-Heiles).

1. Proof of exponential distribution of equilibrium wave function [11]

Consider N complex numbers α_i that satisfy normalization condition $\sum_{i=1}^N |\alpha_i|^2 = 1$ and that 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 $\{\alpha_1, \alpha_2, \dots, \alpha_N\}$ 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 α_j at $|\alpha_j|^2 = \gamma$ is

$$P(\gamma) = \frac{\int d^2\alpha_1 \dots d^2\alpha_N \delta(\gamma - |\alpha_j|^2) \delta(1 - \sum_{i=1}^N |\alpha_i|^2)}{d^2\alpha_1 \dots d^2\alpha_N \delta(1 - \sum_{i=1}^N |\alpha_i|^2)} \tag{A1}$$

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 that the $2N$ -dimensional hypersphere of radius R has an area of $S_{2N}(R) = \frac{2\pi^N}{\Gamma(N)} \times (R)^{2N-1}$. We have

$$P(\gamma) = \frac{\int_0^\infty \pi dx \delta(x - \gamma) \frac{2\pi^{N-1}}{\Gamma(N-1)} (1-x)^{\frac{2N-3}{2}}}{2\pi^N / \Gamma(N)} = (N-1)(1-\gamma)^{N-3/2} \tag{A2}$$

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

$$p(n(\vec{r}))dn(\vec{r}) = \lim_{N \rightarrow \infty} \frac{A}{N} P(\gamma) d\gamma \lim_{N \rightarrow \infty} \frac{A}{N} (N-1) \times \left[1 - \frac{A}{N}n(\vec{r})\right]^N \left[1 - \frac{A}{N}n(\vec{r})\right]^{-3/2} dn(\vec{r}) = Ae^{-An(\vec{r})} dn(\vec{r}) \tag{A3}$$

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

$$p(n) = e^{-n/n_0} / n_0 \tag{A4}$$

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

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

$$P(\gamma) = \frac{\int d\alpha_1 \dots d\alpha_N \delta(\gamma - \alpha_j^2) \delta(1 - \sum_{i=1}^N \alpha_i^2)}{d\alpha_1 \dots d\alpha_N \delta(1 - \sum_{i=1}^N \alpha_i^2)} \tag{A5}$$

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

$$P(\gamma) = \frac{\int_0^\infty dx x^{-1/2} \delta(\gamma - x) \frac{2\pi^{(N-1)/2}}{\Gamma((N-1)/2)} (\sqrt{1-x})^{N-2}}{2\pi^{N/2} / \Gamma(N/2)} = \sqrt{\frac{1}{\gamma\pi}} (\sqrt{1-\gamma})^{N-2} \frac{\Gamma(N/2)}{\Gamma((N-1)/2)} \tag{A6}$$

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

$$p(n) = \sqrt{\frac{A}{2\pi n}} e^{-\frac{A}{2}n} \tag{A7}$$

where we have used $\lim_{N \rightarrow \infty} \frac{\Gamma(N/2)}{\Gamma((N-1)/2)\sqrt{N}} = \frac{1}{\sqrt{2}}$.

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