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LETTER TO THE EDITOR

Thermal fluctuations in quantized chaotic systems

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Abstract. We consider a quantum system with N degrees of freedom which is classically chaotic. When N is large, and both \hbar and the quantum energy uncertainty ΔE are small, quantum chaos theory can be used to demonstrate the following results: (i) given a generic observable A , the infinite time average \bar{A} of the quantum expectation value $\langle A(t) \rangle$ is independent of all aspects of the initial state other than the total energy, and equal to an appropriate thermal average of A ; (ii) the time variations of $\langle A(t) \rangle - \bar{A}$ are too small to represent thermal fluctuations; (iii) however, the time variations of $\langle A^2(t) \rangle - \langle A(t) \rangle^2$ can be consistently interpreted as thermal fluctuations, even though these same time variations would be called quantum fluctuations when N is small.

In this letter we examine the compatibility of certain results in quantum chaos theory with standard results in statistical mechanics. We consider a bounded, isolated, many-body quantum system whose classical limit is chaotic. Given an initial state $|\psi(0)\rangle$ and a generic observable A , we ask the following questions. What is the infinite time average of $\langle A(t) \rangle \equiv \langle \psi(t) | A | \psi(t) \rangle$? Is it independent of the initial state $|\psi(0)\rangle$? If so, is it equal to an appropriate thermal average of A ? What are the root-mean-square fluctuations, in time, of $\langle A(t) \rangle$ about its infinite time average? Are these fluctuations correctly predicted by statistical mechanics?

We begin by noting that the energy spectrum of a bounded quantum system is purely discrete; if the system is classically chaotic, and also has no discrete symmetries, then the energy eigenvalues E_α are almost always non-degenerate [1]. Since we assume that the system is isolated, its state at time t is

$$|\psi(t)\rangle = \sum_{\alpha} C_{\alpha} e^{-iE_{\alpha}t/\hbar} |\alpha\rangle \quad (1)$$

where the C_{α} 's specify the initial state, and we assume the usual normalization

$$\sum_{\alpha} |C_{\alpha}|^2 = 1. \quad (2)$$

The expectation value of an observable A at time t is

$$\begin{aligned} \langle A(t) \rangle &\equiv \langle \psi(t) | A | \psi(t) \rangle \\ &= \sum_{\alpha\beta} C_{\alpha}^* C_{\beta} e^{i(E_{\alpha}-E_{\beta})t/\hbar} A_{\alpha\beta} \end{aligned} \quad (3)$$

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where

$$A_{\alpha\beta} \equiv \langle \alpha | A | \beta \rangle \quad (4)$$

are the matrix elements of A in the energy eigenstate basis. The infinite time average of $\langle A(t) \rangle$ is given by

$$\begin{aligned} \bar{A} &\equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \langle A(t) \rangle \\ &= \sum_{\alpha} |C_{\alpha}|^2 A_{\alpha\alpha}. \end{aligned} \quad (5)$$

The time-averaged fluctuations of $\langle A(t) \rangle$ about \bar{A} are given by

$$\begin{aligned} \overline{[\langle A(t) \rangle - \bar{A}]^2} &\equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt [\langle A(t) \rangle - \bar{A}]^2 \\ &= \sum_{\alpha, \beta \neq \alpha} |C_{\alpha}|^2 |C_{\beta}|^2 |A_{\alpha\beta}|^2. \end{aligned} \quad (6)$$

We now turn to a discussion of what can be inferred about (5) and (6) from quantum chaos theory.

Quantum chaos theory is largely based on semiclassical arguments; to make use of it, we will have to assume that Planck constant is ‘small.’ This means that there is some dimensionless combination of parameters, with a single power of Planck’s constant in the numerator, which serves as an expansion parameter for quantities such as $A_{\alpha\beta}$. The relevant combination of parameters, which we will call \hbar , obviously depends on the system under consideration. How small \hbar has to be depends on both A and the range of energies which are of interest. It is particularly difficult to determine the dependence of \hbar on N , the number of degrees of freedom in the system. This question is irrelevant when N is small, but crucial when N is large. We will not discuss this important problem any further here, however; we will simply assume that the correct expansion parameter \hbar , whatever its dependence on N , is sufficiently small.

Given a classically chaotic system with N degrees of freedom, we consider an observable A which is a smooth function of the classical coordinates and momenta, and which has no explicit dependence on \hbar . Then quantum chaos theory predicts that the matrix elements $A_{\alpha\beta}$ are given by

$$A_{\alpha\beta} = \mathcal{A}(E_{\alpha}) \delta_{\alpha\beta} + \hbar^{(N-1)/2} R_{\alpha\beta}. \quad (7)$$

Here $\mathcal{A}(E)$ is a smooth function of energy whose leading term in the \hbar expansion is $\mathcal{O}(\hbar^0)$. The matrix elements $R_{\alpha\beta}$ are also $\mathcal{O}(\hbar^0)$ to leading order, and their values are characterized by a smooth distribution, often assumed to be Gaussian. Equation (7) has not been demonstrated rigorously, but it follows from a variety of different arguments, including Berry’s random-wave conjecture for the energy eigenfunctions [2–4], the analogy between quantized chaotic systems and random matrix theory [5], and the semiclassical periodic orbit expansion, assuming a certain randomness for the periodic orbits [6]. There is, however, one aspect of (7) which has been proven rigorously; specifically

$$\lim_{\alpha \rightarrow \infty} A_{\alpha\alpha} = \frac{\int d^N p d^N q \delta(H(p, q) - E_{\alpha}) A(p, q)}{\int d^N p d^N q \delta(H(p, q) - E_{\alpha})} \quad (8)$$

where $H(p, q)$ is the classical Hamiltonian, and $A(p, q)$ is the classical form of the operator A [7]. The limit holds for all energy eigenstates $|\alpha\rangle$ except possibly a subsequence of density zero. The right-hand side of (8) is the $\mathcal{O}(\hbar^0)$ contribution to $\mathcal{A}(E_{\alpha})$.

For later use, we must also examine the matrix elements of A^2 . Consider first the diagonal elements $(A^2)_{\alpha\alpha} = \sum_{\beta} A_{\alpha\beta} A_{\beta\alpha}$; using equation (7) gives

$$(A^2)_{\alpha\alpha} = \left[\mathcal{A}^2(E_{\alpha}) + \hbar^{N-1} \sum_{\beta} |R_{\alpha\beta}|^2 \right] + \hbar^{(N-1)/2} 2\mathcal{A}(E_{\alpha})R_{\alpha\alpha}. \quad (9)$$

We have grouped the terms as shown because the second term in square brackets is actually $\mathcal{O}(\hbar^0)$, despite the explicit factor of \hbar^{N-1} . This is because the sum over β can be converted to an integral over the quantum density of states, and the quantum density of states is $\mathcal{O}(\hbar^{-N})$ [1]. One more factor of \hbar then arises from converting a quantum energy integral into a classical frequency integral [3]. Thus, the diagonal matrix elements of A^2 have the same general structure (7) as the diagonal matrix elements of A ; this is of course required for internal consistency, since there was nothing special about A .

Now consider the off-diagonal elements $(A^2)_{\alpha\gamma} = \sum_{\beta} A_{\alpha\beta} A_{\beta\gamma}$; using equation (7) gives

$$(A^2)_{\alpha\gamma} = \hbar^{(N-1)/2} [\mathcal{A}(E_{\alpha}) + \mathcal{A}(E_{\gamma})] R_{\alpha\gamma} + \hbar^{N-1} \sum_{\beta} R_{\alpha\beta} R_{\beta\gamma} \quad (10)$$

when $\alpha \neq \gamma$. This time, however, the sum over β in the last term does not contribute a factor of \hbar^{-N+1} , because $R_{\alpha\beta} R_{\beta\gamma}$ is not positive definite. Instead, we expect $R_{\alpha\beta} R_{\beta\gamma}$ to have a phase (or perhaps just a sign) which varies erratically with β . This implies that the sum over β of $R_{\alpha\beta} R_{\beta\gamma}$ is the same order in \hbar as the square root of the sum over β of $|R_{\alpha\beta} R_{\beta\gamma}|^2$; this latter sum is $\mathcal{O}(\hbar^{-N+1})$. Thus we conclude that, overall, the second term on the right-hand side of (10) is $\mathcal{O}(\hbar^{(N-1)/2})$, just like the first term, and just like the off-diagonal matrix elements of A . Again this is required for the consistency of (7) with the generic character of A .

Returning to equation (5), if we insert (7) we get

$$\bar{A} = \sum_{\alpha} |C_{\alpha}|^2 \mathcal{A}(E_{\alpha}) + \mathcal{O}(\hbar^{(N-1)/2}). \quad (11)$$

We now assume that the expected value of the total energy

$$\langle E \rangle = \sum_{\alpha} |C_{\alpha}|^2 E_{\alpha} \quad (12)$$

has a quantum uncertainty

$$\Delta E = \left[\sum_{\alpha} |C_{\alpha}|^2 (E_{\alpha} - \langle E \rangle)^2 \right]^{1/2} \quad (13)$$

which is small, in a sense which we will make more precise shortly. This is a natural assumption if N is large, since states of physical interest typically have $\Delta E \sim N^{-1/2} \langle E \rangle$. Note, however, that in this case the smallness of ΔE does not imply or require the smallness of \hbar .

Assuming ΔE is small, we can expand $\mathcal{A}(E_{\alpha})$ about $\langle E \rangle$ to get

$$\mathcal{A}(E_{\alpha}) = \mathcal{A}(\langle E \rangle) + (E_{\alpha} - \langle E \rangle) \mathcal{A}'(\langle E \rangle) + \frac{1}{2} (E_{\alpha} - \langle E \rangle)^2 \mathcal{A}''(\langle E \rangle) + \dots \quad (14)$$

Substituting this expansion in (11), we find

$$\bar{A} = \mathcal{A}(\langle E \rangle) + \frac{1}{2} (\Delta E)^2 \mathcal{A}''(\langle E \rangle) + \mathcal{O}((\Delta E)^3) + \mathcal{O}(\hbar^{(N-1)/2}). \quad (15)$$

Thus, the infinite time average \bar{A} depends on the expected value of the total energy $\langle E \rangle$, but is independent of all other aspects of the initial state, provided that \hbar is small enough to make the $\mathcal{O}(\hbar^{(N-1)/2})$ term negligible, and provided that

$$(\Delta E)^2 \left| \frac{\mathcal{A}''(\langle E \rangle)}{\mathcal{A}(\langle E \rangle)} \right| \ll 1. \quad (16)$$

This is the more precise criterion for the smallness of ΔE .

We are now able to make a connection with statistical mechanics. Mathematically, we can choose the $|C_\alpha|^2$ to represent a microcanonical average over an energy range ΔE centred on $\langle E \rangle$. If this ΔE is chosen to satisfy (16), then \bar{A} is equal to this microcanonical average of A . Alternatively, we can choose the $|C_\alpha|^2$ to be canonical Boltzmann weights; the canonical energy dispersion ΔE is usually smaller than $\langle E \rangle$ by a factor of $N^{-1/2}$, and therefore the canonical ΔE should satisfy (16) when N is large. If so, then \bar{A} is equal to the canonical thermal average of A at whatever temperature results in a total energy of $\langle E \rangle$. Thus, the function $\mathcal{A}(E)$ can in principle be calculated, at least up to corrections which are $O(\hbar^{(N-1)/2})$ and $O(N^{-1})$, by the methods of canonical statistical mechanics.

Some time ago, Jaynes [8] pointed out that a canonical calculation of the size of the thermal fluctuations in some observable A must ultimately be based on demonstrating that A exhibits time variations with the same root-mean-square amplitude. To study this issue in the present context, we first consider the time variations of $\langle A(t) \rangle - \bar{A}$. From (6), (7), and (2), we find

$$\overline{[\langle A(t) \rangle - \bar{A}]^2} = O(\hbar^{N-1}). \quad (17)$$

We see that the fluctuations of $\langle A(t) \rangle$ about \bar{A} are small. This tells us that, whatever the initial value $\langle A(0) \rangle$ happens to be, $\langle A(t) \rangle$ must eventually approach its thermal average \bar{A} , and then remain near \bar{A} most of the time. (We do not, however, learn anything about the time scale of this approach.) Apparently, under appropriate circumstances quantum chaos can serve as the dynamical underpinning of certain basic results of statistical mechanics, an idea which has already appeared in various guises [4, 9].

On the other hand, equation (17) is too small to represent the expected thermal fluctuations of A , which are $O(\hbar^0)$. To find thermal fluctuations, we must look at the infinite time average of $\langle A^2(t) \rangle$; this is given by

$$\begin{aligned} \overline{A^2} &\equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \langle A^2(t) \rangle \\ &= \sum_\alpha |C_\alpha|^2 (A^2)_{\alpha\alpha}. \end{aligned} \quad (18)$$

We have already seen that the matrix elements of A^2 have the same general structure as the matrix elements of A . Therefore, we can immediately conclude that $\overline{A^2}$ is equal to a thermal average of A^2 , up to corrections which are $O(\hbar^{(N-1)/2})$ and $O(N^{-1})$.

Putting everything together, we conclude that, up to corrections which are $O(\hbar^{(N-1)/2})$ and $O(N^{-1})$, the infinite time average of $\langle A^2(t) \rangle - \langle A(t) \rangle^2$ is equal to a thermal average of $(A - \bar{A})^2$. Thus, variations with time of $\langle A^2(t) \rangle - \langle A(t) \rangle^2$ can be interpreted as representing thermal fluctuations. It is interesting to note that, in a few-body system, these same time variations would be called quantum fluctuations.

In summary, results from quantum chaos theory are compatible with results from statistical mechanics; quantum chaos theory can even be used as a basis from which one can demonstrate, for example, that the quantum expectation value of an observable must approach its thermal average, at least when the number of degrees of freedom N is large, the quantum energy uncertainty ΔE is small, and the semiclassical expansion parameter \hbar is small. Just how small \hbar needs to be is a question to which we hope to return. Also, we have seen that the variations with time of a quantum expectation value are too small to account for the expected thermal fluctuations; instead, what would be called quantum fluctuations when N is small have just the right amplitude to be identified as thermal fluctuations when N is large.

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