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The approach to thermal equilibrium in quantized chaotic systems

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Abstract. We consider many-body quantum systems that exhibit quantum chaos, in the sense that the observables of interest act on energy eigenstates like banded random matrices. We study the time-dependent expectation values of these observables, assuming that the system is in a definite (but arbitrary) pure quantum state. We induce a probability distribution for the expectation values by treating the zero of time as a uniformly distributed random variable. We show explicitly that if an observable has a non-equilibrium expectation value at some particular moment, then it is overwhelmingly likely to move towards equilibrium, both forwards and backwards in time. For deviations from equilibrium that are not much larger than a typical quantum or thermal fluctuation, we find that the time dependence of the move towards equilibrium is given by the Kubo correlation function, in agreement with Onsager's postulate. These results are independent of the details of the system's quantum state.

1. Introduction

Many-body systems typically exhibit certain dynamical properties that are studied under the subject headings of thermodynamics and statistical mechanics. These properties include the following.

(1) Given an arbitrary initial state, the system almost always evolves towards an identifiable condition known as thermal equilibrium, and then remains in this condition at almost all subsequent times.
(2) When the system is in thermal equilibrium, observables of interest take on values that depend only on the nature of the system and its total energy, but not on any other details of the specific state of the system.
(3) When the system is in thermal equilibrium, the measured value of an observable of interest at any particular time fluctuates about its equilibrium value, with fluctuations whose amplitude is suppressed by a factor of $N^{-1/2}$, where N is the number of degrees of freedom.
(4) During the approach to thermal equilibrium, the values of observables of interest are governed by equations that are not time reversal invariant. These equations typically depend on the values of other observables, possibly at different times. The information about the system that is included in these equations is not sufficient to reconstruct the complete physical state of the system.
(5) Often (but not always), these equations are markovian; that is, they depend only on the values of the observables in question, and their first time derivatives, at any given moment.

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There is a vast literature on the derivation of these properties from an underlying deterministic, time reversal invariant dynamics, classical or quantum. In this paper (closely related earlier work includes [1–16]), we explore to what extent these properties can be deduced as consequences of *quantum chaos*. This means that we will assume that the energy eigenvalues and (more importantly) the matrix elements of typical observables have certain properties. These properties are believed (and, in some cases, rigorously proven) to hold for a canonically quantized system whose classical phase space is fully chaotic at the energies of interest, and they are likely to hold at least approximately for a broader array of systems.

The outline of this paper is as follows. In section 2 we state our basic assumptions, and briefly discuss their origins in quantum chaos theory. Some previous work that is directly relevant is summarized in section 3. Sections 4 and 5 present new results concerning the approach to thermal equilibrium. Section 6 discusses the main conclusions.

2. Quantum chaos

We assume that the quantum system of interest is bounded and isolated, with N degrees of freedom, where $N \gg 1$. Since the system is bounded, the energy eigenvalues are discrete, and since it is isolated, its time evolution is governed by the Schrodinger equation. Let E_α denote the energy eigenvalue corresponding to the energy eigenstate $|\alpha\rangle$; the state of the system at any time t is then given by

$$|\psi_t\rangle = \sum_\alpha c_\alpha \mathrm{e}^{-\mathrm{i}E_\alpha t}|\alpha\rangle. \tag{2.1}$$

We emphasize that $|\alpha\rangle$ is an eigenstate of the full, many-body Hamiltonian. The c_α's specify the state at any one time (say, $t = 0$), and we assume the usual normalization

$$\langle\psi_t|\psi_t\rangle = \sum_\alpha |c_\alpha|^2 = 1. \tag{2.2}$$

Note that we have set $\hbar = 1$ to simplify the notation. We will, however, point out how various quantities scale with $\hbar$ when this information is useful.

We now make two key assumptions about the system.

Our first assumption is not strictly necessary, but it will simplify some of the subsequent analysis. We assume that if any two sums of equal numbers of energy eigenvalues are equal,

$$E_{\alpha_1} + \cdots + E_{\alpha_n} = E_{\beta_1} + \cdots + E_{\beta_n} \tag{2.3}$$

then $\{\beta_1, \ldots, \beta_n\}$ is a permutation of $\{\alpha_1, \ldots, \alpha_n\}$; that is, the corresponding eigenstates are the same for both sides. In particular, $E_\alpha = E_\beta$ implies that $|\alpha\rangle = |\beta\rangle$, so that all the energy eigenvalues are non-degenerate. This assumption is expected to hold in general for a quantized chaotic system in which all unitary symmetries (such as invariance under any discrete or continuous reflection or rotation) have been removed by suitable changes (such as by putting the system in an irregularly shaped box). In this case, the energy eigenvalues have the same statistical properties as the eigenvalues of Gaussian random matrices [17]. The system may or may not be invariant under the anti-unitary transformation of time reversal; we will assume that it is, because one of the most interesting aspects of thermodynamics is the appearance of an 'arrow of time' even when the underlying dynamics is time reversal invariant.

Our second assumption is the crucial one. Let A be a hermitian operator corresponding to an observable of interest that is a smooth, $\hbar$-independent function of the classical coordinates and momenta. We assume that the matrix elements of A in the energy eigenstate basis take the form [6, 18]

$$A_{\alpha\beta} = \mathcal{A}(E)\delta_{\alpha\beta} + \mathrm{e}^{-S(E)/2} f(E, \omega) R_{\alpha\beta}. \tag{2.4}$$

All the factors in this formula need explanation.

First, for notational convenience we have defined

$$E \equiv \tfrac{1}{2}(E_\alpha + E_\beta) \qquad \text{and} \qquad \omega \equiv E_\alpha - E_\beta. \tag{2.5}$$

$S(E)$ is the thermodynamic entropy at energy E, given by

$$\mathrm{e}^{S(E)} \equiv E \sum_\alpha \delta_\varepsilon(E - E_\alpha) \tag{2.6}$$

where $\delta_\varepsilon(x)$ is a Dirac delta function that has been smeared just enough to render $S(E)$ monotonic. $\mathcal{A}(E)$ and $f(E,\omega)$ are smooth functions of their arguments whose physical implications will be the main focus of this paper. Finally, $R_{\alpha\beta}$ is a numerical factor that varies erratically with α and β. It is helpful to think of the real and imaginary parts of $R_{\alpha\beta}$ as random variables, each with zero mean and unit variance. Without loss of generality, we can take $f(E,\omega)$ to be real, positive, and an even function of ω; then hermiticity of A implies $R_{\beta\alpha} = R^*_{\alpha\beta}$. Also, in many cases of physical interest, $R_{\alpha\beta}$ is purely real.

Equation (2.4) is semiclassical in nature; the factor of $\mathrm{e}^{-S(E)/2}$ scales like $\hbar^{(N-1)/2}$. Thus the validity of equation (2.4) requires $\hbar$ to be 'small', which in practice means that the energy E must be 'large'. The appropriate definitions of 'small' and 'large' are a key problem of quantum chaos theory. For systems with few degrees of freedom, it is now well established [19] that a necessary condition for quantum chaos is $\delta \ll \hbar/\tau_{\mathrm{Th}}$, where $\delta \sim \mathrm{e}^{-S}E$ is the mean spacing between energy eigenvalues near E, and τ_{Th} is the Thouless time [20] (roughly speaking, the timescale by which all diffusive classical processes have saturated). For many-body systems in general, less is known. Studies of nonlinearly coupled oscillators [7, 14] and of fermions with pseudo-random single-particle energies and two-body matrix elements [11, 15] both suggest a threshold energy for quantum chaos that goes to zero in the thermodynamic limit like $N^{-\nu}$, with $0 < \nu \leqslant 1$. We may therefore hope that equation (2.4) will enjoy a wide range of validity.

An important feature of equation (2.4) is that the general structure that it describes is preserved under multiplication [6]. Thus, for example, the matrix elements of any power of A are given by

$$(A^n)_{\alpha\beta} = \mathcal{A}_n(E)\delta_{\alpha\beta} + \mathrm{e}^{-S(E)/2} f_n(E,\omega) R^{(n)}_{\alpha\beta} \tag{2.7}$$

where $\mathcal{A}_n(E)$, $f_n(E,\omega)$, and $R^{(n)}_{\alpha\beta}$ can be expressed in terms of $\mathcal{A}(E)$, $f(E,\omega)$, and $R_{\alpha\beta}$. The precise relationship will not be needed, however; the key point is the generic character of equation (2.4).

Finally, the function $\mathcal{A}(E)$ can be related to a standard expression in statistical mechanics: the equilibrium value of A, as given by the canonical thermal average

$$\langle A\rangle_T \equiv \frac{\mathrm{Tr}\,\mathrm{e}^{-H/T}A}{\mathrm{Tr}\,\mathrm{e}^{-H/T}}. \tag{2.8}$$

Here T is the temperature, and we have set Boltzmann's constant to one. To see the relation between $\langle A\rangle_T$ and $\mathcal{A}(E)$, we use equations (2.4) and (2.6) in equation (2.8) to get

$$\langle A\rangle_T = \frac{\int_0^\infty \frac{\mathrm{d}E}{E}\mathrm{e}^{S(E)-E/T}\mathcal{A}(E)}{\int_0^\infty \frac{\mathrm{d}E}{E}\mathrm{e}^{S(E)-E/T}} + \mathrm{O}(\mathrm{e}^{-S/2}). \tag{2.9}$$

When N is large, the entropy is extensive: $S(E,N) = Ns(E/N) + \mathrm{O}(\log N)$. In this case the integrals in equation (2.9) can be evaluated by steepest descent. We see that their ratio is $\mathcal{A}(E) + \mathrm{O}(N^{-1})$, where E is now fixed in terms of T by the steepest-descent condition $\partial S/\partial E = 1/T$; this also implies $E = \langle H\rangle_T$. Turning around equation (2.9) then gives us the expression for $\mathcal{A}(E)$ that we want [6],

$$\mathcal{A}(E) = \langle A\rangle_T + \mathrm{O}(N^{-1}) + \mathrm{O}(\mathrm{e}^{-S/2}). \tag{2.10}$$

We will always assume that N is large enough to make the indicated corrections negligible.

Note also that equation (2.10) is consistent with, but not identical to, Shnirelman's theorem [21]. This theorem essentially states that $\mathcal{A}(E)$ is given by the classical, microcanonical average of A, up to corrections which are expected to be $O(\overline{h}^{1/2})$. Equation (2.10), on the other hand, already includes corrections up to $O(\overline{h}^{(N-2)/2})$, but has in addition corrections of $O(N^{-1})$.

3. Thermal equilibrium

The expectation value of an observable A in the state specified by equation (2.1) is given by

$$\begin{aligned} A_t &\equiv \langle\psi_t|A|\psi_t\rangle \\ &= \sum_{\alpha\beta} c_\alpha^* c_\beta \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)t} A_{\alpha\beta}. \end{aligned} \tag{3.1}$$

We will take A_t as the main object of study. It is not obvious that this is the right thing to do, since short-time measurements do not generally yield quantum expectation values. However, our main goal is to compare with the results of conventional non-equilibrium statistical mechanics, in which time-dependent expectation values are the basic ingredients (see, e.g., [22–24], and section 5, below). A detailed discussion of the quantum measurement problem would be needed to address this issue properly, but this is beyond the scope of the present paper.

If we now take the infinite time average of A_t, we find

$$\begin{aligned} \overline{A} &\equiv \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \mathrm{d}t\, A_t \\ &= \sum_\alpha |c_\alpha|^2 A_{\alpha\alpha} \end{aligned} \tag{3.2}$$

where the last line requires non-degeneracy of the energy eigenvalues. It also requires that the averaging time τ be much larger than the Heisenberg time $\tau_{\mathrm{H}} \equiv 2\pi\overline{h}/\delta \sim \mathrm{e}^S$. This timescale is much too large to be physically relevant, and thus the infinite time average must be regarded as a purely theoretical device. Nevertheless, if the system comes to thermal equilibrium, then A_t should be near its equilibrium value $\langle A\rangle_T$ most of the time, and thus we should have $\overline{A} = \langle A\rangle_T$.

To check whether or not this is the case, we first substitute equation (2.4) into equation (3.2) to get

$$\overline{A} = \sum_\alpha |c_\alpha|^2 \mathcal{A}(E_\alpha) + O(\mathrm{e}^{-S/2}). \tag{3.3}$$

We now make a mild assumption about the state $|\psi_t\rangle$. We assume that the expectation value of the total energy

$$E \equiv \sum_\alpha |c_\alpha|^2 E_\alpha \tag{3.4}$$

has a quantum uncertainty

$$\Delta \equiv \left[\sum_\alpha |c_\alpha|^2 (E_\alpha - E)^2 \right]^{1/2} \tag{3.5}$$

that is small, in the sense that $\Delta^2 |\mathcal{A}''(E)/\mathcal{A}(E)| \ll 1$. This is a natural assumption when N is large, since states of physical interest typically have $\Delta \sim N^{-1/2}E$. If we now expand $\mathcal{A}(E_\alpha)$ in equation (3.3) in powers of $E_\alpha - E$, we get $\overline{A} = \mathcal{A}(E) + O(\Delta^2)$; combining this with equation (2.10), we find

$$\overline{A} = \langle A\rangle_T + O(\Delta^2) + O(N^{-1}) + O(\mathrm{e}^{-S/2}). \tag{3.6}$$

Thus we have shown that the infinite time average of A_t is indeed equal to its equilibrium value at the appropriate temperature. Note that this key property follows entirely from the matrix element structure of equation (2.4), and does not depend on the details of the initial quantum state.

We now turn to an examination of the fluctuations of A_t about its equilibrium value $\overline{A}$. The mean squared amplitude of the these fluctuations is

$$\begin{aligned}\overline{(A_t - \overline{A})^2} &= \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau \mathrm{d}t\,(A_t - \overline{A})^2 \\ &= \sum_{\alpha,\beta\neq\alpha} |c_\alpha|^2|c_\beta|^2|A_{\alpha\beta}|^2 \\ &= \mathrm{O}(\mathrm{e}^{-S}). \end{aligned} \tag{3.7}$$

We see that the fluctuations of A_t about $\overline{A}$ are very small. This tells us that, whatever the initial value A_0 happens to be, A_t must eventually approach its equilibrium value, and then remain near it most of the time.

On the other hand, equation (3.7) is too small to represent the expected thermal fluctuations of A. To find them, we must look at what are usually called quantum fluctuations. The mean squared amplitude of the quantum fluctuations is

$$\begin{aligned}\overline{\langle\psi_t|(A - \overline{A})^2|\psi_t\rangle} &= \overline{\langle A^2\rangle_t} - \overline{A}^2 \\ &= \langle A^2\rangle_T - \langle A\rangle_T^2 + \mathrm{O}(\Delta^2) + \mathrm{O}(N^{-1}) + \mathrm{O}(\mathrm{e}^{-S/2}). \end{aligned} \tag{3.8}$$

In the last line, we have used the fact that the matrix elements of A^2 have the same general structure as the matrix elements of A, as shown in equation (2.7), and that this structure implies that the infinite time average is the same as the thermal average, as shown in equation (3.6). Equation (3.8) tells us that the quantum fluctuations in A have the right magnitude to be identified as thermal fluctuations [6].

Note, however, that $\langle A^2\rangle_T - \langle A\rangle_T^2$ is itself expected to be $\mathrm{O}(N^{-1})$ for typical observables of interest (see, e.g., [25]), and so the first two correction terms on the right-hand side of equation (3.8) are not necessarily smaller than the leading term. This is not a point of concern, however; we used the canonical ensemble to define thermal averaging, and the result would in general change by a factor of order one if we were to use instead the grand canonical or microcanonical ensemble. Since the exact size of the thermal fluctuations in any particular observable depends on the choice of ensemble, our claimed identification of quantum fluctuations as thermal fluctuations can be meaningful only up to a numerical factor. This is what is established in equation (3.8).

Another point of interest is the nature of the classical limit. Recalling that $\mathrm{e}^{-S} \sim \hbar^{N-1}$, we see that equation (3.7) predicts that $\overline{(A_t - \overline{A})^2}$ vanishes in the classical limit. This is in fact a reasonable result if the classical system is chaotic. To see why, first note that the classical limit of a generic quantum state (to the extent that such a thing exists at all) is a probability density on phase space. Then the time dependent expectation value A_t is given (in the classical limit) by $A_t = \int \mathrm{d}^{2N}X\, U_t\rho(X)A(X)$, where X is a point in phase space, $\rho(X)$ is the probability density associated with the quantum state at $t = 0$, and U_t is the Frobenius–Perron evolution operator for phase-space densities. When suitably regulated and renormalized, this formally unitary operator acquires eigenvalues (known as Ruelle resonances) inside the unit circle that are associated with irreversible decay to the ergodic distribution [26]. If both $A(X)$ and $\rho(X)$ are smooth functions, A_t approaches a fixed limit as $t \to \infty$, and $\overline{(A_t - \overline{A})^2}$ vanishes. The mean squared amplitude of the classical thermal fluctuations is then given by the infinite time average of $\int \mathrm{d}^{2N}X\, U_t\rho(X)[A(X) - \overline{A}]^2$, which is the classical limit of the quantum expression $\langle\psi_t|(A - \overline{A})^2|\psi_t\rangle$.

4. Approaching equilibrium

We now turn to our main topic, the approach to thermal equilibrium. Suppose we have an initial state $|\psi_0\rangle = \sum_\alpha c_\alpha |\alpha\rangle$ such that the initial expectation value $A_0 = \langle\psi_0|A|\psi_0\rangle$ of an observable A is far from its equilibrium value $\overline{A} = \langle A\rangle_T$. What, then, is the behaviour of $A_t = \langle\psi_t|A|\psi_t\rangle$ at later times?

It is obvious that the answer depends on the details of the initial state. Without knowing them, we can only make a probabilistic analysis. There are two basic methods for doing so. One is to introduce a probability distribution for the initial state itself, and to average relevant quantities over it. The issue then becomes the justification of the procedure (e.g., maximum entropy) for choosing this particular distribution. The second method, which we will adopt, is to fix the initial state, and then study the values of interesting observables as functions of time. We treat the observation time as a uniformly distributed random variable, thus inducing a probability distribution for each observable. We then attempt to determine to what extent these probability distributions depend on the initial state. Ideally, there would be no dependence at all, thus rendering the choice of the initial state irrelevant.

The moments of the probability distribution for A_t (which is induced by assuming a uniform probability distribution for t) are given by the infinite time averages

$$\overline{(A_t)^n} = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau \mathrm{d}t\,(A_t)^n. \tag{4.1}$$

Again we note that we are using the infinite time average simply as a mathematical tool; in this context, the fact that astronomically long averaging times are necessary is not relevant. By using equation (3.1), and the non-degeneracy assumption discussed after equation (2.3), we can express these moments as products of traces of powers of the matrix

$$\tilde{A}_{\alpha\beta} \equiv c_\alpha^* A_{\alpha\beta} c_\beta. \tag{4.2}$$

It will simplify the notation considerably if we first shift the operator A by a constant, so that the infinite time average of A_t is zero. This entails no loss of generality, and so from here on we will take

$$\overline{A} = \mathrm{Tr}\,\tilde{A} = 0. \tag{4.3}$$

The first few moments $\overline{(A_t)^n}$ can then be expressed as

$$\begin{aligned}
\overline{(A_t)^2} &= \mathrm{Tr}\,\tilde{A}^2 \\
\overline{(A_t)^3} &= 2\,\mathrm{Tr}\,\tilde{A}^3 \\
\overline{(A_t)^4} &= 3(\mathrm{Tr}\,\tilde{A}^2)^2 + 6\,\mathrm{Tr}\,\tilde{A}^4 \\
\overline{(A_t)^5} &= 20\,\mathrm{Tr}\,\tilde{A}^2\,\mathrm{Tr}\,\tilde{A}^3 + 24\,\mathrm{Tr}\,\tilde{A}^5 \\
\overline{(A_t)^6} &= 15(\mathrm{Tr}\,\tilde{A}^2)^3 + 90\,\mathrm{Tr}\,\tilde{A}^2\,\mathrm{Tr}\,\tilde{A}^4 + 40(\mathrm{Tr}\,\tilde{A}^3)^2 + 120\,\mathrm{Tr}\,\tilde{A}^6.
\end{aligned} \tag{4.4}$$

Determining these coefficients is a straightforward but tedious combinatoric problem; it involves counting the number of different ways that the time-dependent phases can cancel against each other, and so survive the infinite time average. Generalizing from equation (4.4), the coefficient of a term of the form $\prod_i (\mathrm{Tr}\,\tilde{A}^{m_i})^{p_i}$ in the expansion of $\overline{(A_t)^n}$ is given by $n!/(\prod_i p_i! m_i^{p_i})$, where $n = \sum_i m_i p_i$.

We now wish to estimate the magnitude of $\mathrm{Tr}\,\tilde{A}^m$ for different values of m. Necessary inputs include the quantum uncertainty Δ in the total energy E, given by equation (3.5); the energy bandwidth W of the matrix $A_{\alpha\beta}$ near energy E, given by

$$W \equiv \frac{\int_{-\infty}^{+\infty} \mathrm{d}\omega\,|f(E,\omega)|^2}{|f(E,0)|^2} \tag{4.5}$$

where $f(E,\omega)$ is defined in equation (2.4); the typical size a of the quantum/thermal fluctuations in A, given by

$$a^2 \equiv \overline{(A^2)_t} = \sum_\alpha |c_\alpha|^2 (A^2)_{\alpha\alpha} = \sum_{\alpha\beta} |c_\alpha|^2 |A_{\alpha\beta}|^2 \tag{4.6}$$

and the inverse participation ratio

$$\mathcal{I} \equiv \frac{1}{\sum_\alpha |c_\alpha|^4} \tag{4.7}$$

which counts the effective number of different energy levels that are present in the quantum state of the system. Also, $\mathcal{I}^{-1}$ can be regarded as the average value of $|c_\alpha|^2$. Given $\mathcal{I}$, it is helpful to define an effective level spacing between the participating energy eigenstates,

$$\delta_{\rm eff} \equiv \frac{\Delta}{\mathcal{I}}. \tag{4.8}$$

In general, $\delta_{\rm eff}$ must be greater than or equal to the actual level spacing $\delta \sim {\rm e}^{-S} E$.

Before proceeding to evaluate ${\rm Tr}\, \tilde{A}^m$, we must order the various energy scales. We expect that 'typical' states of physical interest will have $\delta_{\rm eff} \sim \delta$ and $\Delta \sim N^{-1/2} E \sim N^{1/2} T$, since these are properties of a thermal density matrix. We also expect that W will be independent of N. To see why, we turn to the formula for A_t, equation (3.1). From it, we can see that the timescale for the initial evolution of A_t is either $\overline{h}/W$ or $\overline{h}/\Delta$, whichever is larger. (Before this time, no relative phases have changed significantly.) For an observable A of interest, this timescale should be finite and non-zero in the thermodynamic limit, and hence independent of N. Since we expect $\Delta \sim N^{1/2} T$, it must be W that is independent of N. We therefore conclude that

$$\delta_{\rm eff} \ll W \ll \Delta \ll E \tag{4.9}$$

is the regime of interest.

With these considerations in place, we note that we can regard $\tilde{A}$ as a banded random matrix of overall size $(\Delta/\delta_{\rm eff}) \times (\Delta/\delta_{\rm eff})$ and bandwidth $W/\delta_{\rm eff}$. Within the band of non-zero matrix elements, the magnitude of a typical entry is

$$\tilde{A}_{\rm typ} \sim \mathcal{I}^{-1} (W/\delta)^{-1/2} a. \tag{4.10}$$

This comes from equation (4.6), whose last equality demonstrates that a typical value of $|A_{\alpha\beta}|^2$ is $(W/\delta)^{-1} a^2$; the extra factor of $\mathcal{I}^{-1}$ in equation (4.10) comes from the c_α's in equation (4.2). We can now estimate ${\rm Tr}\, \tilde{A}^m$ for even $m \equiv 2k$ as

$$\begin{aligned} {\rm Tr}\, \tilde{A}^{2k} &\sim \left(\frac{\Delta}{\delta_{\rm eff}}\right) \left(\frac{W}{\delta_{\rm eff}}\right)^k (\tilde{A}_{\rm typ})^{2k} \\ &\sim \left(\frac{\Delta}{\delta_{\rm eff}}\right) \left(\frac{\delta_{\rm eff}}{\Delta}\right)^{2k} \left(\frac{\delta}{\delta_{\rm eff}}\right)^k a^{2k}. \end{aligned} \tag{4.11}$$

For odd $m \equiv 2k+1$, the expected value of ${\rm Tr}\, \tilde{A}^{2k+1}$ can be positive or negative; a root-mean-square estimate of its magnitude is

$$\begin{aligned} {\rm Tr}\, \tilde{A}^{2k+1} &\sim \left(\frac{\Delta}{\delta_{\rm eff}}\right)^{1/2} \left(\frac{W}{\delta_{\rm eff}}\right)^k \left(\tilde{A}_{\rm typ}\right)^{2k+1} \\ &\sim \left(\frac{\Delta}{W}\right)^{1/2} \left(\frac{\delta_{\rm eff}}{\Delta}\right)^{2k+1} \left(\frac{\delta}{\delta_{\rm eff}}\right)^{(2k+1)/2} a^{2k+1}. \end{aligned} \tag{4.12}$$

However, this estimate should be regarded as less trustworthy than equation (4.11).

Equations (4.11) and (4.12) imply that the probability distribution for A_t has the form

$$P(A_t) \propto \exp\left[-\left(\frac{\Delta}{\delta_{\rm eff}}\right) F_+\left(\frac{A_t}{(\delta/\delta_{\rm eff})^{1/2}a}\right) - \left(\frac{\Delta}{W}\right)^{1/2} F_-\left(\frac{A_t}{(\delta/\delta_{\rm eff})^{1/2}a}\right)\right] \tag{4.13}$$

where $F_+(x)$ and $F_-(x)$ are even and odd functions (respectively) whose Taylor expansions involve purely numerical coefficients. Equation (4.13) can be verified by via a Feynman-diagram expansion for the moments; the quadratic term from F_+ provides the propagator, and the remaining terms (in both F_+ and F_-) give the vertex coefficients.

For $A_t \lesssim (\delta/\delta_{\rm eff})^{1/2}a$, we can neglect F_- and all but the quadratic term in F_+; we then have

$$P(A_t) \propto \exp\left[-\frac{\xi_2}{2}\left(\frac{\Delta}{\delta}\right)\left(\frac{A_t}{a}\right)^2\right] \tag{4.14}$$

where $F_+(x) = \frac{1}{2}\xi_2 x^2 + {\rm O}(x^4)$, and ξ_2 is a number of order one. Thus, for sufficiently small values of A_t, its probability distribution (as induced by a uniform distribution for t) is Gaussian, and independent of the details of the initial state; only the energy width Δ of this state is relevant. Furthermore, we see again that the fluctuations of A_t about its infinite time average (which is zero, by construction) are suppressed by a factor of $(\delta/\Delta)^{1/2} \sim {\rm e}^{-S/2}$.

For $A_t \gtrsim (\delta/\delta_{\rm eff})^{1/2}a$, the non-universal behaviour of the functions $F_\pm$ becomes relevant. Initial states that are 'typical' according to most any reasonable criterion would all have $\delta_{\rm eff} \sim \delta$. In this case the non-universal corrections are important for $A_t \gtrsim a$.

So far, our analysis has not addressed our original question: given the initial value A_0, what is the behaviour of A_t at later times? To answer this question, we must compute the conditional probability $P(A_t|A_0)$ to find the value A_t at time t, given the value A_0 at time zero. By the usual rules of probability theory, this conditional probability can be expressed as

$$P(A_t|A_0) = \frac{P(A_t, A_0)}{P(A_0)} \tag{4.15}$$

where $P(A_t, A_0)$ is the joint probability for the observable A to have the expectation values A_t at time t and A_0 at time zero. This joint probability is induced by assuming a uniform distribution for the initial time; hence the moments of $P(A_t, A_0)$ are given by $\overline{(A_{t+t'})^n (A_{t'})^m}$, where the time averaging is done with respect to t', with t held fixed. To compute these moments, we need an expansion analogous to equation (4.4). Let us focus on the universal regime. In this case, the dominant terms in the expansion, as in equation (4.4), are those with the largest number of traces. Keeping only these terms results in a Gaussian distribution. As always for a Gaussian distribution, it is completely determined by its second moments,

$$\begin{aligned} \overline{A_{t+t'}A_{t'}} &= \sum_{\alpha\beta} |\tilde{A}_{\alpha\beta}|^2 {\rm e}^{{\rm i}(E_\alpha - E_\beta)t} \\ \overline{(A_{t+t'})^2} &= \overline{(A_{t'})^2} = \sum_{\alpha\beta} |\tilde{A}_{\alpha\beta}|^2. \end{aligned} \tag{4.16}$$

To streamline the notation a little we define a correlation function

$$C(t) \equiv \overline{A_{t+t'}A_{t'}}/\overline{(A_{t'})^2}. \tag{4.17}$$

Note that, by construction, $C(0) = 1$.

These considerations lead to

$$P(A_t, A_0) \propto \exp\left[-\frac{\xi_2}{2}\left(\frac{\Delta}{\delta}\right)\frac{(A_t)^2 + (A_0)^2 - 2C(t)A_tA_0}{[1-C(t)]^2 a^2}\right] \tag{4.18}$$

which has the correct second moments. Then, equations (4.14), (4.15), and (4.18) give us the conditional probability

$$P(A_t|A_0) \propto \exp\left[-\frac{\xi_2}{2}\left(\frac{\Delta}{\delta}\right)\frac{[A_t - C(t)A_0]^2}{[1-C(t)]^2 a^2}\right] \tag{4.19}$$

in the universal regime. Recalling that $\Delta/\delta \sim \mathrm{e}^S$, equation (4.19) shows us that it is overwhelmingly likely that we will find $A_t = C(t)A_0$. In the next section, we will see that the correlation function $C(t)$ does not depend on the quantum state of the system. Thus, for all practical purposes, A_t is fully determined just by the initial value A_0; no other information about the state of the system is needed.

For $A_0 \gtrsim (\delta/\delta_{\mathrm{eff}})^{1/2}a$, the non-universal corrections can become important. We then expect a formula for $P(A_t|A_0)$ that is similar to equation (4.13). Because the large prefactor of $\Delta/\delta \sim \mathrm{e}^S$ should still be present, we still expect to get an effectively deterministic equation for A_t as a function of t and A_0, although it will no longer take the simple form $A_t = C(t)A_0$.

Returning to the universal regime, we need to study the properties of $C(t)$. This we do in the next section.

5. Linear response

Equations (4.16) and (4.17) imply that the correlation function $C(t)$ is real, even, and has a maximum magnitude of one. Also, it is quasiperiodic on the scale of the Heisenberg time $\tau_{\mathrm{H}} = 2\pi\hbar/\delta \sim \mathrm{e}^S$. However, this timescale is much too long to be of physical interest, and so we can justifiably ignore the quasiperiodicity of $C(t)$. Then, also using equations (2.4) and (4.2), we get

$$\begin{aligned} C(t) &\propto \sum_{\alpha\beta} |c_\alpha|^2 |c_\beta|^2 |A_{\alpha\beta}|^2 \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)t} \\ &\propto \int_{-\infty}^{+\infty} \mathrm{d}\omega\, |f(E,\omega)|^2 \mathrm{e}^{\mathrm{i}\omega t}. \end{aligned} \tag{5.1}$$

The last line shows that $C(t)$ does not depend on the initial state, and that the bandwidth W of $f(E,\omega)$ sets the timescale for $C(t)$.

Equation (5.1) can be compared with the results obtained through more standard methods. For example [22], we can give A a non-zero expectation value at $t = 0$ by supposing that, for $t < 0$, the system's hamiltonian was perturbed to $H + \lambda A$, where λ is a constant. For $t \leqslant 0$, we assume that the quantum state of the system is described by a thermal density matrix $\rho_0 \sim \mathrm{e}^{-(H+\lambda A)/T}$. For $t \geqslant 0$, this state is evolved forward in time with the original hamiltonian H, so that $\rho_t = \mathrm{e}^{-\mathrm{i}Ht}\rho_0 \mathrm{e}^{\mathrm{i}Ht}$; the time-dependent expectation value of A is then $A_t \equiv \mathrm{Tr}\,\rho_t A$. To leading order in λ, this procedure results in $A_t = C_{\mathrm{Kubo}}(t)A_0$, where

$$C_{\mathrm{Kubo}}(t) \propto \int_0^{1/T} \mathrm{d}\mu\, \langle A_H(-\mathrm{i}\mu)A_H(t)\rangle_T. \tag{5.2}$$

Here $A_H(t) \equiv \mathrm{e}^{\mathrm{i}Ht}A\mathrm{e}^{-\mathrm{i}Ht}$ is the operator A in the Heisenberg picture, and the angle brackets denote canonical thermal averaging as in equation (2.8). Equation (5.2) can be written in terms of the matrix elements $A_{\alpha\beta}$ as

$$\begin{aligned} C_{\mathrm{Kubo}}(t) &\propto \sum_{\alpha\beta} \frac{\mathrm{e}^{-E_\alpha/T} - \mathrm{e}^{-E_\beta/T}}{E_\beta - E_\alpha} |A_{\alpha\beta}|^2 \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)t} \\ &\propto \int_{-\infty}^{+\infty} \mathrm{d}\omega\, \frac{\sinh(\omega/2T)}{\omega} |f(E,\omega)|^2 \mathrm{e}^{\mathrm{i}\omega t}. \end{aligned} \tag{5.3}$$

This is not the same as equation (5.1). Suppose, however, that the bandwidth W of $f(E,\omega)$ is smaller than the temperature T, and that the falloff of $f(E,\omega)$ for $\omega \gg W$ is fast enough to make the integral in equation (5.3) converge. Then the factor of $\sinh(\omega/2T)/\omega$ will be approximately constant over the relevant range of ω, and so we will get

$$C_{\text{Kubo}}(t) = C(t) + \text{O}(W^2/T^2). \tag{5.4}$$

In this case, equation (4.19) may be viewed as a verification of Onsager's postulate [27] that a random fluctuation (in the value of some quantity) will dissipate in the same way as an initial value that is produced by an applied force.

Let us now consider the circumstances under which the time evolution will be markovian. In the linear regime, and for $t > 0$, a markovian equation has the form $(\text{d}/\text{d}t)A_t = -\Gamma A_t$, where the parameter Γ must be real and positive. Given $A_t = C(t)A_0$, this implies $C(t) = \exp(-\Gamma|t|)$. From equation (5.1), we see that this corresponds to $|f(E,\omega)|^2 \propto 1/(\omega^2 + \Gamma^2)$, and hence $W \sim \Gamma$. However, $1/(\omega^2 + \Gamma^2)$ does not fall off fast enough at large ω for convergence of the integral in equation (5.3), and so we expect some additional suppression of $|f(E,\omega)|^2$ when ω is greater than the temperature T. If it happens that Γ is much less than T, then the time evolution will still be approximately markovian, but with 'memory' effects on timescales less than $\hbar/T$. This is consistent with other analyses [24, 28], which find that the time evolution of expectation values is always non-markovian on timescales less than $\hbar/T$, essentially because of the energy-time uncertainty principle. The overall conclusion is that markovian time evolution is associated with an isolated pole in $|f(E,\omega)|^2$ at $\omega = \pm\text{i}\Gamma$, with $\Gamma \ll T$. However, this structure for $|f(E,\omega)|^2$ is not required by any general principles, and so non-markovian behaviour on all timescales is an open possibility.

6. Discussion

Our major result is equation (4.19), which gives the probability to find that an observable A has a quantum expectation value of A_t at time t, given that its expectation value is A_0 at time zero (and assuming that A has been shifted, if necessary, so that the infinite time average of A_t is zero). This probability is computed for a particular quantum state $|\psi_t\rangle$, but with the zero of time treated as a uniformly distributed random variable.

To understand the essential features of equation (4.19), it is helpful to rewrite it more schematically as

$$P(A_t|A_0) \propto \exp\{-\text{O}(\text{e}^S)[A_t - C(t)A_0]^2/a^2\}. \tag{6.1}$$

Here $A_t \equiv \langle\psi_t|A|\psi_t\rangle$ is the time-dependent quantum expectation value of A; a^2 is the mean squared amplitude of the quantum fluctuations (which are also to be identified as thermal fluctuations) in A; S is the thermodynamic entropy at energy $E = \langle\psi_t|H|\psi_t\rangle$; and $C(t)$ is the correlation function (normalized to one at $t = 0$) given in equation (5.1), which, under favourable circumstances, is the same as the Kubo correlation function $C_{\text{Kubo}}(t)$ given in equation (5.3). The range of validity of equation (6.1) is $A_0 \lesssim (\delta/\delta_{\text{eff}})^{1/2}a$, where $\delta \sim \text{e}^{-S}E$ is the mean energy-level spacing near E, and $\delta_{\text{eff}} \geqslant \delta$ is the mean level spacing for those eigenstates that participate significantly in $|\psi_t\rangle$. Maximum participation (such as would be predicted by a thermal density matrix) corresponds to $\delta_{\text{eff}} \sim \delta$.

Equation (6.1) implies an effectively deterministic evolution equation for A_t, given only A_0 as input: $A_t = C(t)A_0$. The probability that this equation is not satisfied is $\text{O}(\text{e}^{-S})$. Since $C(t)$ is an even function of time, the effective evolution equation is invariant under time reversal. However, $C(t) \leqslant C(0)$ for all t, and $C(t)$ decays to zero if the bandwidth W, defined in equation (4.5), is finite. (There will be quasiperiodic resurgences of $C(t)$ on the scale of

the Heisenberg time $\tau_{\rm H} = 2\pi\hbar/\delta \sim {\rm e}^S$, but this is much too long to be relevant.) Thus a non-zero initial value A_0 is overwhelmingly likely to evolve, both forwards and backwards in time, towards the equilibrium value of zero. This is of course entirely consistent with the heuristic picture of statistical mechanics originally proposed by Boltzmann.

If the envelope function $|f(E,\omega)|^2$, defined in equation (2.4), has an isolated pole at $\omega = \pm{\rm i}\Gamma$, then the time evolution will be approximately markovian, with $C(t) \simeq \exp(-\Gamma|t|)$. This is consistent with $C(t) \simeq C_{\rm Kubo}(t)$ only if $\Gamma \ll T$, where T is the temperature corresponding to a thermodynamic energy of E. There will still be non-markovian 'memory' effects on timescales less than $\hbar/T$, which is consistent with the results of other analyses [24, 28].

To get equation (6.1) (or, more precisely, (4.19)), we had to make a fairly strong assumption about the quantum matrix elements of A, equation (2.4). However, this equation is well grounded in quantum chaos theory, and is likely to be at least approximately valid under a fairly wide range of circumstances.

Naturally it would be useful to extend our results to the nonlinear regime, and naturally this is much harder to do. Still, we hope to return to this question in future work. A combination of our methods (which easily demonstrate the ubiquity of thermal equilibrium) with projection-operator methods (which easily generate equations for expectation values, assuming appropriately forced thermal density matrices as the starting point [23, 24]) might be a fruitful approach.

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