Equilibration of isolated macroscopic quantum systems under experimentally realistic conditions

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Received 12 June 2012
Accepted for publication 4 September 2012
Published 19 October 2012
Online at stacks.iop.org/PhysScr/86/058512

Abstract
In how far does a non-equilibrium initial ensemble evolve towards a stationary long time behavior for an isolated macroscopic quantum system? We demonstrate that deviations from a steady state indeed become unmeasurably small or exceedingly rare after initial transients have died out under the following conditions: the Hamiltonian does not exhibit exceedingly large degeneracies of energy eigenvalues and energy gaps. A large number of energy levels are significantly populated by the initial ensemble. The system is observed by a measurement device with a reasonably bound working range compared to the resolution limit. The entire experiment, ending in the quantum mechanical measurement process, can only be repeated a ‘reasonable’ number of times. It is argued that all these prerequisites for equilibration are fulfilled under many, if not all, experimentally realistic conditions.

PACS numbers: 05.30.d, 05.30.Ch, 03.65.-w

1. Introduction
According to textbook statistical physics, all the properties of a macroscopic system at thermal equilibrium are perfectly described by the canonical ensemble when weakly coupled to a thermal bath and by the microcanonical ensemble when isolated from the rest of the world. However, there still seems to be no truly satisfying explanation of why this is so [1, 2].

Here we adopt the most common viewpoint that investigations of this problem should be based on standard quantum mechanics and should start with the treatment of isolated systems. Indeed, it is widely believed that by considering a system in contact with a thermal bath as a single, isolated ‘supersystem’, the canonical formalism should be deducible from the microcanonical one. In turn, to directly describe an open system alone (without the bath to which it is coupled) by means of standard quantum mechanics does not seem possible.

Excellent reviews of the large number of pertinent ‘classical’ (i.e. older) works are provided, e.g., by [1, 2], while more recent developments are covered, e.g., by [4, 5]. In this work, we summarize and further develop a recently developed new approach [6–12] to the fundamental question: in how far does a non-equilibrium initial ensemble evolve towards a stationary long time behavior? Besides this problem of equilibration, a second fundamental issue is the problem of thermalization, i.e. the question whether, and to what extent, such a steady state is in agreement with the microcanonical ensemble predicted by equilibrium statistical mechanics. This important issue, either for an isolated system per se or for an isolated system-plus-bath composite, has recently been addressed, e.g., in [4–9, 13–35] but will not be considered here in any further detail.

A first key point of our approach is the modeling concept [2] that any given experimental system gives rise to a specific, well-defined statistical ensemble (density operator) the details of which are, however, unknown in practice. Typically, one only knows that in the initial state certain (usually macroscopic) observables are relatively sharply distributed about some approximately known mean values. A main challenge of the theory is to properly cope with this lack of knowledge. A second key point is not to modify or approximate in any way the exact quantum mechanical time evolution. The third key point is to focus on experimentally realistic observables, exhibiting a finite range and a finite resolution.

For the rest, our present approach still covers essentially arbitrary (generic) systems and as such is complementary to...
many recent investigations on different specific model classes, observables and initial conditions—often with a main focus on the so-called eigenstate thermalization hypothesis and the role of (non-)integrability in this context—see, e.g., [4, 5, 14–35]. In particular, our present approach is not restricted to macroscopic observables, in contrast to, e.g., [13, 36, 37]. The reason is that equilibrium statistical mechanics, in fact, also covers microscopic observables, e.g. the position, velocity, etc of one specific ‘tracer’ particle within a fluid, and its pertinent (probabilistic) predictions are in perfect agreement with numerical simulations and with the rapidly increasing number of experiments on single molecules, nano-particles, etc.

2. Model assumptions

We consider a large (macroscopic but finite), isolated system, modeled in terms of a Hilbert space \( \mathcal{H} \) and a time-independent Hamiltonian \( H : \mathcal{H} \rightarrow \mathcal{H} \) of the form

\[
H = \sum_n E_n P_n,
\]

where \( P_n \) are the projectors onto the eigenspaces of \( H \) with mutually different eigenvalues \( E_n \) and multiplicities

\[
\mu_n := \text{Tr}(P_n).
\]

For the sake of simplicity, we restrict ourselves throughout this paper to Hilbert spaces \( \mathcal{H} \) of arbitrarily large but finite dimensions. Generalizations to infinite dimensions are readily possible along the lines of [12]. In particular, the number of distinct energy eigenvalues is given by some finite integer \( N_E \) and the indices \( n \) in (1) and (2) run from 1 to \( N_E \).

Besides the multiplicities/denegeracies of the energy levels from (2), a related further quantity of central importance will be the maximal degeneracy of energy gaps

\[
g := \max_{m, n} |\langle (k, l) : E_k - E_l = E_m - E_n \rangle|,
\]

where \( |S| \) denotes the number of elements contained in the (finite) set \( S \). In other words, \( g \) is the maximal number of (exactly) coinciding energy differences among all possible pairs of distinct energy eigenvalues. In particular, \( g = 1 \) is tantamount to the absence of any degenerate energy gaps: for a given \( m \neq n \) and (thus \( E_m \neq E_n \)) all energy gaps \( E_k - E_l \) are different from \( E_m - E_n \), except for \( k = m \) and \( l = n \).

System states are described by density operators \( \rho(t) \), evolving according to \( \dot{\rho}(t) = U_t \rho(0) U_t^\dagger \) with propagator \( U_t := \exp[-iHt] \) and \( h = 1 \). With (1) we can thus conclude that

\[
\rho(t) = \sum_{m,n} \rho_{mn}(0) \exp[-i(E_m - E_n)t],
\]

where we have introduced the auxiliary operators

\[
\rho_{mn}(t) := P_m \rho(t) P_n.
\]

Observables are modeled by self-adjoint operators \( A \) with expectation values \( \text{Tr}(\rho(t) A) \). Similarly to (1), any such \( A \) can be written in the form

\[
A = \sum_v a_v Q_v,
\]

where \( Q_v \) are the projectors onto the eigenspaces of \( A \) with \( N_A \) mutually different eigenvalues \( a_v \).

A single quantum mechanical measurement process of the observable \( A \) on the system in the state \( \rho(t) \) thus results in one of the \( N_A \) possible outcomes \( a_v \), and the probability of obtaining the specific outcome \( a_v \) is given by

\[
q_v(t) := \text{Tr}(\rho(t) Q_v).
\]

Upon repeating the same experiment (the same measurement and system state) \( N_{\text{rep}} \) times, every outcome \( a_v \) is thus obtained approximately \( N_v := q_v(t) N_{\text{rep}} \) times with typical statistical fluctuations/uncertainties of the order of \( \sqrt{N_v} \). In other words, the ‘true’ values of \( q_v(t) \) can be determined by means of \( N_{\text{rep}} \) measurements up to a statistical uncertainty of approximately

\[
\delta q_v(t) = \frac{\sqrt{q_v(t)} / N_{\text{rep}}.}
\]

While, in principle, one and the same experiment can be repeated arbitrarily often, in practice (under experimentally realistic conditions) the number of repetitions \( N_{\text{rep}} \) must remain ‘reasonable’. To be on the safe side, we will henceforth take for granted the quite weak bound

\[
N_{\text{rep}} \leq 10^{20}.
\]

In fact, also \( N_{\text{rep}} \leq 10^{10} \) or \( N_{\text{rep}} \leq 10^{1000} \) would still be no problem in our later considerations, and it seems convincing that a theory that does not go very much beyond that will do.

As pointed out, e.g., in [36, 38–44], it is not necessary to admit any arbitrary self-adjoint operator \( A \) in order to model real experimental measurements. Rather, it is sufficient to focus on experimentally realistic observables in the following sense [6, 9, 45]: any observable \( A \) must represent an experimental device with a finite range of possible outcomes of a measurement,

\[
\Delta_A := \max_{|\psi, \psi\rangle} (|\langle \psi | A | \psi \rangle| - \min_{|\psi, \psi\rangle} (|\langle \psi | A | \psi \rangle| = a_{\text{max}} - a_{\text{min}}.
\]

where the maximization and minimization are over all normalized vectors \( |\psi\rangle \in \mathcal{H} \) and where \( a_{\text{max}} \) and \( a_{\text{min}} \) are the largest and smallest eigenvalues of \( A \). Moreover, this working range \( \Delta_A \) of the device must be limited to experimentally reasonable values compared to its resolution limit \( \delta A \). Due to the manifold and often not very well understood contributions to the uncertainty \( \delta A \) of a real experimental measurement, quantitative estimates are not easy. However, it seems reasonable to claim that uncertainties of less than, say, \( 10^{-20} \), of the instrumental range \( \Delta_A \) are impossible to achieve, i.e.

\[
\Delta_A / \delta A \leq 10^{20}.
\]

Similarly as below (9), also exponents of 100 or 1000 are still admissible, and to go even far beyond that does not seem to be necessary to faithfully model any real or numerical experiment.

A particularly interesting and important example is a digital instrument, displaying \( d \) decimal places. In this case, we have that \( N_A = 10^d \) and we can assume without loss of generality that \( a_v = \delta A (v - 1) \) with \( v = 1, \ldots, N_A = 10^d \) and thus \( \Delta_A = (N_A - 1) \delta A \). It is quite convincing that every experimentally realistic measurement device, both digital and
analogue, can be satisfactorily modeled along these lines. Moreover, all measurements known to the present author yield less than 20 relevant digits, i.e.
\[ \Delta A / \delta A = N_A - 1 \approx 10^{30}, \]  
(12)
in accordance with our general estimate (11).

Next we focus on the specific observable \( A = P_n \), describing according to (1) the population of the (possibly degenerate) energy level \( E_n \) with expectation value (occupation probability)
\[ p_n := \text{Tr}[P_n \rho(t)]. \]  
(13)
Note that \( P_n \) commutes with \( H \) from (1) and hence the level populations \( p_n \) are conserved quantities.

For a system with \( f \) degrees of freedom there are roughly \( 10^{3(f/2)} \) energy eigenstates with eigenvalues in every interval of 1 \( J \) beyond the ground state energy, see, e.g., [46] or section 2.1 in [9]. The same estimate carries over to the number of energy eigenvalues under the assumption that their multiplicities (2) are much smaller than \( 10^{3(f/2)} \). For a macroscopic system with \( f = \mathcal{O}(10^{23}) \), the energy levels are thus unimaginably dense on any decent energy scale and even the most careful experimentalist will not be able to populate only a few of them with significant probabilities \( p_n \), in particular after averaging over the ensemble, i.e. over many repetitions \( N_{\text{rep}} \) of the experiment. In the generic case, we can thus conclude [6, 9, 45] that even if the system’s energy is fixed to an extremely small experimental uncertainty and even if the energy levels are populated extremely unequally, we still expect that even the largest ensemble-averaged level population \( p_n \) will be extremely small (compared to \( \sum_n p_n = 1 \)) and typically satisfy the very rough estimate
\[ \max_n p_n = 10^{-3(f/2)}. \]  
(14)

3. Definition of equilibration

Generically, the statistical ensemble \( \rho(t) \) is not stationary right from the beginning, in particular for an initial condition \( \rho(0) \) out of equilibrium. But if the right-hand side of (4) depends on \( t \) initially, it cannot approach for large \( t \) any time-independent ‘equilibrium ensemble’ whatsoever. In fact, any mixed state \( \rho(t) \) returns arbitrarily close (with respect to some suitable distance measure in Hilbert space) to its initial state \( \rho(0) \) for certain, sufficiently large times \( t \), as demonstrated, for instance, in appendix D of [47]. We emphasize that these arbitrarily close recurrences do not refer to pure states only (as in the classical Poincaré recurrences) but rather to arbitrary statistical ensembles \( \rho(t) \).

As an example, we focus on the simplest case that all eigenvalues \( E_n \) in (1) are non-degenerate and thus every projector \( P_n \) is of the form \(| n \rangle \langle n | \), where \(| n \rangle \) is the (unique) eigenvector belonging to the eigenvalue \( E_n \). Next, we consider any \( \rho(t) \) which is (at least initially) not completely independent of \( t \). So, according to (4) there must exist a pair of indices \( m, n \) with the property that \( \langle m | \rho(0) | n \rangle \neq 0 \) and \( \Omega := [E_n - E_m] / \hbar \neq 0 \). Then, by focusing on the specific observable
\[ A = B + B^\dagger, \quad B := | m \rangle \langle n | / \langle m | \rho(0) | n \rangle, \]  
(15)
it readily follows from (4) that
\[ \text{Tr}[\rho(t)A] = 2 \cos(\Omega t). \]  
(16)
In other words, the ensemble \( \rho(t) \) exhibits permanent oscillations rather than equilibration, at least as far as the specific observable (15) is concerned.

The main implication of the two previous paragraphs is that equilibration cannot be true (and hence cannot be proven) in full generality and rigor. Put differently, Quantum Mechanics and equilibration are strictly speaking incompatible. Equilibration can at most approximately hold true for a restricted class of observables \( A \) and initial conditions \( \rho(0) \). We therefore focus on the weaker notion of equilibration from [6–12], which merely requires the existence of a time-independent ‘equilibrium state’ \( \bar{\rho} \) (density operator) with the property that the difference
\[ \sigma(t) := \text{Tr}[\rho(t)A] - \text{Tr}[\bar{\rho}A] \]  
(17)
between the true expectation value \( \text{Tr}[\rho(t)A] \) and the equilibrium reference value \( \text{Tr}[\bar{\rho}A] \) is unsolvably small for the overwhelming majority of times \( t \) contained in any sufficiently large (but finite) time interval \([0, T] \). In other words, the expectation values \( \text{Tr}[\rho(t)A] \) may still exhibit everlasting small fluctuations around their ‘equilibrium values’ \( \text{Tr}[\bar{\rho}A] \), as well as very rare large excursions away from equilibrium (including the above-mentioned recurrences [2]), but quantitatively these fluctuations are either unobservably small or exceedingly rare on any realistic time scale after initial transients have died out. (Note that those initial transients become irrelevant if \( T \) is chosen large enough.) The compatibility of the specific example (15) and (16) with this notion of equilibration will be further discussed in section 6.

As we will see below, such an equilibrium ensemble \( \bar{\rho} \) indeed exists under quite weak conditions, and is given by the following definition:
\[ \bar{\rho} := \sum_n \rho_{nn}, \]  
(18)
where the operators \( \rho_{nn} := \rho_{nn}(t) \) are defined via (5) and where the time arguments of \( \rho_{nn}(t) \) have been omitted since these operators are in fact time independent according to (4) and (5).

Intuitively, (18) may be viewed as the infinite-time average of \( \rho(t) \) from (4), but also as the time-independent or the ‘diagonal’ part of \( \rho(t) \). However, it should be emphasized that the definition (18) is formally self-contained and unambiguous without any such ‘interpretation’. In particular, \( \bar{\rho} \) in (18) is well defined, independently of whether the infinite-time average of \( \rho(t) \) actually exists or not. Note that also physically, the ‘equilibrium state’ \( \bar{\rho} \) is mainly a theoretical ‘vehicle’ without a direct correspondence in the real system.

In the following, we will see that the above-mentioned ‘equilibration properties’ of \( \sigma(t) \) from (17) indeed can be demonstrated by adopting this specific choice (18) of the ‘equilibrium state’ \( \bar{\rho} \).
interest turns out (as one might have expected) to be the time-averaged variance
\[
\langle \sigma^2(t) \rangle_T := \frac{1}{T} \int_0^T dt \sigma^2(t)
\]  
(19)
following from (17) and (18). Considering and estimating such averages has a long tradition, see, e.g., [3, 14, 48–52]. Substantial progress along this line has been achieved quite recently in the works [6–12]. In the following, we summarize and further develop this approach.

4. Equilibration of mean values
Closely following the line of reasoning of Short and Farrelly [11], we introduce (4), (17), (18) into (19) to conclude that
\[
\langle \sigma^2(t) \rangle_T = \left( \sum_{m \neq \alpha} \text{Tr}[\rho_{mn}A] \exp \left[ -i(E_m - E_n)T \right] \right)^2
\]  
(20)
where \( \rho_{mn}(0) \) is abbreviated as \( \rho_{mn} \) and the sum runs over the finite set of pairs of labels
\[
\mathcal{G} := \{(m, n) : m, n \in [1, \ldots, N_E], m \neq n \}.
\]  
(21)
Defining for any \( \alpha \in \mathcal{G} \) with \( \alpha = (m, n) \) the two quantities
\[
G_\alpha := E_m - E_n, \quad v_\alpha := \text{Tr}[\rho_{mn}A]
\]  
(22)
and introducing the self-adjoint, non-negative matrix \( M \) with matrix elements
\[
M_{\alpha \beta} := \langle \exp \left[ i(G_\alpha - G_\beta)t \right] \rangle_T,
\]  
(23)
we can rewrite (20) as
\[
\langle \sigma^2(t) \rangle_T = \left( \sum_{\alpha} v_\alpha \exp \left[ -iG_\alpha T \right] \right)^2 = \sum_{\alpha, \beta} v_\alpha^* M_{\alpha \beta} v_\beta.
\]  
(24)
Denoting by \( \| M \| \) the standard operator norm of the matrix \( M \) (tantamount to the largest eigenvalue of \( M \)) it follows that [11]
\[
\langle \sigma^2(t) \rangle_T \leq \| M \| \sum_{\alpha} |v_\alpha|^2 = \| M \| \sum_{m \neq \alpha} |\text{Tr}[\rho_{mn}A]|^2.
\]  
(25)
Obviously, every matrix element (23) exhibits a well-defined limit as the averaging time \( T \) (cf (19)) tends to infinity. Thanks to our restricting ourselves to finite dimensions below (1), it then follows that also the norm \( \| M \| \) converges for \( T \to \infty \). Hence, \( \| M \| \) can be bounded from above for all sufficiently large (but finite) \( T \). Quantitatively, for non-degenerate energy gaps, i.e. \( g = 1 \) in (3), one can infer from (23) that \( M \) approaches the unit matrix for \( T \to \infty \) and hence \( \| M \| \to 1 = g \). As demonstrated in [11, 12], the same result \( \| M \| \to g \) for \( T \to \infty \) remains valid for arbitrary \( g \). We can thus conclude that \( \| M \| \leq 2g \) for all sufficiently large \( T \), where \( g \) is the maximal degeneracy of energy levels from (3). Observing that the sum in (25) can only grow by extending it to all \( m, n \in [1, \ldots, N_E] \), it follows that
\[
\langle \sigma^2(t) \rangle_T \leq 2g \sum_{m, n} |\text{Tr}[\rho_{mn}A]|^2
\]  
(26)
for all sufficiently large \( T \). We remark that this is the only place where our restriction to finite dimensions below (1) is essential. While it is quite plausible that everything still ‘goes well’ in the limit of infinite dimensions [6, 9], a more detailed justification is actually not so obvious and has been worked out in [12].

Next we employ (5) for \( \rho_{nn} = \rho_{mn}(0) \), the property \( P_n^2 = P_m \) of any projector \( P_m \), and the cyclic invariance of the trace to conclude that
\[
\text{Tr}[\rho_{mn}A] = \text{Tr}[P_m \rho(0) P_n A P_m].
\]  
(27)
Since \( \rho := \rho(0) \) is a self-adjoint, non-negative operator, one can infer that there exists a self-adjoint, non-negative operator, which we denote by \( \rho^{1/2} \), and which satisfies the relation \( \rho^{1/2} \rho^{1/2} = \rho \). Observing that
\[
P_m P_n A P_m = (P_m \rho^{1/2})(\rho^{1/2} P_n A P_m),
\]  
(28)
and exploiting the Cauchy–Schwarz inequality
\[
|\text{Tr}[B^\dagger C]|^2 \leq \text{Tr}[B^\dagger B] \text{Tr}[C^\dagger C],
\]  
(29)
for the scalar product \( \text{Tr}[B^\dagger C] \) of arbitrary operators \( B \) and \( C \), it follows from (5), (13), and (27) that
\[
|\text{Tr}[\rho_{mn}A]|^2 \leq p_m \text{Tr}[\rho_{mn} A P_m A]
\]  
(30)
and hence
\[
\sum_{m, n} |\text{Tr}[\rho_{mn}A]|^2 \leq \text{Tr} \left( \sum_n \rho_n A \left( \sum_m p_m P_m \right) A \right).
\]  
(31)
Introducing
\[
\omega := \sum_m p_m P_m
\]  
(32)
and taking into account (18) we thus obtain
\[
\sum_{m, n} |\text{Tr}[\rho_{mn}A]|^2 \leq \text{Tr}[\rho A \omega A] = \text{Tr} [\omega A \bar{\rho} A].
\]  
(33)
Finally, we observe that
\[
\text{Tr}[B C] \leq \| B \| \text{Tr}[C],
\]  
(34)
for arbitrary self-adjoint, non-negative operators \( B \) and \( C \), where
\[
\| B \| := \max \{ |\langle \psi | B | \psi \rangle : \langle \psi | \psi \rangle = 1 \}
\]  
(35)
denotes the standard operator norm (the largest eigenvalue of \( B \)). Since both \( \omega \) and \( A \bar{\rho} A \) are self-adjoint and non-negative, it follows that
\[
\text{Tr}[\omega A \bar{\rho} A] \leq \| \omega \| \text{Tr}[A \bar{\rho} A] = \| \omega \| \text{Tr}[\bar{\rho} A^2].
\]  
(36)
The first term on the right-hand side equals \( \max_n p_n \), according to (32). In view of (26) and (33) we can thus conclude that
\[
\langle \sigma^2(t) \rangle_T \leq 2 \text{Tr}[\bar{\rho} A^2] g \max_n p_n,
\]  
(37)
for all sufficiently large $T$. Since both $\tilde{\rho}$ and $A^2$ are self-adjoint and non-negative we can exploit (34) to conclude that $\text{Tr}(\tilde{\rho} A^2) \leq \|A^2\| \|\tilde{\rho}\|$. With $\text{Tr}(\tilde{\rho}) = 1$ it follows that $\text{Tr}(\tilde{\rho} A^2) \leq \|A^2\|$. Next we note that $\sigma(t)$ in (17) and thus $\{\sigma^2(t)\}$ in (19) remain unchanged if $A$ is replaced by $A + c 1$, where $c$ is an arbitrary real number and 1 the identity operator. Choosing $c$ so that $a_{\min} = -a_{\max}$ and thus $a_{\max} = \Delta_A/2$ in (10), it follows from (35) that $\|A\| = \Delta_A/2$. Altogether, we finally obtain the result
\[
\{\sigma^2(t)\}_T \leq \frac{1}{2} \Delta_A^2 g \max_n p_n, \quad (38)
\]
for all sufficiently large $T$.

Next we define for any given $\delta A > 0$ and $T > 0$ the quantity
\[
T_{\delta A} := \left\{ 0 < t < T : |\text{Tr}(\rho(t) A) - \text{Tr}(\tilde{\rho} A)| \geq \delta A \right\}, \quad (39)
\]
where $|S|$ denotes the size (Lebesgue measure) of the set $S$. According to (17), $T_{\delta A}$ thus denotes the measure of all times $t \in [0, T]$ for which $|\sigma(t)| \geq \delta A$ holds true. It follows that $\sigma^2(t) \geq \Delta_A^2$ for a set of times $t$ of measure $T_{\delta A}$ and $\sigma^2(t) \geq 0$ for all remaining times $t \in [0, T]$. Hence the temporal average (19) must be at least $\delta A^2 T_{\delta A}/T$ and we can conclude from (38) that
\[
\frac{T_{\delta A}}{T} \leq \frac{1}{2} \left( \frac{\Delta_A}{\delta A} \right)^2 g \max_n p_n, \quad (40)
\]
for all sufficiently large $T$. This is the first main result of the present paper. A more detailed discussion of its physical content is postponed to section 6.

5. Equilibration of individual measurement outcomes

Next we focus on the special case when $A$ happens to coincide with one of the projectors $Q_v$ in (6). Similarly to (39), we define for any given $\epsilon > 0$ and $T > 0$ the quantity
\[
T_{\epsilon, v} := \left\{ 0 < t < T : |\text{Tr}(\rho(t) Q_v) - \text{Tr}(\tilde{\rho} Q_v)| \geq \epsilon \right\}, \quad (41)
\]
and similarly to (40) we can conclude from (37) and $Q_v^2 = Q_v$ that
\[
\frac{T_{\epsilon, v}}{T} \leq \frac{2}{\epsilon^2} \text{Tr}(\tilde{\rho} Q_v) g \max_n p_n, \quad (42)
\]
for all sufficiently large $T$.

Returning to general observables $A$ of the form (6), we denote, similarly to (7), by
\[
\tilde{q}_v := \text{Tr}(\tilde{\rho} Q_v) \quad (43)
\]
the probability that a single measurement of $A$ would result in the outcome $a_v$ if the system were in the state $\tilde{\rho}$. Similarly to (8), upon repeating the same experiment $N_{\text{rep}}$ times, the ‘true’ frequency $\tilde{q}_v N_{\text{rep}}$ of the outcome $a_v$ can thus be determined up to a statistical uncertainty of approximately
\[
\delta \tilde{q}_v := \sqrt{\tilde{q}_v / N_{\text{rep}}} \quad (44)
\]
Focusing on the special choice $\epsilon = \delta \tilde{q}_v$, we can conclude from (42)–(44) that
\[
\frac{T_{\delta \tilde{q}_v}}{T} \leq 2 N_{\text{rep}} g \max_n p_n, \quad (45)
\]
for all sufficiently large $T$. According to (41), the left-hand side of (45) quantifies the fraction of all times $t \in [0, T]$ for which one may find by means of $N_{\text{rep}}$ measurements a statistically significant difference between the two frequencies $q_v(t) = \text{Tr}(\rho(t) Q_v)$ and $\tilde{q}_v = \text{Tr}(\tilde{\rho} Q_v)$ of observing the outcome $a_v$. For all other times $t \in [0, T]$, the ‘true’ frequency $q_v(t)$ cannot be distinguished from the one theoretically predicted by means of $\tilde{\rho}$. Denoting by $T^*$ the measure of all times $t \in [0, T]$ for which such a distinction is possible at least for one of the $N_A$ different indices $v$, one readily sees that $T^* \leq \sum_v T_{\tilde{q}_v, v}$ and thus with (45) that
\[
\frac{T^*}{T} \leq 2 N_{\text{rep}} N_A g \max_n p_n, \quad (46)
\]
for all sufficiently large $T$. For all other times $t \in [0, T]$, it is impossible to observe by means of $N_{\text{rep}}$ measurements of $A$ any kind of statistically significant difference between $\rho(t)$ and $\tilde{\rho}$.

6. Discussion

The first main result of this paper is relation (40). In fact, the same result has already been obtained before by Short and Farrelly in [11], but by means of quite a different line of reasoning.

In particular, these authors focus, in a first step, solely on pure states and only in the end extend their result to mixed states via purification. On the other hand, our present line of reasoning is very similar to that from [12], but the final result is significantly stronger.

According to (39), the left-hand side of (40) represents the fraction of all times $t \in [0, T]$ for which there is an experimentally resolvable difference between the true expectation value $\text{Tr}(\rho(t) A)$ and the time-independent equilibrium expectation value $\text{Tr}(\tilde{\rho} A)$. On the right-hand side of (40), $\Delta_A/\delta A$ is the range-to-resolution ratio, which may be very large but remains bounded according to (11) for experimentally realistic observables. The next factor, $g$, is the maximal degeneracy of energy gaps from (3). Finally, $\max_n p_n$ represents the largest, ensemble-averaged occupation probability of the (possibly degenerate) energy eigenvalues $E_n$, see (13). Typically, one expects that the rough upper bound (14) applies, except if certain energy eigenvalues are so extremely highly degenerate that the multiplicities defined in (2) severely reduce the pertinent energy level density compared to the non-degenerate case, see above (14).

For a system with sufficiently many degrees of freedom $f$ and no exceedingly large degeneracies of energy eigenvalues and energy gaps$^2$, we can thus conclude from (40) with (11) and (14) that the system behaves with respect to any experimentally measurable expectation value exactly as if it were in the equilibrium state $\tilde{\rho}$ for the overwhelming majority of times within a sufficiently large (but finite) time interval $[0, T]$. In particular, $T$ must obviously be much larger than

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1. In fact, the estimate obtained in [11] is even somewhat tighter than that in (40).

2. Note that no such degeneracies are actually encountered in the generic case [6, 7, 9, 14, 15, 50, 53], i.e. in the absence of special reasons like additional conserved quantities (e.g. due to (perfect) symmetries or when the system consists of non-interacting subsystems) or fine-tuning of parameters (‘accidental degeneracies’).
the relaxation time in the case of a far-from-equilibrium initial condition \( \rho(0) \).

Next we turn to the second main result of this paper, namely equation (46). Its left-hand side represents the fraction of all times \( t \in [0, T] \) for which one may find by means of \( N_{\text{rep}} \) measurements of \( A \) a statistically significant difference between the ‘true’ probabilities \( q_\theta(t) = \text{Tr} [\rho(t) Q_\theta] \) and the corresponding ‘equilibrium probabilities’ \( \tilde{q}_\theta = \text{Tr} [\rho_0 Q_\theta] \) of observing \( \theta \) of the \( N_A \) different possible outcomes \( a_\nu \) of the quantum mechanical measurement process. According to (9), (12) and (14) we can conclude from (46) that for a system with sufficiently many degrees of freedom \( f \) and no exceedingly large degeneracies of energy eigenvalues and energy gaps, the true state \( \rho(t) \) is practically indistinguishable from the equilibrium state \( \rho \) after initial transients have died out. More precisely, since a real experiment can only be repeated a ‘reasonable’ number of times (see (9)), the observable differences between \( \rho(t) \) and \( \rho \) are either smaller than the remnant statistical uncertainties or so unimaginably rare in time that they never actually occur in practice.

The main difference between (40) and (46) is that the former refers to the expectation value of \( A \), i.e. the mean value over all the actually observed outcomes \( a_\nu \) of the single repetitions of the experiment. In particular, statistical uncertainties due to finite numbers of experiments are not taken into account, i.e. \( N_{\text{rep}} \to \infty \) is implicitly taken for granted. The result (46) goes substantially beyond (40) in two respects. Firstly, it properly accounts for a finite number of experiments. Secondly and even more importantly, not only the first moment (mean value) but actually the full probability distribution of the different possible measurement outcomes is covered by the result (46).

It is instructive to illustrate the above general considerations by means of our specific example from (15) and (16). Recalling that in this example we are dealing with a non-degenerate Hamiltonian (1) with eigenvectors \( |n\rangle \), one readily sees that the spectrum of \( A \) from (15) consists of the two (non-degenerate) eigenvalues \( a_\pm = \pm |\rho_0(0)|^{-1} \), and one (highly degenerate) eigenvalue \( a_0 = 0 \). In other words, we have \( N_A = 3 \) distinct eigenvalues in (6). Furthermore, one can infer, similarly to (28) and exploiting (29), that \( |\langle m | \rho(0) |n\rangle|^2 \leq |\langle m | \rho(0) |m\rangle | \langle n | \rho(0) |n\rangle| \). According to (13), the latter product equals \( p_m p_n \). It follows that \( |a_\pm| \geq 1/\max p_n \) and hence from (10) that \( \Delta_A \geq 2/\max p_n \). For experimentally realistic initial conditions, we can infer from (14) that \( \Delta_A = O(1/\epsilon) \). On the other hand, in order to resolve the oscillations from (16), the experimental uncertainty \( \Delta A \) must not exceed unity.

In other words, while it is clearly impossible to deny the existence of the permanently oscillating expectation values (16), they cannot be actually ‘seen’ without admitting unrealistically large range-to-resolution ratios \( \Delta A/\delta A \) or statistical ensembles with unrealistically large energy level populations \( \max p_n \).

The same thing may alternatively be viewed as follows: any single (ideal) measurement process always results in one of the three outcomes \( a_+, a_- \) or \( a_0 \). Recalling that \( a_+ = -a_- \geq 1/\max p_n \) and \( a_0 = 0 \) it follows that an infeasible number of measurements \( N_{\text{rep}} \) would be needed to resolve the order-one variations of the ensemble average (16).

The above example also suggests that our assumptions of experimentally realistic observables, numbers of measurements and initial conditions (or some similar restrictions) are unavoidable for taming the oscillations in (4) and thus overcoming the fundamental incompatibility of basic quantum mechanics with rigorous equilibration, as detailed in section 3. In other words, it seems to be not an artifact of our present (or any other) specific line of reasoning, but rather a feature of ‘physical reality’ (within the realm of standard quantum mechanics) that invoking ‘our human inability’ is unavoidable in order to demonstrate and understand equilibration.

Acknowledgments

Collaboration with Michael Kastner on closely related issues is gratefully acknowledged. This work was supported by Deutsche Forschungsgemeinschaft under grant no. RE1344/7-1.

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