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On the speed of fluctuations around thermodynamic equilibrium

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Abstract. We study the speed of fluctuations of a quantum system around its equilibrium state, and show that the speed is extremely small at almost all times in typical thermodynamic cases. This suggests an alternative view on the nature of thermal equilibrium and, in particular, of the origin of thermal fluctuations. We argue that instead of equilibrium being a dynamical process in which the system actively fluctuates in time, the fluctuations are due to quantum uncertainties in an essentially static state.

The nature of thermal equilibrium is one of the most fundamental questions in statistical mechanics. Invariably, equilibrium is described as a dynamic process in which the system actively fluctuates in time. Here we argue that this image is essentially wrong and, in fact, unnecessary when taking into account quantum mechanics. We present an image of thermal equilibrium that is essentially static—it does fluctuate, but the fluctuations are on a far smaller scale than is usually assumed—instead, the usual fluctuations are almost entirely attributable to quantum uncertainty in an almost time-independent state. Part of this argument is already

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implied in [9], where the absolute magnitude of the fluctuations was analyzed and shown to become infinitesimal in the limit of large systems. Here, we prove that the speed of fluctuations also becomes infinitesimal.

The present work is part of a recent series of interesting results concerning the fundamental principles of statistical mechanics [1]–[8]. Underlying this progress is the realization that quantum mechanics allows individual quantum states to exhibit statistical properties and that ensemble or time averages are not needed to obtain a mixed equilibrium state for the system under consideration. This is a purely quantum phenomenon, and the key is entanglement, which leads to *objective* uncertainty—even when we have complete knowledge of the state of the whole system, a subsystem that is entangled with the rest of the system will be best described by a mixed state (i.e. a probabilistic mixture of pure states).

This progress led to a proof from first principles that virtually any subsystem of any large enough system will reach equilibrium and fluctuate around it at almost all times [9]. In order to better understand the nature of these fluctuations and to help understand the timescales involved, here we investigate the speed of fluctuations around equilibrium: does the state of the subsystem oscillate rapidly around equilibrium or remain relatively static? Our main result is to put a universal upper bound on the average speed of fluctuations, showing that the speed is extremely small at almost all times in typical thermodynamic cases.

Consider a large quantum system, described by a Hilbert space $\mathcal{H}$. We decompose this system into two parts: a small subsystem S and the rest of the system that we refer to as the bath B. Correspondingly, we decompose the total Hilbert space as $\mathcal{H} = \mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{B}}$, where $\mathcal{H}_{\mathrm{S}}$ and $\mathcal{H}_{\mathrm{B}}$ (of dimensions d_{S} and d_{B}) are the Hilbert spaces of the subsystem and bath, respectively. If the subsystem or bath has infinite dimension, we bound its volume and energy to render the dimension finite and project the interaction Hamiltonian onto the restricted Hilbert space $\mathcal{H}$.

Let the subsystem and the bath evolve under a Hamiltonian H that we decompose into a constant, subsystem, bath and interaction term

$$H = H_0 + H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{int}}. \tag{1}$$

The decomposition is made unique by taking H_0 proportional to the identity, H_{S} the tensor product of a traceless operator on the subsystem and the identity on the bath, H_{B} the tensor product of the identity on the subsystem and a traceless operator on the bath, and H_{int} traceless for both the subsystem and bath. We take the total system, i.e. subsystem plus bath, to be in a pure state $|\Psi(t)\rangle$; let $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ be the density matrix representation of the state of the total system and let $\rho_{\mathrm{S}}(t) = \mathrm{tr}_{\mathrm{B}}\rho(t)$ be the density matrix of the subsystem.

Our results can easily be extended to the case in which the subsystem and bath are in a mixed state $\rho(t)$, as may arise if they are entangled with an additional non-interacting environment (if this additional system is interacting, then we just include it in the bath itself). For a non-interacting additional environment, we do not need to know anything about its dynamics. Rather, as far as S and B are concerned, we can formally extend the bath to include an additional system B′ (of dimension $d_{\mathrm{S}}d_{\mathrm{B}}$), and consider a purification of $\rho(t)$ on $\mathcal{H} \otimes \mathcal{H}_{\mathrm{B}'}$ evolving under the Hamiltonian $H' = H \otimes I_{\mathrm{B}'}$.

Following the notation in [9], we define the time-averaged state of the whole system ω, which is given by

$$\omega = \langle\rho(t)\rangle_t = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^{\tau} \rho(t)\,\mathrm{d}t. \tag{2}$$

Similarly, we define $\omega_S = \mathrm{tr}_B\omega$ and $\omega_B = \mathrm{tr}_S\omega$ as the time-averaged states of the subsystem and bath, respectively. It is also convenient to introduce the notion of the *effective dimension* of a (mixed) state ρ by

$$d^{\mathrm{eff}}(\rho) = \frac{1}{\mathrm{tr}(\rho^2)}. \tag{3}$$

This is a measure of the number of states over which ρ is spread (e.g. for an equal mixture of N orthogonal states, $d^{\mathrm{eff}} = N$).

Clearly, ω_S is the canonical candidate for the equilibrium state, but we need to pause here to clarify what is meant by the statement that the system reaches equilibrium. Namely, note that due to the finiteness of the Hilbert spaces involved, there will be recurrences (on timescales exponential in $d^{\mathrm{eff}}(\omega)$), so a relaxation of $\rho_S(t)$ toward ω_S is out of the question. The best thing we can hope for in the current setting is that $\rho_S(t)$ remains close to ω_S at most times t.

To put our present results in a proper context, we first recall the key ideas and results of our previous work [9]. A key observation we made was that the process of thermalization actually contains many different aspects and we can decompose it into the following elements of analysis.

1. Equilibration. We say that a system equilibrates if its state evolves toward some particular state (in general, mixed) and remains in that state (or close to it) at almost all times. As far as equilibration is concerned, it is irrelevant what the equilibrium state actually is.
2. Bath state independence. The equilibrium state of the system should depend not on the precise initial state of the bath but only on its macroscopic parameters (e.g. its temperature).
3. Subsystem state independence. If the subsystem is small compared to the bath, the equilibrium state of the subsystem should be independent of its initial state.
4. Boltzmann form of the equilibrium state. Under certain additional conditions on the Hamiltonian (especially the interaction term) and on the initial state, the equilibrium state of the subsystem can be written in the familiar Boltzmannian form $\rho_S = (1/Z)\exp\left(-\widetilde{H}_S/k_BT\right)$.

Realizing that thermalization can be decomposed in this way had major consequences. Firstly, it allowed us to address each aspect separately. Secondly, and more important, it allowed us to greatly expand the scope of our study. Indeed, we now consider equilibration as a general quantum phenomenon that may occur in situations other than those usually associated with thermalization. In particular, we need not restrict ourselves to any of the following: standard thermal baths (that are described by a given temperature or restricted energy range), weak or short range interactions between the system and the bath, Boltzmannian distributions, situations in which energy is an extensive quantity, etc. Furthermore, we can consider situations in which the subsystem does not reach equilibrium and prove results about the bath or subsystem independence properties of the time-averaged state.

In [9], we made substantial progress on items 1–3 above, under very weak assumptions. The only real constraint we impose on the Hamiltonian is that it should have non-degenerate energy gaps. That is, any four energy eigenvalues satisfy $E_1 - E_2 = E_3 - E_4$ if and only if $E_1 = E_2$ and $E_3 = E_4$, or $E_1 = E_3$ and $E_2 = E_4$. This assumption rules out non-interacting Hamiltonians of the form $H_S \neq 0$, $H_B \neq 0$, $H_{\mathrm{int}} = 0$, which obviously do not equilibrate. These conditions are essentially the same as those in [9] but allow greater flexibility. Indeed, they

allow the Hamiltonian to have degenerate energy levels, as long as the gaps between levels are non-degenerate, whereas in [9], degenerate levels were not allowed. Yet, it can be easily shown that even under these more general conditions the results of our previous work [9] hold, namely that any small subsystem will reach equilibrium and fluctuate around it at almost all times[6].

More precisely, in [9, theorem 1], we show that the average distance between $\rho_S(t)$ and its time average ω_S is bounded by

$$\langle D(\rho_S(t), \omega_S)\rangle_t \leqslant \frac{1}{2}\sqrt{\frac{d_S}{d^{\mathrm{eff}}(\omega_B)}} \leqslant \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathrm{eff}}(\omega)}}, \tag{4}$$

where $D(\rho_1, \rho_2) = \frac{1}{2}\|\rho_1 - \rho_2\|_1 = \frac{1}{2}\mathrm{tr}\sqrt{(\rho_1 - \rho_2)^2}$ denotes the trace distance between two density matrices (see footnote 6). This is a natural distance measure on density matrices, giving the maximum difference in probability for any measurement on the two states[7]. The meaning of equation (4) is that the average distance between the instantaneous state of the subsystem $\rho_S(t)$ and the fixed state ω_S will be small whenever the total dimension explored by the state (or the dimension explored in the bath) is much larger than the subsystem dimension. In typical thermodynamic situations, this will indeed be the case. Indeed, as dimensions typically grow exponentially with particle number, we would expect any expression of the form $\mathrm{poly}(d_S)/d_{\mathrm{eff}}(\omega)$ to tend to zero in the thermodynamic limit (where the fraction of particles in the system tends to zero), as long as the energy distribution of $|\Psi(0)\rangle$ is reasonable. This addresses point 1 in our programme; in practice, one has to check that an initial state leads to large enough $d^{\mathrm{eff}}(\omega)$; however, in [9, theorem 2], we show that this is the case for typical states from any sufficiently large subspace (for instance, a subspace of states with similar macroscopic properties).

Regarding item 2, it is proven in [9, theorem 3] that initial states of tensor product form of a fixed state on the subsystem with a typical state of a large enough subspace on the bath yield very similar equilibrium states.

Finally, regarding item 3, we have similarly proven in [9, theorem 3] that if the energy eigenstates of the Hamiltonian are sufficiently entangled, then also initial states of tensor product form of a typical state on the system with a fixed state on the bath have very similar equilibrium states. Furthermore, simple examples, such as Hamiltonians with tensor product eigenstates, show that without any additional assumptions on the correlation properties of the eigenstates, one cannot expect subsystem independence to hold.

We emphasize, as in [9], that in the above discussion, the 'equilibrium' state ω_S is not necessarily Boltzmannian, and may depend on details of the Hamiltonian and the initial state (in particular, strong interactions, or conserved quantities for the subsystem, will generate different equilibrium states). However, the equilibration results still hold.

We now come to a crucial additional issue, namely timescales. This issue needs to be a part of the general programme of investigating thermalization. Again, this issue can be decomposed into a number of different questions (see the discussion at the end of this paper). The one that concerns us here is 'What is the speed of fluctuations around equilibrium?'.

[6] To see this, consider a basis for the energy eigenstates containing the (normalized) projection of $|\Psi(0)\rangle$ onto each energy eigenspace.

[7] We will make use of several norms on Hermitian operators, in particular the trace norm $\|A\|_1 = \mathrm{tr}|A| = \sum_i |a_i|$, where a_i are the eigenvalues of A; the Hilbert–Schmidt norm $\|A\|_2 = \sqrt{\mathrm{tr}(A^\dagger A)} = \sqrt{\sum_i |a_i|^2}$; and the standard operator norm $\|A\| = \max_i |a_i|$.

While the magnitude of the fluctuations from equilibrium may be small according to equation (4), this does not say anything about their speed. Mathematically, the speed of change of the subsystem state is given by

$$v_{\mathrm{S}}(t) = \lim_{\delta t \to 0} \frac{D(\rho_{\mathrm{S}}(t), \rho_{\mathrm{S}}(t+\delta t))}{\delta t} = \frac{1}{2} \left\| \frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} \right\|_1 . \tag{5}$$

We will show that $v_{\mathrm{S}}(t)$ is small at almost all times in typical thermodynamic cases, as follows.

Theorem 1. *For the average rate of change of ρ_{S},*

$$\langle v_{\mathrm{S}}(t) \rangle_t \leqslant \| H_{\mathrm{S}} + H_{\mathrm{int}} \| \sqrt{\frac{d_{\mathrm{S}}^3}{d_{\mathrm{eff}}(\omega)}}, \tag{6}$$

where we take $\hbar = 1$ and use the operator norm (see footnote 7).

Proof. The time evolution of the subsystem state is given by

$$\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} = \mathrm{tr}_{\mathrm{B}}(\mathrm{i}[\rho(t), H]) = \sum_k c_k(t) e_k, \tag{7}$$

where e_k with $k = \{1, 2, \ldots, d_{\mathrm{S}}^2\}$ is a Hermitian orthonormal operator basis for the system, i.e. $tr(e_k e_\ell) = \delta_{k\ell}$. Hence,

$$\begin{aligned} c_k(t) &= \mathrm{tr}_{\mathrm{S}} \left(\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} e_k \right) \\ &= \mathrm{tr}\,(\mathrm{i}\,[\rho(t), H]\, e_k \otimes I) = \mathrm{tr}\,(\rho(t)\mathrm{i}[H, e_k \otimes I]) \\ &= \mathrm{tr}\,(\rho(t)\mathrm{i}[H_{\mathrm{S}} + H_{\mathrm{int}}, e_k \otimes I])\,. \end{aligned} \tag{8}$$

Using our notation, but with a slight modification to use the operator norm, Reimann [7] shows that for a Hamiltonian with non-degenerate energy gaps, and a Hermitian observable A,

$$\langle (\mathrm{tr}(\rho(t)A) - \langle \mathrm{tr}(\rho(t)A) \rangle_t)^2 \rangle_t \leqslant \frac{\|A\|^2}{d_{\mathrm{eff}}(\omega)}. \tag{9}$$

Taking $A = \mathrm{i}[H_{\mathrm{S}} + H_{\mathrm{int}}, e_k \otimes I]$ and noting that

$$\|\mathrm{i}[H_{\mathrm{S}} + H_{\mathrm{int}}, e_k \otimes I]\| \leqslant 2\|H_{\mathrm{S}} + H_{\mathrm{int}}\|, \tag{10}$$

we obtain

$$\left\langle (c_k(t) - \langle c_k(t) \rangle_t)^2 \right\rangle_t \leqslant \frac{4\|H_{\mathrm{S}} + H_{\mathrm{int}}\|^2}{d_{\mathrm{eff}}(\omega)}. \tag{11}$$

However,

$$\langle c_k(t) \rangle_t = \langle \mathrm{tr}\,(i\,[\rho(t), H]\, e_k \otimes I) \rangle_t = \mathrm{tr}\,(\mathrm{i}\,[\omega, H]\, e_k \otimes I) = 0$$

and hence

$$\langle (c_k(t))^2 \rangle_t \leqslant \frac{4\|H_{\mathrm{S}} + H_{\mathrm{int}}\|^2}{d_{\mathrm{eff}}(\omega)}. \tag{12}$$

This implies

$$\left\langle \left\| \frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} \right\|_2^2 \right\rangle_t = \left\langle \mathrm{tr}\left(\sum_k c_k(t) e_k \right)^2 \right\rangle_t$$

$$= \sum_{kl} \langle c_k(t) c_l(t) \rangle_t \, \mathrm{tr}\,(e_k e_l)$$

$$= \sum_k \left\langle (c_k(t))^2 \right\rangle_t \leqslant \frac{4 \| H_{\mathrm{S}} + H_{\mathrm{int}} \|^2 d_{\mathrm{S}}^2}{d_{\mathrm{eff}}(\omega)}.$$

On the other hand, the trace norm and the Hilbert–Schmidt norm are connected by the elementary relation $\|X\|_1^2 \leqslant (\mathrm{rank}\, X) \|X\|_2^2$. Hence, using the concavity of the square root function,

$$\left\langle \left\| \frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} \right\|_1 \right\rangle_t \leqslant \sqrt{\left\langle \left\| \frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} \right\|_1^2 \right\rangle_t}$$

$$\leqslant \sqrt{d_{\mathrm{S}} \left\langle \left\| \frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} \right\|_2^2 \right\rangle_t}$$

$$\leqslant 2 \| H_{\mathrm{S}} + H_{\mathrm{int}} \| \sqrt{\frac{d_{\mathrm{S}}^3}{d_{\mathrm{eff}}(\omega)}}. \tag{13}$$

From the definition of $v_{\mathrm{S}}(t)$ given by (5), we obtain the desired result

$$\langle v_{\mathrm{S}}(t) \rangle_t = \frac{1}{2} \left\langle \left\| \frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} \right\|_1 \right\rangle_t \leqslant \| H_{\mathrm{S}} + H_{\mathrm{int}} \| \sqrt{\frac{d_{\mathrm{S}}^3}{d_{\mathrm{eff}}(\omega)}}.$$

□

This result can be interpreted as follows. Firstly, the speed of fluctuations varies in time and, of course, there may—and in general will—be times when the speed is extremely high. What our theorem shows is that, on average, the instantaneous speed is bounded by the expression given in equation (6). Since speed is a positive quantity, this also means that the fraction of times for which $v_{\mathrm{S}}(t) > K \| H_{\mathrm{S}} + H_{\mathrm{int}} \| \sqrt{d_{\mathrm{S}}^3 / d_{\mathrm{eff}}(\omega)}$ must be less than $1/K$.

Secondly, our bound depends linearly on the magnitude of the Hamiltonian and, more precisely, on the subsystem and interaction Hamiltonian. Clearly the speed depends linearly on the Hamiltonian since multiplying the Hamiltonian by a constant factor $H \to \lambda H$ makes the entire time evolution faster by a factor λ. Furthermore, the speed of change of the state of the subsystem depends only on the part of the Hamiltonian that acts directly on it; in particular, it is independent of the bath Hamiltonian H_{B}. Of course, since the subsystem interacts with the bath, the time evolution of the subsystem depends on the state of the bath and thus implicitly on the bath Hamiltonian. However, as is already evident from equation (8), the instantaneous change in the state of the subsystem (and hence the speed of its evolution) depends only on the instantaneous state of the bath and not directly on the bath Hamiltonian. Also, obviously,

the time evolution is completely independent of the constant part of the Hamiltonian H_0 that only defines a reference point for the energy. These being said, the bound (6) should be better interpreted as a bound on the speed of fluctuations as measured in 'natural units', i.e.

$$\frac{\langle v_S(t)\rangle_t}{\|H_S + H_{\text{int}}\|} \leqslant \sqrt{\frac{d_S^3}{d_{\text{eff}}(\omega)}}. \tag{14}$$

The main result of this paper is therefore that the average speed, as measured in natural units, is bounded by $\sqrt{d_S^3/d_{\text{eff}}(\omega)}$. As mentioned earlier, because dimension generally grows exponentially with the number of particles, we would expect any fixed power of d_S to be much smaller than $d_{\text{eff}}(\omega)$ in the thermodynamic limit. (Note that similar arguments can be made for any finite derivative of $\rho_S(t)$, with higher powers of the Hamiltonian in the upper bound depending on the degree of derivative.)

Thirdly, as far as the value of the speed is concerned, we note that in most natural systems the magnitude of the Hamiltonian governing the speed, i.e. $\|H_S + H_{\text{int}}\|$, scales relatively slowly (i.e. polynomially) with the number of particles. For example, in a system of n particles in which the Hamiltonian only contains two-particle interactions, we would expect the norm of the Hamiltonian to grow at most quadratically in n. Hence in the thermodynamic limit, when the total number of particles in the system increases, we would expect the exponential dependence of the dimensional term $\sqrt{d_S^3/d_{\text{eff}}(\omega)}$ to dominate, causing the absolute value of the average speed to tend to zero.

To summarize, we have shown that in the thermodynamic regime not only every subsystem spends almost all its time fluctuating very closely around a fixed state—the equilibrium state ω_S—but also that the speed of fluctuations becomes vanishingly small. To be precise, they are of an exponentially small order in the number of elements of the system rather than inverse polynomial. Both of these results suggest a view on equilibrium that is essentially static, with ω_S describing the objective state of a subsystem at equilibrium, rather than an average based on our subjective uncertainty.

This static viewpoint appears, at first glance, to contradict the established view that a system has non-vanishing fluctuations around equilibrium. However, what are generally thought to be time fluctuations are just the result of quantum uncertainty (the probabilistic nature of the outcomes of quantum measurements), which would be present even if the subsystem's state were truly constant and we had perfect knowledge of the global state $|\Psi(t)\rangle$. When we perform a measurement on a subsystem at equilibrium, we will generally disturb its state, causing it to 'collapse' from ω_S to an eigenstate of the measurement that is a fluctuation from the average. It would be interesting to see how long the subsystem would take to re-equilibrate after such a disturbance (or indeed to equilibrate initially). Such a timescale is the closest equivalent to the timescale of fluctuations in the usual picture, which has no meaning for a static equilibrium state. Without external measurement there are only two steady motions: the constant speed of the global state $|\Psi(t)\rangle$ and the near-standstill of $\rho_S(t)$. An important, more general, question for future work is to understand the timescales for the approach to equilibrium starting from arbitrary initial states.

As in [9], our results hold not only for the standard statistical mechanical setting with Boltzmannian equilibrium, but also under extremely general conditions.

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