

TYPICALITY APPROACH TO QUANTUM THERMODYNAMICS

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ABSTRACT

Why do thermodynamical systems reach (more or less universal) final states that no longer exhibit any macroscopically visible evolution while the underlying microscopic equations of motion do not feature any attractive fixed points? The quantum typicality approach to thermodynamics is at present intensely debated. If Hilbert space is considered as the quantum analogue of phase space, any pure state is represented by a point which ventures eternally through this Hilbert space without coming to a halt. The apparent non-evolving equilibrium state of the macroscopic system is now explained by the following concept: Almost all states from some accessible region in Hilbert space may exhibit very similar properties such as expectation values of pertinent observables, probabilities to measure certain values, reduced density matrices corresponding to smaller parts of a larger system, etc. Thus as long as some concrete pure state ventures through regions in Hilbert space that are entirely filled with such typical states this motion will never be visible from considering only the above properties. Of course it is inherent to such a theory of thermalization that it cannot directly predict thermalizing dynamics of specific initial states as generated by specific Hamiltonians, it primarily addresses relative frequencies.

INTRODUCTION

Despite the fact that some call it a “tired old question” [1] the search for the origin and the true nature of the second law of thermodynamics has recently regained considerable impact. Although all researches are utterly used to the second law, the idea of almost any system always approaching a state (equilibrium) which is in accord with the concept of the system occupying an immense multitude of micro states at the same time (ensemble) is still quite puzzling. How can the system end up in a multitude of states given that there is conservation of phase space volume? And, even worse, always in the same well defined multitude? How can this be explained on the basis of an underlying theory? The traditional answers are of course well known: Some are based on the the microstate of the system wandering rapidly through all accessible phase space (ergodicity), others are based on the idea of the system occupying an initial multitude of states due to inevitable imperfections of measurements, that then effectively, in a coarse grained consideration, grows in time (mixing).

Although not really being new, lately the concept of “typicality” has also attracted some attention. The idea is that there are different, individual microstates each of which which leads for a set of observables to the same outcomes as if the system was in a multitude of states which form the ensemble. Furthermore these micro states are supposed to fill almost the entire accessible phase space such that, drawing states at random, they appear as being “typical”. Or, from a more dynamical point of view, a generic evolution will likely eventually lead to and proceed inside a region in phase space which is filled with the above mentioned typical states if this region is overwhelmingly large. This concept immediately raises some questions: For what class of observables can this concept hold at all? How can the overwhelming relative frequency of the above mentioned states be proven?

A number of publications [2; 3; 4; 5; 6; 7] aim at show-

ing that the typicality-principle applies to quantum physics in a quite general sense. Some of these papers consider a quantum system in contact with some quantum environment. Instead of considering one or a few observables the authors consider the reduced density matrix for the system which is tantamount to considering the set of all observables that may be locally defined for the system. These papers convincingly show that for a large majority of pure states drawn from an energy interval $E, E - \Delta E$ (of the full system) the reduced local density matrix assumes the same form as the one resulting from a microcanonical ensemble corresponding to the same interval. In the case of standard environment spectra and weak couplings this accounts for the typicality of the canonical equilibrium state. Other papers intend to avoid the system-environment partition as well as the restriction of the states onto energy intervals. They essentially analyze the (Hilbert space-) variance of a distribution of expectation values $\langle \psi | \hat{A} | \psi \rangle$ corresponding to a more general distribution of states ψ in Hilbert space. This way an upper bound to this variance based on the difference between the highest and the lowest eigenvalue of \hat{A} and the purity of the averaged density matrix is established.

In the paper at hand we consider both, the typicality of observables and of reduced states. The fashion according to which we “draw” our states from Hilbert space is neither just given by a restriction onto a projective subspace as in [2; 4; 3] nor is it defined by a rather general probability distribution as in [5]. Instead we consider a region in Hilbert space which is in accord with the system, occupying different projective (invariant) subspaces with different probabilities. We define these subspaces (labeled by α) by projectors

$$\hat{\Pi}_\alpha = \sum_i |\alpha, i\rangle \langle \alpha, i|, \quad W_\alpha = \langle \psi | \hat{\Pi}_\alpha | \psi \rangle \quad (1)$$

i.e. the probability to find the system in state ψ in some subspace α is W_α . The accessible region (AR) we are going to con-

sider may now be defined by a set of probabilities W_α . If and only if ψ is in accord with Eq. (1) it belongs to the AR. This choice of AR has primarily dynamical reasons: If the $\hat{\Pi}_\alpha$ correspond to natural invariants of the system (e.g. particle number, magnetization, etc.) the (pure) state of the system $\psi(t)$ can never leave the AR it started in. Of course subspaces that correspond to energy eigenstates are invariants of motion. However, if there is a small perturbation of strength ϵ , one can nevertheless expect subspaces spanned by the eigenstates of the unperturbed system corresponding to an energy interval $\Delta E > \epsilon$ to be approximately invariant. I.e. even the perturbed system will not substantially leave the AR defined on the basis of such subspaces.

TYPICALITY OF OBSERVABLES

In the following we are interested in the Hilbert Space Average (HA) of an expectation value of an arbitrary Hermitian operator \hat{A} (an observable) restricted to the above defined AR. The average is defined as a mean of the expectation value over all states of AR with respect to the unitary invariant measure (Haar measure), $[\langle \psi | \hat{A} | \psi \rangle]_{\text{AR}} = [\langle \hat{A} \rangle]_{\text{AR}}$. For details how to concretely compute such integrals see [6].

According to the partitioning in subspaces α the general operator \hat{A} can be decomposed in subspaces defined by the projection operators Eq. (1) finding

$$\hat{A} = \sum_{\alpha\beta} \hat{\Pi}_\alpha \hat{A} \hat{\Pi}_\beta =: \sum_{\alpha\beta} \hat{A}_{\alpha\beta}. \quad (2)$$

Using this decomposition the HA yields

$$\begin{aligned} [\langle \hat{A} \rangle]_{\text{AR}} &= \text{Tr}\{\hat{A}[\hat{\rho}_\psi]_{\text{AR}}\}, \quad \hat{\rho}_\psi \equiv |\psi\rangle\langle\psi| \\ [\hat{\rho}_\psi]_{\text{AR}} &\equiv \hat{\omega} = \sum_\alpha \frac{W_\alpha}{N_\alpha} \hat{\Pi}_\alpha \end{aligned} \quad (3)$$

where $N_\alpha := \text{Tr}\{\hat{\Pi}_\alpha\}$ is the dimension of the corresponding subspace. We have skipped some calculations and used some averages which can be found in [6]. Here $\hat{\omega}$ is simply the state that corresponds to the Boltzmann ‘‘a priori principle of equal weights’’, a state for which probability in each subspace W_α is uniformly distributed onto all states that span the subspace $\hat{\Pi}_\alpha$.

So far, however, this does not classify an $\langle \hat{A} \rangle$ in accord with the Boltzmann ensemble as being typical. To quantify this typicality, i.e., whether or not a concrete the expectation value of \hat{A} is most frequently close to the average, we furthermore introduce the Hilbert space variance (HV)

$$\Delta_{\text{H}}^2(\langle \hat{A} \rangle) := [(\langle \hat{A} \rangle)^2]_{\text{AR}} - [\langle \hat{A} \rangle]_{\text{AR}}^2. \quad (4)$$

Using again the decomposition given in Eq. (2), carefully calculating these HV’s using techniques described in [6] yields

$$\begin{aligned} \Delta_{\text{H}}^2(\langle \hat{A} \rangle) &= \sum_{\alpha\beta} \frac{W_\alpha W_\beta}{N_\alpha(N_\beta + \delta_{\alpha\beta})} \left(\text{Tr}\{\hat{A}_{\alpha\beta} \hat{A}_{\alpha\beta}^\dagger\} - \frac{\delta_{\alpha\beta}}{N_\alpha} \text{Tr}\{\hat{A}_{\alpha\alpha}\}^2 \right). \end{aligned} \quad (5)$$

This is a rigid result and may in principle be evaluated for any given AR, \hat{A} . Whenever it is small, the average result (3) can

be considered as being typical. For what scenarios can such typicality be expected? Specializing without substantial loss of generality to observables with $\text{Tr}\{\hat{A}\} = 0$ the variance of the spectrum of \hat{A} reads:

$$\Delta_{\text{S}}^2(\hat{A}) = \frac{1}{N} \sum_{\alpha\beta} \text{Tr}\{\hat{A}_{\alpha\beta} \hat{A}_{\alpha\beta}^\dagger\} \quad N \equiv \sum_\alpha N_\alpha \quad (6)$$

where N is simply the total dimension of the system. A HV is by construction positive, so are both terms that appear in the difference in (5) thus omitting the second of those will only make the outcome larger. Hence an upper bound to the HV written in a suggestive way reads:

$$\Delta_{\text{H}}^2(\langle \hat{A} \rangle) \leq \frac{1}{N^2} \sum_{\alpha\beta} \left(\frac{W_\alpha W_\beta}{n_{\alpha n\beta}} \right) \text{Tr}\{\hat{A}_{\alpha\beta} \hat{A}_{\alpha\beta}^\dagger\} \quad (7)$$

with $n_{\alpha(\beta)} \equiv N_{\alpha(\beta)}/N$. Thus, whenever the system occupies with significant probability only subspaces that are large enough to represent a substantial fraction of the full dimension of the system the HV is roughly by a factor N smaller than the variance of the spectrum. Thus, a result for $\langle \hat{A} \rangle$ as calculated from $\hat{\omega}$ classifies as typical for a wide range of accessible regions if \hat{A} has a bounded spectrum and is defined on a large-dimensional Hilbert space. This essentially reflects results by Reimann [5]

In which cases can this be expected? Consider as an instructive example the case of no restriction, i.e., the AR being all Hilbert space. One may be interested in a ‘‘local’’ variable \hat{A} which should really be written as $\hat{A} \otimes \hat{1}_E$, where $\hat{1}_E$ denotes the unit operator acting on the (for this inquiry irrelevant) rest of the system. If this rest of the system is enlarged N increases drastically while $\Delta_{\text{S}}^2(\hat{A})$ remains constant. Thus the corresponding HV will decrease according to Eq. (7). This means whenever a bounded local variable of interest is embedded in a large surrounding featuring a high dimensionality, typicality can be expected. Such a scenario is naturally implemented if a considered system is coupled to a large environmental system. One may then even observe a set of local variables which determine the reduced (local) state of the considered system completely, finding that they all relax to equilibrium due to all their HV’s being small. Such a scenario will be considered in more detail below. However, since the above reasoning does not require weak coupling, it also applies in principle to scenarios in which the system-environment partition in the traditional sense is absent. If one, e.g., considers a many particle system of some solid state type, one may be interested in the number of particles that can be expected in some spatial region of the system. The variance of the corresponding number operator surely remains unchanged if the whole system is increased (at constant particle density) but the dimension on which the number operator is defined increases exponentially. Thus a strongly typical occupation number will result from this scenario.

The same overall picture can be considered more or less appropriate even if there are restrictions to different subspaces $\hat{\Pi}_\alpha$. Thus, in very many scenarios and for many observables one finds small HV’s and in all those cases the typicality argument applies.

TYPICALITY OF STATES

Thus, measuring only one (or a few) observable(s) \hat{A} one is most likely not able to distinguish some ψ from the AR from $\hat{\omega}$.

However, measuring more and more observables on will eventually be able to determine the full, true quantum state of the system (ψ). Thus one may ask the question whether a true quantum state from the AR is typically close to the state that represents the ensemble, i.e., $\hat{\omega}$? To quantify this question we use as a measure for the “size” of an operator $D^2(\hat{O}) \equiv \text{Tr}\{\hat{O}\hat{O}^\dagger\}$ thus the distance between, two operators \hat{A}, \hat{B} is simply $D^2(\hat{A} - \hat{B})$. As the HV of $\langle \hat{A} \rangle$ is simply the HA over the squared distance between $\langle \hat{A} \rangle$ and $\text{Tr}\{\hat{A}\hat{\omega}\}$, we define

$$\Delta_H^2(\hat{\rho}_\psi) \equiv \llbracket D^2(\hat{\rho}_\psi - \hat{\omega}) \rrbracket_{\text{AR}} = \llbracket D^2(\hat{\rho}_\psi) \rrbracket_{\text{AR}} - D^2(\hat{\omega}) \quad (8)$$

For the situation discussed above this HV is easy to calculate since $D^2(\hat{\rho}_\psi)$ is simply the purity of $\hat{\rho}_\psi$. Since in this example the purity of $\hat{\rho}_\psi$ is always one, regardless of the actual ψ , we find: $\Delta_H^2(\hat{\rho}_\psi) = 1 - D^2(\hat{\omega})$. If the purity of $\hat{\omega}$ is low, which will be the case for most realistic scenarios, the HV will be close to one and thus not small at all. This means that regardless of $\text{Tr}\{\hat{A}\hat{\rho}_\psi\} \approx \text{Tr}\{\hat{A}\hat{\omega}\}$ for very many \hat{A} the states $\hat{\rho}_\psi$ from the HA are not close to $\hat{\omega}$, i.e., there is no typical state in the HA. This also obviously includes the purities or entropies (e.g. Von Neumann entropy) of states $\hat{\rho}_\psi$ from the HA being very different from the purity or entropy of $\hat{\omega}$.

In the following we analyze whether or not there is a typical state for a considered system which is in contact with some environment E . Here we require the pure state of the full system to be confined to some HA which is also defined in the full system. The considered state however is now a reduced state, i.e., $\hat{\rho}_\psi \equiv \text{Tr}_E\{|\psi\rangle\langle\psi|\}$. Its possibly typical outcome, i.e., its HA is

$$\llbracket \hat{\rho}_\psi \rrbracket = \text{Tr}_E\{\llbracket |\psi\rangle\langle\psi| \rrbracket\} = \text{Tr}_E\{\hat{\omega}\} \quad (9)$$

To analyze typicality in this case it is more convenient to write $\Delta_H^2(\hat{\rho}_\psi)$ in terms of matrix elements of $\hat{\rho}_\psi$, i.e., $\rho_\psi^{lm} := \langle l|\hat{\rho}_\psi|n\rangle$, where $|l\rangle, |n\rangle$ are energy eigenstates of the local system. Defining $X_{lm} \equiv \text{Re}(\rho_\psi^{lm})$ and $Y_{lm} \equiv \text{Im}(\rho_\psi^{lm})$, we straightforwardly find

$$\Delta_H^2(\hat{\rho}_\psi) = \sum_{lm} \Delta_H^2(X_{lm}) + \Delta_H^2(Y_{lm}) \quad (10)$$

The quantities X_{lm}, Y_{lm} may be expressed as expectation values of the corresponding (local) operators $\hat{X}_{lm}, \hat{Y}_{lm}$ with

$$\hat{X}_{lm} := \frac{1}{2}(|l\rangle\langle m| + |m\rangle\langle l|) \otimes \hat{1}, \quad (11)$$

$$\hat{Y}_{lm} := \frac{i}{2}(|l\rangle\langle m| - |m\rangle\langle l|) \otimes \hat{1} \quad (12)$$

Writing it this way we can use Eq. (7) to compute an upper bound to the HV as given by Eq. (10). Concentrating for simplicity on the case of the HA consisting of a restriction onto just one projective subspace, we may write, $\Delta_H^2(X_{lm}) \leq \Delta_S^2(\hat{X}_{lm})/N_\alpha$ and the corresponding for Y_{lm} . Since $\Delta_S^2(\hat{X}_{lm}), \Delta_S^2(\hat{Y}_{lm}) \leq 1/N_S$ (N_S being the dimension of the considered system) for all l, m we find plugging all this into Eq. (10)

$$\Delta_H^2(\hat{\rho}_\psi) \leq \frac{2N_S}{N_\alpha} \quad (13)$$

for this situation. Hence, whenever the dimension of the subspace onto which the full system is confined is much larger than

the dimension of the Hilbert space of the considered system, $\hat{\omega}$ will be the most likely, typical reduced state of the considered system for almost all pure states from the AR. In this case also the local entropies and purities of the $\hat{\rho}_\psi$'s are close to those of $\hat{\omega}$. In short: in this case there is a typical state. This essentially reflects the results by Popescu et. al. [7]

EIGENSTATE THERMALIZATION HYPOTHESIS AND TYPICALITY

So far everything stated above referred to the relative frequency of states featuring certain typical properties in Hilbert space. However, this does not imply directly anything rigorous on the dynamics, especially not on whether they may be classified as equilibrating, thermalizing, etc. Even though almost all of Hilbert space may be filled with typical states, concrete evolutions may never reach this giant region of typical states. Or depending on the initial state, some evolutions may do so while others may not. It is thus instructive to consider the link between typicality and concrete quantum dynamics. Let us start by considering a generic evolution of a quantum expectation value (QEV):

$$\langle \psi(t)|\hat{A}|\psi(t) \rangle = \sum_{mn} \psi_m^* \psi_n \langle m|\hat{A}|n \rangle \exp(-i(E_n - E_m)t) \quad (14)$$

with $|m\rangle, |n\rangle$ being energy eigenstates of the system corresponding to eigenvalues E_m, E_n and ψ_m, ψ_n being amplitudes of the initial wave function $|\psi(0)\rangle$ with respect to the energy eigenbasis. If the QEV reaches a more or less constant value at all after a (possibly very long) time, this value can only be the time average over an even longer time. Denoting this average (somewhat vaguely) as $\overline{\langle \psi(t)|\hat{A}|\psi(t) \rangle}$ and specializing to cases without degeneracy yields:

$$\overline{\langle \psi(t)|\hat{A}|\psi(t) \rangle} = \sum_n |\psi_n|^2 \langle n|\hat{A}|n \rangle \quad (15)$$

For a thermodynamical system one would expect the expectation value of a relevant variable to reach an equilibrium value that is independent of the details of the initial state, even though it may depend e.g., on the overall energy, etc. This equilibrium value would be given by the r.h.s. of Eq. (15) This, however, can only be independent of the initial state if $\langle n|\hat{A}|n \rangle$ does not (strongly) depend on n , at least not for energy eigenstates within a given energy region of a pertinent width. Such an independence has become popular under the name of “eigenstate thermalization hypothesis” [8; 9; 10]. But it may also be rephrased from the perspective of typicality: This approximate independence results if the energy eigenstates belong to the typical set. This in turn is to be expected in an unbiased guess. Simply because if the energy region is high-dimensional and the spectrum of \hat{A} is bounded, there are much more typical states than there are non-typical ones. This, however is only an unbiased guess. Whether or not it holds for a concrete Hamiltonian and a concrete observable within a concrete energy regime cannot be answered on the basis of typicality arguments.

DYNAMICAL TYPICALITY

So far we have been concerned with the question whether or not certain QEV's (or reduced states) will reach constant values

that are independent of the details of the initial states, possibly after a very long time. The experiences with non-equilibrium thermodynamics are, however, even more far reaching. Thermodynamical observables do not only reach final equilibrium values that are independent of the details of the initial states, but starting from the same non-equilibrium values, all evolutions, at any point in time, will be more or less the same irrespective of the details of the initial state. In the following we turn towards the question how this can be understood on the basis of typicality. More specifically we demonstrate that pure states from a set $\{|\phi\rangle\}$ featuring a common QEV of some observable \hat{A} at some time t , i.e. $\langle\phi|\hat{A}(t)|\phi\rangle = a$, most likely yield very similar QEV's at any later time, i.e. $\langle\phi|\hat{A}(t+\tau)|\phi\rangle \approx \langle\phi'|\hat{A}(t+\tau)|\phi'\rangle$ (with $|\phi\rangle, |\phi'\rangle$ both being states from the above set). We present some analytical derivations based on the above considerations, in particular on Eqs. (3 and 7) and we additionally support the results with numerical calculations. Finally, we discuss what consequences arise for the validity of projection operator methods (Nakajima-Zwanzig (NZ), etc. [12; 13; 14]) w.r.t. initial states and the corresponding inhomogeneities. Furthermore, we comment on the irreversibility of QEV's corresponding to individual pure states.

We specify our considered observable \hat{A} only by the moments, c_i of its spectrum ($c_i := \text{Tr}\{\hat{A}^i\}/n$, with n being the dimension of the relevant Hilbert space), and specialize without substantial loss of generality to observables which are trace-free, $c_1 = 0$, and normalized to $c_2 = 1$. Furthermore we require the c_i with $i = 2, \dots, 8$ to be of the order 1. Next, we introduce an ensemble of pure states $|\phi\rangle$ which is characterized as follows: All its states must feature the same QEV of the observable \hat{A} , $\langle\phi|\hat{A}|\phi\rangle = a$, must be normalized ($\langle\phi|\phi\rangle = 1$), and uniformly distributed otherwise. That means the ensemble has to stay invariant under all unitary transformations in Hilbert space that leave the expectation value of \hat{A} unchanged, i.e. those transformations that commute with \hat{A} , or, concretely, transformations of the form $e^{i\hat{B}}$, with $[\hat{B}, \hat{A}] = 0$. This specifies the most general ensemble consistent with the restriction that all its state should yield a given a .

For the following calculations we further introduce some kind of ‘‘substitute’’ ensemble $\{|\omega\rangle\}$, which is much easier to handle. As will be shown below, this ensemble approximates the exact ensemble $\{|\phi\rangle\}$ described above very well for large Hilbert spaces.

The ensemble $\{|\omega\rangle\}$ is generated by

$$|\omega\rangle = (1/\sqrt{1+d^2})(1+d\hat{A})|\psi\rangle, \quad (16)$$

where $|\psi\rangle$ are pure states drawn from a uniform distribution of normalized states without further restriction as described above Eq. (3). d is some small parameter which describes the deviation from the ‘‘equilibrium’’ ensemble $\{|\psi\rangle\}$. Since it is essentially the operator \hat{A} itself that generates $\{|\omega\rangle\}$ from the entirely uniform distribution, $\{|\omega\rangle\}$ is invariant under the above uniform transformations that leave a invariant.

The construction (16) allows for an evaluation of moments of the distribution of $\langle\omega|\hat{C}|\omega\rangle$ based on results on moments of the distribution of $\langle\psi|\hat{D}|\psi\rangle$, or concretely (for simplicity of notation we denote in the remainder of this paper Hilbert space averages

as $\text{HA}[\dots]$ and Hilbert space variances as $\text{HV}[\dots]$):

$$\begin{aligned} \text{HA}[\langle\omega|\hat{C}|\omega\rangle^i] &= \text{HA}[\langle\psi|\hat{D}|\psi\rangle^i] \\ \text{with } \hat{D} &= \frac{1}{1+d^2}(1+d\hat{A})\hat{C}(1+d\hat{A}). \end{aligned} \quad (17)$$

(Of course the average on the l.h.s. corresponds to the substitute ensemble $\{|\omega\rangle\}$ while the average on the r.h.s is based on the completely uniform ensemble $\{|\psi\rangle\}$). Exploiting this, average and variance of $\langle\omega|\hat{C}|\omega\rangle$ may be evaluated with the help of Eqs. (3,7).

To assure that the ensemble $\{|\omega\rangle\}$ indeed approximates the ensemble $\{|\phi\rangle\}$, in the limit of large n , we evaluate the following four quantities

$$\begin{aligned} \text{HA}[\langle\omega|\omega\rangle], & & \text{HA}[\langle\omega|\hat{A}|\omega\rangle], \\ \text{HV}[\langle\omega|\omega\rangle], & & \text{HV}[\langle\omega|\hat{A}(t)|\omega\rangle], \end{aligned} \quad (18)$$

where $\hat{A}(t)$ denotes the time dependence according to the Heisenberg picture. (For clarity: the results are given in Eqs. (19), (20), (21) and (23).)

The states $|\omega\rangle$ are not exactly normalized which would render them unphysical, of course. However, one finds from Eqs. (3) and (17) (by implementing $\hat{C} = \hat{1}$) that

$$\text{HA}[\langle\omega|\omega\rangle] = 1. \quad (19)$$

By exploiting Eq. (7) and Eq. (17) one finds analogously for the variance

$$\text{HV}[\langle\omega|\omega\rangle] = \frac{1}{n+1} \cdot \frac{4d^2 + 4d^3c_3 + d^4(c_4 - 1)}{(1+d^2)^2}. \quad (20)$$

As defined above, the c_i are of the order 1, i.e. the HV of the norms scales with $1/n$ and becomes small for large Hilbert spaces. Therefore, the vast majority of the states $|\omega\rangle$ are approximately normalized for large n .

The average of the QEV's of \hat{A} w.r.t. the ensemble $\{|\omega\rangle\}$ (which is meant to correspond to the above a) is calculated by exploiting Eq. (3) and Eq. (17) (by implementing $\hat{C} = \hat{A}$)

$$\text{HA}[\langle\omega|\hat{A}|\omega\rangle] = \frac{2d + d^2c_3}{1+d^2}. \quad (21)$$

That is, the mean QEV can be adjusted through the choice of the parameter d . However, the replacement ensemble is restricted on expectation values not too far away from zero (i.e. the average expectation value of the ‘‘equilibrium’’ ensemble $\{|\psi\rangle\}$) because by sweeping through all possible d not all possible expectation values up to the maximum eigenvalue of \hat{A} are reachable.

The evaluation of $\text{HV}[\langle\omega|\hat{A}(t)|\omega\rangle]$ turns out to be somewhat more complicated, since we, in general, cannot fully diagonalize the Hamiltonian and thus do not know $\hat{A}(t)$ in detail. However, we are able to perform an estimation for an upper bound. For this purpose we make use of the Hilbert Schmidt scalar product for complex matrices defined as $(\hat{X}, \hat{Y}) := \text{Tr}\{\hat{X}^\dagger \hat{Y}\}$.

Thus, one can formulate a Cauchy-Schwarz inequality of the form

$$\text{Tr}\{\hat{X}^\dagger \hat{Y}\} \leq \sqrt{\text{Tr}\{\hat{X}^\dagger \hat{X}\} \text{Tr}\{\hat{Y}^\dagger \hat{Y}\}}. \quad (22)$$

Particularly, one obtains $\text{Tr}\{\hat{A}(t)\hat{A}\} \leq \text{Tr}\{\hat{A}^2\}$. Evaluating $\text{HV}[\langle \omega | \hat{A}(t) | \omega \rangle]$ based on Eq. (7) and Eq. (17) (by implementing $\hat{C} = \hat{A}(t)$), realizing that $\text{Tr}\{\hat{D}\}^2$ is always positive and repeatedly applying the Cauchy-Schwarz inequality Eq. (22) yields the inequality

$$\text{HV}[\langle \omega | \hat{A}(t) | \omega \rangle] \leq \frac{1}{n+1} \cdot \frac{1 + 4d\sqrt{c_4} + 6d^2c_4 + 4d^3\sqrt{c_4}\sqrt[4]{c_4c_8} + d^4\sqrt{c_4c_8}}{(1+d^2)^2}. \quad (23)$$

Again, since the c_i are of the order 1, the upper bound decreases as $1/n$. Thus, the variance Eq. (23) becomes small for large Hilbert spaces, just like the variance of the norms Eq. (20). This result yields two major direct implications.

First, if one evaluates (23) at $t = 0$, one finds that the majority of the states $|\omega\rangle$ feature approximately the same QEV of the observable \hat{A} for large n . From this property together with the result that the states $|\omega\rangle$ are nearly normalized one concludes that the replacement ensemble $\{|\omega\rangle\}$ indeed approximates the exact ensemble $\{|\phi\rangle\}$ very well for large Hilbert spaces (with $a = \text{HA}[\langle \omega | \hat{A} | \omega \rangle]$ as given in Eq. (21)).

Second, the upper bound from Eq. (23) is valid for any time t . Thus, for large enough systems, the dynamical curves for $a_\omega(t) := \langle \omega | \hat{A}(t) | \omega \rangle$ of the vast majority of pure states from the initial ensemble $\{|\omega\rangle\}$ are very close to each other and thus to the evolving ensemble average at any time t . Due to the similarity of $\{|\omega\rangle\}$ and $\{|\phi\rangle\}$ this should also hold true for the “exact” ensemble $\{|\phi\rangle\}$. Thus, there is a typical evolution for the expectation values $\langle \phi | \hat{A}(t) | \phi \rangle$ or, to rephrase, there is “dynamical typicality”. This statement represents the main result of this paper. Particularly, this typicality is independent of the concrete form of the dynamics, which may be a standard exponential decay into equilibrium or something completely different. For more details on and a numerical demonstration of dynamical typicality see [11]

The mean QEV, i.e., essentially a , can alternatively be reformulated using the notion of a density matrix as usually done in the framework of projection operator formalisms

$$a = \text{HA}[\langle \omega | \hat{A} | \omega \rangle] = \text{HA}[\text{Tr}\{\hat{A}|\omega\rangle\langle\omega|\}] = \text{Tr}\{\hat{A} \text{HA}[|\omega\rangle\langle\omega|]\}. \quad (24)$$

The $\text{HA}[|\omega\rangle\langle\omega|]$ takes the role of the density matrix. Further evaluation gives (using the “substitute” ensemble $\{|\omega\rangle\}$) (see [6])

$$\text{HA}[|\omega\rangle\langle\omega|] = \frac{1 + 2d\hat{A} + d^2\hat{A}^2}{n(1+d^2)}. \quad (25)$$

For ensembles close to equilibrium, i.e., small d , which is fulfilled in the examples presented here, one can neglect the terms which grow quadratically in d . In this case, the density matrix takes approximately the same form as the initial state which is often used in projection operator calculations which aim at determining the dynamics of expectation values like $a(t)$ ([15]).

There, for reasons given below, the (mixed) initial state is simply taken to be $\rho(0) = 1/n + c\hat{A}$ such that $c = a(0)$. That means, correct dynamical results from the projection operator methods based on the above initial state describe the dynamics of the ensemble average of $\{|\omega\rangle\}$.

From this point of view some consequences on the applicability of projection operator theories (NZ, time-convolutionless, Mori formalism etc.), which are standard tools for the description of reduced dynamics, arise. These methods have in common the occurrence of an inhomogeneity in the central equations of motion that typically has to be neglected in order to solve them. Generally, the inhomogeneity depends on the true initial state, it, however, vanishes if the true initial state indeed is of some specific form determined by the pertinent projector [13; 16; 14]. For the above mentioned case the above $\hat{\rho}(0)$ is exactly of that form, which means the dynamics of the ensemble are equal to the dynamics generated by the pertinent projected equation of motion without the inhomogeneity. However, the evolution of the ensemble is typical, this implies that the inhomogeneity, as generated by most of the true initial states, should be negligible.

On the other hand, there are investigations in the field of open quantum systems, e.g., [17] and [18], suggesting that the true initial states may have an utterly crucial influence on the dynamics, such that, e.g., some correlated initial states may yield projected dynamics which are entirely different from the ones obtained by corresponding product states.

Nevertheless, to rephrase, the results of this paper indicate that in the limit of large (high dimensional) systems the inhomogeneity should become more and more irrelevant in the sense that the statistical weight of initial states, which yield an inhomogeneity that substantially changes the solution of the projected equation of motion, should decrease to zero. Note that this does not contradict the concrete results of [17] and [18].

The above results also shed some light on the relation of the apparently irreversible dynamics of QEV’s to the, in some sense, reversible dynamics of the underlying Schrödinger equation. If a mean QEV as generated by some initial non-equilibrium ensemble (pertinent density matrix) relaxes to equilibrium (which can often be reliably shown [13]), then for the majority of the individual states that form the ensemble, the corresponding individual QEV’s will relax to equilibrium in the same way. Thus, for the relaxation of the QEV’s, the question whether or not the initial ensemble truly exists is largely irrelevant. Of course, there may be individual initial states giving rise to QEV evolutions that do not (directly) relax to equilibrium, but, to repeat, for high dimensional systems, their statistical weight is low.

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