

# Equilibration of isolated many-body quantum systems with respect to general distinguishability measures

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We demonstrate equilibration of isolated many-body systems in the sense that, after initial transients have died out, the system behaves practically indistinguishable from a time-independent steady state, i.e., non-negligible deviations are unimaginably rare in time. Measuring the distinguishability in terms of quantum mechanical expectation values, results of this type have been previously established under increasingly weak assumptions about the initial disequilibrium, the many-body Hamiltonian, and the considered observables. Here, we further extend these results with respect to generalized distinguishability measures which fully take into account the fact that the actually observed, primary data are not expectation values but rather the probabilistic occurrence of different possible measurement outcomes.

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## I. INTRODUCTION

Does a macroscopic system, prepared in a nonequilibrium initial state, and evolving in isolation from the rest of the world, approach a steady state in the long time limit? Due to quantum revivals, time inversion invariance, and other quite obvious reasons (see Sec. III A), such a relaxation towards an equilibrium state can certainly not be true in the strict sense. On the other hand, “practical equilibration” has been established in Refs. [1–4] under quite weak conditions in the sense that the expectation value of quantum mechanical observables remains extremely close to a constant value for the overwhelming majority of all sufficiently late times. In other words, deviations of expectation values from a steady long time limit are either so small or so rare that they can be safely neglected in any real experiment.

Yet, it has been pointed out by Short [2] that these findings are still not fully satisfactory since the primary data in a quantum mechanical measurement are not expectation values but rather the probabilistic occurrence of different possible measurement outcomes. Indeed, the exact probabilities of those outcomes are generically not strictly identical to the presumed steady state values, hence the difference unavoidably must become statistically resolvable when repeating the measurement sufficiently many times. If such a difference would already be recognizable by an experimentally feasible number of repetitions, then practical equilibration in the above sense would thus no longer hold true. The main purpose of our present paper is to exclude the latter possibility by further developing the approach from Refs. [2–4].

Two immediate next questions are as follows: Does the steady long time limit agree (at least approximately) with the value predicted by one of the canonical ensembles from textbook statistical physics? What is the characteristic time scale governing the relaxation towards equilibrium? Both questions are clearly of great conceptual as well as practical importance, and they have been recently addressed by numerous analytical, numerical, and experimental works (see Refs. [5–8] for a few representative examples). Yet, these questions are beyond the scope of this paper.

## II. GENERAL FRAMEWORK

We focus on time-independent Hamiltonians of the form

$$H = \sum_n E_n P_n, \quad (1)$$

where the  $P_n$  are projectors onto the eigenspaces of  $H$  with mutually different eigenvalues  $E_n$ , and where  $n$  runs from 1 to infinity or to some finite upper limit.

The main examples we have in mind are isolated macroscopic systems with, say,  $f \approx 10^{23}$  degrees of freedom. Compound systems, consisting of a subsystem of actual interest and a much larger environmental bath, are thus included as special cases. While the precise requirements on  $H$  will be provided later, we anticipate that, similarly as in Refs. [1–4], those rather weak requirements do *not* imply that the system must be “non-integrable” or “chaotic” in the sense of Refs. [6]. Moreover, our explorations may also be of interest, e.g., for systems with few degrees of freedom [9] but with a high dimensional “active Hilbert space.”<sup>1</sup>

As usual, system states (pure or mixed) are described by density operators  $\rho$  and observables by Hermitian operators  $A$ . Expectation values are given by  $\langle A \rangle_\rho := \text{Tr}\{\rho A\}$  and the time evolution by  $\rho(t) = \mathcal{U}_t \rho(0) \mathcal{U}_t^\dagger$  with propagator  $\mathcal{U}_t := e^{-iHt}$  ( $\hbar = 1$ ), implying with (1) that  $\mathcal{U}_t := \sum_n P_n e^{-iE_n t}$  and hence that

$$\langle A \rangle_{\rho(t)} = \sum_{m,n} A_{mn} e^{i(E_n - E_m)t}, \quad (2)$$

$$A_{mn} := \text{Tr}\{P_m \rho(0) P_n A\}. \quad (3)$$

<sup>1</sup>Here, “a high dimensional active Hilbert space” means that, analogously as in Eqs. (7) and (8), the energy level populations  $p_n$  must be small for all but one  $n$ . Apart from trivial cases this implies that there must be many levels which are non-negligibly populated by the system state (“active”), and which thus span a high dimensional Hilbert space.

Similarly as in (1), any given observable  $A$  can be written in the form

$$A = \sum_v a_v K_v, \quad (4)$$

where  $K_v$  are the projectors onto the eigenspaces of  $A$  with mutually different eigenvalues  $a_v$ . According to textbook quantum mechanics, given a system in state  $\rho(t)$ , any single measurement of the observable  $A$  results in one of the possible outcomes  $a_v$ , and the probability to obtain the specific outcome  $a_v$  is given by

$$k_v(t) := \text{Tr}\{\rho(t)K_v\}. \quad (5)$$

As an aside, we remark that our present approach could be readily extended to the so-called positive-operator valued measure (POVM) formalism [10]: The only formal difference would be that the pertinent operators  $K_v$  are then in general no longer mutually orthogonal, a property which we never actually exploit in the following.

Finally, we adopt the viewpoint that no experimentally realistic measurement yields more than, say, 20 relevant digits. Hence, it is sufficient to consider observables with less than  $10^{20}$  different measurement outcomes  $a_v$ , i.e., we can and will restrict ourselves from now on to observables  $A$  which satisfy the conditions

$$v \in \{1, 2, \dots, N_A\}, \quad N_A < 10^{20}. \quad (6)$$

In view of Eq. (1), the specific observable  $A = P_n$  describes the population of the (possibly degenerate) energy level  $E_n$  with expectation value (occupation probability)

$$p_n := \text{Tr}\{\rho(t)P_n\}. \quad (7)$$

Since  $P_n$  commutes with  $H$  from (1), the level populations  $p_n$  are  $t$  independent (conserved quantities). Thus, they are entirely determined already by the initial condition (system preparation).

For typical macroscopic systems with  $f \approx 10^{23}$  degrees of freedom, the energy levels are unimaginably dense. Under realistic experimental conditions it is therefore practically unavoidable to notably populate a number of energy levels which is exponentially large in  $f$ . In turn, every single level population  $p_n$  from (7) is expected to be extremely small (compared to  $\sum_n p_n = 1$ ) and to typically satisfy the very rough estimate  $\max_n p_n = 10^{-\mathcal{O}(f)}$ . In the following, we even admit the possibility that one single energy level exhibits a non-small population, for instance, a macroscopically populated ground state. Accordingly, we may still expect that

$$\max'_n p_n = 10^{-\mathcal{O}(f)}, \quad (8)$$

where  $\max'_n p_n$  indicates the second largest energy level population.

### III. PROBLEM OF EQUILIBRATION

#### A. Preliminary results

Our preliminary formulation of the problem of equilibration consists in the question whether, in which sense, and under what conditions the expectation value from (2) approaches a constant value in the long time limit.

It is quite obvious that the expectation value (2) cannot rigorously converge towards any long time limit apart from trivial cases with  $A_{mn} = 0$  for all  $m \neq n$ . Moreover, it is well known that any  $\rho(t)$  returns arbitrarily close to the initial state  $\rho(0)$  for certain, sufficiently late time points  $t$  (quantum revivals).

The only remaining hope is that (2) *approximately* approaches some steady value for *most* sufficiently large times  $t$ . Intuitively, if any such steady asymptotics is approached at all, then the most promising candidate appears to be the value which is obtained by averaging (2) over all times  $t \geq 0$ . Since all energies  $E_n$  are mutually different [see below Eq. (1)], one readily can infer from (2) that this putative steady state should thus be given by  $\langle A \rangle_{\bar{\rho}} := \text{Tr}\{\bar{\rho}A\}$ , where

$$\bar{\rho} := \sum_n P_n \rho(0) P_n \quad (9)$$

is a non-negative Hermitian operator of unit trace and thus a well defined density operator. A result of this type is derived in Appendix A by combining and refining techniques originally due to Refs. [3,4,11]. Namely, it is shown that the following inequality holds for all sufficiently large  $T$ :

$$\frac{1}{T} \int_0^T dt [\sigma(t)]^2 \leq 3 \text{Tr}\{\bar{\rho}A^2\} g \max'_n p_n, \quad (10)$$

$$\sigma(t) := \langle A \rangle_{\rho(t)} - \langle A \rangle_{\bar{\rho}}, \quad (11)$$

where  $\max'_n p_n$  is the second largest energy level population [see around Eq. (8)] and  $g$  represents the maximal degeneracy of energy gaps

$$g := \max_{m \neq n} |\{(k,l) : E_k - E_l = E_m - E_n\}|, \quad (12)$$

with  $|S|$  denoting the number of elements contained in the set  $S$ . In other words,  $g$  is the maximal number of exactly coinciding energy differences among all possible pairs of distinct energy eigenvalues.

In view of (8) and disregarding exceedingly large gap degeneracies  $g$ , the time average on the left hand side in (10) is extremely small, implying that the deviation (11) must be very small in modulus for most times  $t \in [0, T]$ . In order to quantify this argument, we define for any given  $\epsilon > 0$  and  $T > 0$  the quantity

$$T_\epsilon := |\{0 \leq t \leq T : |\sigma(t)| > \epsilon\}|, \quad (13)$$

where  $|S|$  denotes the size (Lebesgue measure) of the set  $S$ . In other words,  $T_\epsilon$  is the measure of all times  $t \in [0, T]$  for which  $|\sigma(t)| > \epsilon$  holds true. It follows that  $[\sigma(t)]^2 > \epsilon^2$  for a set of times  $t$  of measure  $T_\epsilon$  and that  $0 \leq [\sigma(t)]^2 \leq \epsilon^2$  for all remaining times  $t$  contained in  $[0, T]$ . Hence the temporal average on the left hand side of (10) must be bounded from below by  $\epsilon^2 T_\epsilon / T$ . It follows that for any given  $\epsilon > 0$

$$T_\epsilon / T \leq 3 \text{Tr}\{\bar{\rho}A^2\} g \max'_n p_n / \epsilon^2 \quad (14)$$

for all sufficiently large  $T$ .

Note that the left hand side of (10) remains unchanged if  $A$  is replaced by  $A + c 1$ , where  $c$  is an arbitrary real number and  $1$  the identity operator. Accordingly, we may replace also on the right hand side of (10)  $A$  by  $A + c 1$  with an arbitrary  $c$ . Denoting by  $a_{\max}$  and  $a_{\min}$  the largest and smallest eigenvalues

of  $A$  [cf. (4) and (6)], and by  $\Delta_A := a_{\max} - a_{\min}$  the range of  $A$ , we can and will choose  $c$  so that  $|a_\nu - c| \leq \Delta_A/2$  for all eigenvalues  $a_\nu$  of  $A$ . It follows that  $\text{Tr}\{\bar{\rho}(A+c)^2\} \leq (\Delta_A/2)^2$  on the right hand side of (10), and likewise in (14), i.e.,

$$\frac{T_\epsilon}{T} \leq \frac{3\Delta_A^2 g \max_n' p_n}{4\epsilon^2} \quad (15)$$

for all sufficiently large  $T$ .

Relation (15) together with (8), (12), and (13) represents the answer to the above stated, preliminary problem of equilibration: For any given  $\epsilon > 0$  the “true” expectation value  $\langle A \rangle_{\rho(t)}$  deviates from the constant value  $\langle A \rangle_{\bar{\rho}}$  by more than  $\epsilon$  for a set of times  $t \in [0, T]$ , whose measure  $T_\epsilon$  is bounded by (15) for all sufficiently large  $T$ . If  $\epsilon$  as well as the right hand side of (15) are both sufficiently small, which is easily feasible in view of (8), then it follows that  $\langle A \rangle_{\rho(t)}$  is practically (within any experimentally achievable resolution) constant for the overwhelming majority of all times  $t \in [0, T]$ . In particular,  $T$  must be so large that the initial decay process (from the possibly far from equilibrium initial value  $\langle A \rangle_{\rho(0)}$  towards the equilibrium value  $\langle A \rangle_{\bar{\rho}}$ ) is accomplished during a time interval much smaller than  $[0, T]$ .

Note that Hamiltonians with degenerate energy gaps are, loosely speaking, of measure zero among “all” Hamiltonians. They only arise in the presence of special reasons like (perfect) symmetries, additional conserved quantities (besides  $H$ ), or fine tuning of parameters. Generically, all nontrivial energy gaps  $E_m - E_n$  (i.e., those with  $m \neq n$ ) are thus mutually different, implying  $g = 1$  in (12). Our above results remain valid even for nongeneric cases with  $g > 1$ . Likewise, Hamiltonians with degenerate energy eigenvalues are in principle nongeneric, but still admitted in (1).

In summary, the true system state  $\rho(t)$  becomes experimentally indistinguishable from the time-independent approximation  $\bar{\rho}$  for practically all sufficiently late times  $t$  under very weak conditions on the initial state, the observable, and the Hamiltonian.

### B. Reformulation of the problem

So far, the (non)distinguishability of  $\rho(t)$  and  $\bar{\rho}$  was always meant with respect to the corresponding two expectation values of the considered observable  $A$ . As pointed out by Short [2], such a distinguishability criterion is not entirely satisfying since the basic measurable quantities are *not* expectation values, but rather the different possible measurement outcomes  $a_\nu$  [see above Eq. (5)]. Hence, the distinguishability of  $\rho(t)$  and  $\bar{\rho}$  should be based on the actually observed, random occurrence of each outcome  $a_\nu$ . More precisely, one should compare in some suitable way the probabilities  $k_\nu(t)$  from (5) and

$$\bar{k}_\nu := \text{Tr}\{\bar{\rho}K_\nu\} \quad (16)$$

with which the different possible measurement outcomes  $a_\nu$  are observed in the two states  $\rho(t)$  and  $\bar{\rho}$ , respectively. Indeed, it could well be that  $\rho(t)$  and  $\bar{\rho}$  are indistinguishable as far as the expectation value of  $A$  is concerned, yet the two states are clearly distinguishable (with high statistical significance) by the frequencies of observing the different measurement out-

comes  $a_\nu$ , when repeating the same measurement sufficiently often [2].

Here and in the following, the term “repetition” (of a measurement) has the usual meaning, namely, to perform a measurement of the same observable on an ensemble of systems in the same quantum mechanical state, each of them resulting in a random measurement outcome and a concomitant collapse of the system state according to the common rules of quantum mechanics [see also above Eq. (5)].

Put differently, the actual problem of equilibration is to show that the frequencies, with which the different possible measurement outcomes are realized in the true system state  $\rho(t)$ , are not incompatible in any statistically significant way with the approximation  $\bar{\rho}$ .

In this statement of the problem,  $t$  is tacitly considered as being chosen arbitrarily but then kept fixed. (In Sec. V, we will extend the scope of our results also to cases when the measurement is taken at a different time in each repetition.) Moreover, the number of repetitions, henceforth denoted as  $N_{\text{rep}}$ , must remain reasonable, say

$$N_{\text{rep}} < 10^{30}. \quad (17)$$

(This bound is reached for  $10^{12}$  repetitions per second during the age of the universe.) To understand why such an upper bound is needed, we focus on the generic case that the probabilities (5) and (16) with which the outcomes  $a_\nu$  are realized in the two states  $\rho(t)$  and  $\bar{\rho}$ , respectively, are not exactly identical for all  $\nu$ . In the limit  $N_{\text{rep}} \rightarrow \infty$ , it then must become apparent with arbitrary statistical significance that the approximation  $\bar{\rho}$  is incompatible with the observed measurement outcomes, which are sampled according to the true system state  $\rho(t)$ . In other words, without imposing any upper bound on  $N_{\text{rep}}$ , the two states  $\rho(t)$  and  $\bar{\rho}$  would generically be trivially distinguishable.

Important first steps in resolving the above stated problem of equilibration have been achieved in Ref. [2]. In doing so, the distinguishability of  $\rho(t)$  and  $\bar{\rho}$  was quantified as follows: Imagine that one of the two states  $\rho(t)$  and  $\bar{\rho}$  were randomly chosen with probability  $\frac{1}{2}$  and then used to sample one of the different outcomes  $a_\nu$  according to the corresponding probabilities in (5) or (16). Now, the task is to guess from the observed  $a_\nu$  which state [ $\rho(t)$  or  $\bar{\rho}$ ] has been chosen, and the probability that this guess is correct was shown in Ref. [2] to be bounded by  $1/2 + \sum_{\nu=1}^{N_A} |k_\nu(t) - \bar{k}_\nu|/4$ . Hence, the latter quantity was adopted in Ref. [2] as the basic measure to quantify the distinguishability of  $\rho(t)$  and  $\bar{\rho}$  by means of  $A$ .

We think that this approach is still unsatisfying in two respects: (i) The underlying “state guessing task” is not exactly equivalent to the above formulated “actual problem of equilibration”: in the actual problem, the outcomes are always generated by  $\rho(t)$ , and not by either  $\rho(t)$  or  $\bar{\rho}$  with equal probability. Moreover, the actual task is not to guess which of the two states was realized but rather to quantify the compatibility of the state  $\bar{\rho}$  with the observed measurement outcomes. (ii) The entire approach is limited to single shot measurements, i.e., to  $N_{\text{rep}} = 1$ . Indeed, already in the case of two repetitions of the same measurement, resulting in two outcomes  $a_{\nu_1}$  and  $a_{\nu_2}$ , it is not clear at all which of the two states should be guessed according to the above described strategy

from Ref. [2]. While a restriction like in (17) still covers all cases of practical relevance, the same is no longer true for the restriction  $N_{\text{rep}} = 1$  considered in [2].

The main objective of our present paper is to resolve the above issues (i) and (ii). In doing so, we will even admit one more generalization. Namely, in every repetition  $j$ , a measurement of a different observable  $A_j$  may be performed (but the system state remains the same in each repetition). In particular, some or even all  $A_j$  may still be identical, but in general they are admitted to be different. In doing so we denote, similarly as in (5), by  $K_v^{(j)}$  the projectors onto the eigenspaces of  $A_j$  and by  $a_v^{(j)}$  the corresponding eigenvalues, where  $v = 1, \dots, N_{A_j}$ . Furthermore, their probabilities of occurrence are denoted, similarly as in (5) and (16), as

$$k_v^{(j)}(t) := \text{Tr}\{\rho(t)K_v^{(j)}\} \quad (18)$$

if the system is in the state  $\rho(t)$  and as

$$\bar{k}_v^{(j)} := \text{Tr}\{\bar{\rho} K_v^{(j)}\} \quad (19)$$

with respect to the state  $\bar{\rho}$ . Accordingly, the outcome of our  $N_{\text{rep}}$  measurements can be uniquely specified by a  $N_{\text{rep}}$ -dimensional vector  $\vec{s}$ , whose  $j$ th component  $s_j \in \{1, \dots, N_{A_j}\}$  specifies which outcome of  $A_j$  was realized in the  $j$ th measurement. The probability to obtain the outcome  $\vec{s}$  then follows as

$$p_t(\vec{s}) := \prod_{j=1}^{N_{\text{rep}}} k_{s_j}^{(j)}(t) \quad (20)$$

if the system is in the state  $\rho(t)$ , and as

$$\bar{p}(\vec{s}) := \prod_{j=1}^{N_{\text{rep}}} \bar{k}_{s_j}^{(j)} \quad (21)$$

with respect to the state  $\bar{\rho}$ . Finally, with the definition

$$N_{\text{obs}} := \max_j N_{A_j} \quad (22)$$

we can conclude from (6) that

$$N_{A_j} \leq N_{\text{obs}} < 10^{20} \quad (23)$$

for all  $j = 1, \dots, N_{\text{rep}}$ .

#### IV. DISTINGUISHABILITY MEASURES

In essence, the situation encountered above is as follows: There is a true state  $\rho(t)$  ( $t$  arbitrary but fixed) and an approximative state  $\bar{\rho}$ . A series of  $N_{\text{rep}}$  measurements of the observables  $A_j$  ( $j = 1, \dots, N_{\text{rep}}$ ) is performed on the system state  $\rho(t)$ , resulting in one of the possible outcomes  $\vec{s}$ . Within this setup, our key question is as follows: Given the outcome  $\vec{s}$  of such a measurement series, does the approximation  $\bar{\rho}$  explain the observed data  $\vec{s}$  notably worse than the truth  $\rho(t)$  would explain them, or are  $\rho(t)$  and  $\bar{\rho}$  both about equally well (or badly) compatible with the given data  $\vec{s}$ ? If the latter is the case with very high probability when the entire measurement series is repeated many times [i.e., each outcome  $\vec{s}$  is realized with probability  $p_t(\vec{s})$  from (20)], then the two states  $\rho(t)$  and

$\bar{\rho}$  are practically indistinguishable by means of the considered observables  $A_j$ . Put differently, the approximation  $\bar{\rho}$  is as good as it possibly can be since it explains the observed measurement outcomes practically as well as the best possible theory  $\rho(t)$  would explain them.

To further substantiate these ideas, let us focus on an arbitrary but fixed “test” (or “rule,” “strategy,” “criterion,” etc.) by means of which we can (or hope to) quantify (in whatever way) how much worse (or possibly better) the approximation  $\bar{\rho}$  is compatible with a given data set  $\vec{s}$  than  $\rho(t)$ . In doing so, the two states  $\rho(t)$  and  $\bar{\rho}$  are thus considered as known. In particular, all the probabilities from (20) and (21) are explicitly available and may be exploited by our test at hand. In other words,  $\rho(t)$ ,  $\bar{\rho}$ , and  $\vec{s}$  are the input of the test, which then acts like a black box to produce an output in the form of a real number  $q(\rho(t), \bar{\rho}, \vec{s})$ .

Without any significant loss of generality we assume that  $q(\rho(t), \bar{\rho}, \vec{s})$  is standardized so that it only takes values within the interval  $[-1, 1]$ . Furthermore,  $q(\rho(t), \bar{\rho}, \vec{s}) = 0$  indicates that  $\rho(t)$  and  $\bar{\rho}$  are (approximately) equally well (or badly) compatible with  $\vec{s}$ . Finally, increasingly positive  $q$  values correspond to an increasing superiority of  $\rho(t)$  over  $\bar{\rho}$  in explaining the data  $\vec{s}$ , and likewise for negative  $q$  values.

Note that we can never be “100% sure” that  $\bar{\rho}$  is incompatible with the data  $\vec{s}$ .<sup>2</sup> Hence, any (reasonable) test can only make certain probabilistic statements (based on some certain notion of probability, likelihood, confidence, plausibility, ...) about the compatibility of  $\bar{\rho}$  with  $\vec{s}$ , and likewise for  $\rho(t)$ .

We also note that for some “strange” (unlikely but not impossible) outcomes  $\vec{s}$  of the measurement series, even the “reality”  $\rho(t)$  may be incompatible (in the above mentioned probabilistic sense) with  $\vec{s}$  according to the criteria of the given test. Likewise, the compatibility of certain  $\vec{s}$  with  $\bar{\rho}$  may actually be better (or less bad) than with  $\rho(t)$ . Intuitively (or from a Bayesian viewpoint), it seems plausible that such cases may be realized whenever a given outcome  $\vec{s}$  has the property that  $\bar{p}(\vec{s}) > p_t(\vec{s})$ . Quantitatively, such cases are taken into account by the negative  $q$  values.

A particularly simple example is

$$q(\rho(t), \bar{\rho}, \vec{s}) := f[p(\rho(t)|\vec{s}) - p(\bar{\rho}|\vec{s})], \quad (24)$$

$$p(\rho(t)|\vec{s}) := \frac{p_t(\vec{s})}{p_t(\vec{s}) + \bar{p}(\vec{s})}, \quad (25)$$

$$p(\bar{\rho}|\vec{s}) := \frac{\bar{p}(\vec{s})}{p_t(\vec{s}) + \bar{p}(\vec{s})}, \quad (26)$$

where  $f[x]$  is some monotonically increasing function of  $x$  with  $f[-1] = -1$ ,  $f[0] = 0$ ,  $f[1] = 1$ , for instance  $f[x] = x$ . [We tacitly restrict ourselves to outcomes  $\vec{s}$  which are realized with nonvanishing probability, hence, the denominators in (25) and (26) are nonzero. We also note that since  $p(\bar{\rho}|\vec{s}) = 1 - p(\rho(t)|\vec{s})$ , the right hand side of (24) could equally well be written as a function of  $p(\rho(t)|\vec{s})$  alone.]

<sup>2</sup>At first sight, one might think that  $\bar{p}(\vec{s}) = 0$  implies “for sure” that  $\bar{\rho}$  is incompatible with the data  $\vec{s}$ . However, as shown in Appendix A [see below Eq. (A59)],  $\bar{p}(\vec{s}) = 0$  implies  $p_t(\vec{s}) = 0$ , i.e., such an  $\vec{s}$  is never realized.

Within the framework of Bayesian inference,  $p(\rho(t)|\vec{s})$  and  $p(\bar{\rho}|\vec{s})$  in (25) and (26) can be identified with the posterior probabilities of  $\rho(t)$  and  $\bar{\rho}$ , given  $\vec{s}$  has been observed, and assuming equal prior probabilities for  $\rho(t)$  and  $\bar{\rho}$  (i.e., before the observations  $\vec{s}$  are available). Accordingly, (24) may be interpreted as quantifying the likelihood of  $\rho(t)$  compared to that of  $\bar{\rho}$ . We, however, remark that even without adopting a Bayesian viewpoint, all quantities in (24)–(26) remain well defined and admit a decent probabilistic interpretation.

Analogously as in (24), one also could, for example, quantify the compatibility of  $\rho(t)$  and  $\bar{\rho}$  with  $\vec{s}$  in cases when all  $A_j$  are equal by defining  $q(\rho(t), \bar{\rho}, \vec{s})$  in some suitable way via the two values which are obtained by applying a  $\chi^2$  test to the two “null hypotheses”  $\rho(t)$  and  $\bar{\rho}$ .

Returning to the general case of an arbitrary but fixed test, any given such test may still admit many different reasonable choices of  $q$  [e.g., different functions  $f$  in (24)]. Our first key hypothesis is now that for any given test it is possible to choose a function  $q$  so that the quality of this test is reasonably quantified by the distinguishability measure

$$Q(t) := \sum_{\vec{s}} p_t(\vec{s}) q(\rho(t), \bar{\rho}, \vec{s}), \quad (27)$$

i.e., by averaging  $q(\rho(t), \bar{\rho}, \vec{s})$  over many measurement series and weighting every possible outcome  $\vec{s}$  with the frequency  $p_t(\vec{s})$  with which it is realized. More precisely, the existence of at least one  $q$  function is postulated for which a  $Q$  value close to unity indicates that the given test quite reliably recognizes the incompatibility of  $\bar{\rho}$  with the measurement series  $\vec{s}$  [which was sampled according to  $\rho(t)$ ], while a  $Q$  value close to zero indicates that there is no way to recognize by means of the given test any significant difference between the truth  $\rho(t)$  and the approximation  $\bar{\rho}$  when sampling a data set  $\vec{s}$  according to  $\rho(t)$ . Note that small negative  $Q$  still indicates a good compatibility of  $\bar{\rho}$  with the measurements, while nonsmall negative  $Q$  values are also possible but would quite plausibly indicate that the given test is futile, or that one rather should employ  $-q$  instead of  $q$ .

The complete set of all tests which fulfill our above assumptions may still admit some undesirably biased  $q$  functions. The most trivial example is  $q(\rho(t), \bar{\rho}, \vec{s}) := 1$  for all  $\vec{s}$ , yielding the highest possible score of  $Q(t) = 1$ . The only viable way out seems to admit only tests, whose  $q$  function does not exploit the information that the data  $\vec{s}$  were actually sampled according to  $\rho(t)$ . In particular, we may imagine (as a hypothetical *Gedankenexperiment*) that the system was not in the state  $\rho(t)$  but rather in the state  $\bar{\rho}$  without telling this fact to the person working with a given  $q$  function. If we would in this way secretly sample  $\vec{s}$  not according to  $\rho(t)$  but rather according to  $\bar{\rho}$ , then the very same  $q$  function should now be able to recognize that the data are (on the average) better explained by  $\bar{\rho}$  than by  $\rho(t)$ .

Therefore, our second key hypothesis is that it is sufficient to focus on tests, whose  $q$  functions satisfy the following additional symmetry property: imagine many repetitions of our so far considered measurement series. But now, in every repetition, either  $\rho(t)$  or  $\bar{\rho}$  is randomly selected with probability  $\frac{1}{2}$  and then used to randomly generate (via the usual quantum mechanical measurement process) a measurement

series  $\vec{s}$  according to the corresponding probability (20) or (21). In this case, we require that the  $q$  function must be unbiased on the average, i.e.,

$$\sum_{\vec{s}} \frac{p_t(\vec{s}) + \bar{p}(\vec{s})}{2} q(\rho(t), \bar{\rho}, \vec{s}) = 0. \quad (28)$$

While the above two hypotheses seem difficult or impossible to derive from some more fundamental principles, they appear quite reasonable as they stand and are thus taken for granted from now on. Their most important virtue is that they imply, as demonstrated in detail in Appendix B, the general rigorous bound

$$|Q(t)| \leq Q_{\max}(t) := \frac{1}{2} \sum_{\vec{s}} |p_t(\vec{s}) - \bar{p}(\vec{s})| \quad (29)$$

for the distinguishability measure  $Q(t)$  from (27), independently of any further peculiarities of the considered test and the concomitant  $q$  function. This is the first main result of our paper.

In particular, one readily verifies that the example from (24)–(26), with  $f[x] = x$ , exhibits the symmetry (28) and respects the bound (29). More generally, the symmetry (28) imposes a nontrivial constraint on  $f[x]$  and a direct verification of (29) (without recourse to Appendix B) becomes difficult.

In hindsight, the original task to quantify the compatibility of  $\bar{\rho}$  with the measurement series  $\vec{s}$  may have appeared quite daunting since this can be done in so many different ways, most of which one possibly did not even think of in the first place. The appeal of our main result (29) is that it applies independently of the concrete manner in which the compatibility is quantified. In particular, no explicit knowledge is needed about the best possible way to quantify the compatibility of  $\bar{\rho}$  with  $\vec{s}$ . The only, very weak and plausible, requirements are that all considered distinguishability measures can be written in the form (27) for some suitable  $q$  function, and that they respect the symmetry condition (28).

## V. FINAL RESULT AND CONCLUSIONS

The upshot of the previous section is as follows: If we can show that  $Q_{\max}(t)$  from (29) is a small quantity, then there is no way to experimentally detect any statistically significant deviation of the approximation  $\bar{\rho}$  from the true system state  $\rho(t)$ . The latter statement applies for an arbitrary but fixed time  $t$  and for an arbitrary but fixed measurement series  $A_1, \dots, A_{N_{\text{rep}}}$ . Hence, if we can show that the same statement holds simultaneously for all measurement series which satisfy (17) and (23) and for the overwhelming majority of all sufficiently late times  $t$ , then it follows, analogously as in Sec. III A, that approximating  $\rho(t)$  by  $\bar{\rho}$  can be considered as perfect for all practical purposes.<sup>3</sup>

As detailed in Appendix C, it is indeed possible to show that a result of the above type holds true. Quantitatively, the

<sup>3</sup>We recall that (23) follows from our assumption (6) and the definition (22).

result is analogous to Eqs. (13) and (15), stating that

$$T^*/T \leq \epsilon, \quad (30)$$

$$T^* := |\{0 \leq t \leq T : Q_{\max}(t) > \epsilon\}|, \quad (31)$$

$$\epsilon := (122 g \max'_n p_n)^{1/4} N_{\text{obs}}^{1/2} N_{\text{rep}} \quad (32)$$

for all sufficiently large  $T$ . This is the main final result of our paper. Its discussion can be conducted along very similar lines as in Sec. III, hence, we only recapitulate here the main points: On the right-hand side of (32),  $g$  denotes the maximal degeneracy of energy gaps from (12) (with  $g = 1$  for Hamiltonians with a generic spectrum). Furthermore,  $\max'_n p_n$  is the second largest level population and, according to (8), is typically exponentially small in  $f$  for a system with  $f \gg 1$  degrees of freedom. In view of (17) and (23), we thus can conclude that  $\epsilon$  in (32) becomes an extremely small number already for systems with, say, more than  $10^3$  degrees of freedom. In turn, the Lebesgue measure (31) of those times  $t \in [0, T]$ , for which there possibly may exist a non-negligible chance to observe a resolvable difference between  $\rho(t)$  and  $\bar{\rho}$  by some suitable measurement procedure, is [according to (30)] negligibly small compared to all times  $t \in [0, T]$ , provided  $T$  is sufficiently large.

To summarize, the steady state  $\bar{\rho}$  approximates the true state  $\rho(t)$  practically perfectly for all sufficiently large times  $t$ . While the two states are rigorously speaking never close to each other in some mathematically obvious way, the observable differences are either unresolvably small or negligibly rare from all practical points of view.

We finally note that by admitting the possibility to employ in every repetition of the experiment a different observable  $A_j$ , our approach actually also covers the case when the measurement is performed in every repetition at a different time point (which strictly speaking applies to every real experiment). The reason is the usual equivalence of the Schrödinger and Heisenberg pictures, i.e., a temporal change of the system state can be replaced by an equivalent change of the considered observable.

## ACKNOWLEDGMENTS

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## APPENDIX A

In this Appendix, we provide the derivation of Eqs. (10) and (11), i.e., we show that for all sufficiently large  $T$ ,

$$\int_0^T \frac{dt}{T} [\sigma(t)]^2 \leq 3 \text{Tr}\{\bar{\rho} A^2\} g \max'_n p_n, \quad (A1)$$

$$\sigma(t) := \text{Tr}\{\rho(t)A\} - \text{Tr}\{\bar{\rho}A\}, \quad (A2)$$

where  $g$  is the maximal degeneracy of energy gaps from (12), and  $\max'_n p_n$  is the second largest among all energy level populations from (7).

## 1. Preliminaries

We recall that the  $P_n$  in (1) are the projectors onto the eigenspaces of the Hamiltonian  $H$ , where  $n$  runs from 1 to infinity or to some upper finite limit. In other words,  $n \in I$ , where the index set  $I$  is either equal to  $\mathbb{N}$  or of the form  $\{1, \dots, L\}$  with a finite upper limit  $L \in \mathbb{N}$ . Hence, the projectors  $P_n$  satisfy the usual orthogonality and completeness relations, i.e.,

$$P_m P_n = \delta_{mn} P_n \quad (A3)$$

for all  $m, n \in I$  and

$$\sum_n P_n = 1, \quad (A4)$$

where 1 is the identity operator and, as in (1), the sum runs over all  $n \in I$ . Next, we define

$$\rho_n := P_n \rho(0) P_n \quad (A5)$$

and we denote by  $S_O$  the set of operators which contains all the  $P_n$ 's and all the  $\rho_n$ 's. It follows that all operators in  $S_O$  are Hermitian and commute with each other, hence, there must be a common eigenbasis for all operators contained in  $S_O$ . In other words, there is an orthonormalized basis  $\{|\gamma\rangle\}_{\gamma=1}^D$ , whose dimension  $D$  may be either finite or infinite, and whose associated projectors  $P_\gamma := |\gamma\rangle\langle\gamma|$  commute with all operators contained in  $S_O$ . As a consequence, also the projectors

$$X := \sum_{\gamma=1}^d |\gamma\rangle\langle\gamma|, \quad (A6)$$

$$Y := 1 - X = \sum_{\gamma=d+1}^D |\gamma\rangle\langle\gamma| \quad (A7)$$

commute with all  $P_n$  and  $\rho_n$ , i.e.,

$$X P_n = P_n X, \quad X \rho_n = \rho_n X \quad (A8)$$

for all  $n$ , and likewise for  $Y$ . With the definition

$$\tilde{A} := X A X \quad (A9)$$

for arbitrary observables  $A$ , it follows with (A8) that

$$\tilde{P}_n := X P_n X = P_n X = X P_n. \quad (A10)$$

In particular, if one defines  $\tilde{A}_{mn}$  analogously as in (3), then one readily verifies that

$$\tilde{A}_{mn} := \text{Tr}\{P_m \rho(0) P_n \tilde{A}\} = \text{Tr}\{\tilde{P}_m \rho(0) \tilde{P}_n A\} \quad (A11)$$

by exploiting (A9), (A10), and the cyclic invariance of the trace.

For any given basis vector  $|\gamma\rangle$ , one can infer from (A3) and (A4) that  $P_n |\gamma\rangle$  equals  $|\gamma\rangle$  (eigenvalue 1) for exactly one index  $n$ , and equals the null vector  $|0\rangle$  (eigenvalue 0) for all other indices  $n$ . Since  $d$  in (A6) is finite, it follows that at least one and at most  $d$  among all the  $\tilde{P}_n$ 's in (A10) are not identically zero. Without loss of generality, we can and will choose the labels  $n$  and some suitable integer  $N \in \{1, \dots, d\}$  so that  $\tilde{P}_n$  is nonzero if and only if  $n \in \{1, \dots, N\}$ . Furthermore, we can and will choose the labels  $\gamma$  and  $n$  so that the energy

level populations  $p_n$  from (7) assume their maximal value for  $n = 1$ , i.e.,

$$\max_n p_n = p_1. \quad (\text{A12})$$

Accordingly, the second largest level population can be written as

$$\max'_n p_n = \max_{n \geq 2} p_n. \quad (\text{A13})$$

It follows that  $\tilde{A}_{mn}$  in (A11) must vanish unless  $m \leq N$  and  $n \leq N$ . With (2) we thus can conclude that

$$\text{Tr}\{\rho(t)\tilde{A}\} = \sum_{m,n=1}^N \tilde{A}_{mn} e^{i(E_n - E_m)t}. \quad (\text{A14})$$

Likewise, one can infer from (9) and (A9) that

$$\text{Tr}\{\tilde{\rho}\tilde{A}\} = \sum_{n=1}^N \tilde{A}_{nn}. \quad (\text{A15})$$

Together, we thus obtain

$$\tilde{\sigma}(t) := \text{Tr}\{\rho(t)\tilde{A}\} - \text{Tr}\{\tilde{\rho}\tilde{A}\} = \sum_{m \neq n}^N \tilde{A}_{mn} e^{i(E_n - E_m)t}, \quad (\text{A16})$$

where the sum runs over all  $m, n \in \{1, \dots, N\}$  with  $m \neq n$ .

Since  $\rho(0)$  is a Hermitian, non-negative operator, there exists a Hermitian, non-negative operator, which we denote by  $\rho^{1/2}$ , and which satisfies the relation  $\rho^{1/2}\rho^{1/2} = \rho(0)$ . With the Cauchy-Schwarz inequality

$$|\text{Tr}\{B^\dagger C\}|^2 \leq \text{Tr}\{B^\dagger B\}\text{Tr}\{C^\dagger C\} \quad (\text{A17})$$

for the scalar product  $\text{Tr}\{B^\dagger C\}$  of arbitrary operators  $B$  and  $C$  [for which all traces in (A17) exist], and exploiting  $P_m = P_m^2$  [cf. (A3)] and the cyclic invariance of the trace, we can conclude from (A11) that

$$\begin{aligned} |\tilde{A}_{mn}|^2 &= \text{Tr}\{(P_m \rho^{1/2})(\rho^{1/2} P_n \tilde{A} P_m)\} \\ &\leq \text{Tr}\{P_m \rho(0) P_m\} \text{Tr}\{P_n \rho(0) P_n \tilde{A} P_m \tilde{A}\}. \end{aligned} \quad (\text{A18})$$

The first factor in the last line can be identified with the level population  $p_m$  from (7). In combination with (A5), (A9), and (A10), we thus obtain

$$\begin{aligned} |\tilde{A}_{mn}|^2 &\leq p_m \text{Tr}\{\rho_n X A X P_m X A X\} \\ &= p_m \text{Tr}\{X \rho_n A \tilde{P}_m A\}. \end{aligned} \quad (\text{A19})$$

Next, we observe that  $A \tilde{P}_m A$  as well as  $\rho_n$  from (A5) are both Hermitian, non-negative operators, and that every  $|\gamma\rangle$  is an eigenvector of both  $\rho_n$  and  $X$  from (A6). Upon employing the basis  $|\gamma\rangle$  to evaluate the trace in (A19), one thus obtains

$$|\tilde{A}_{mn}|^2 \leq p_m \text{Tr}\{\rho_n A \tilde{P}_m A\}. \quad (\text{A20})$$

With  $P_m^2 = P_m$  [cf. (A3)] and (A10) we can infer that  $\tilde{P}_m = P_m X P_m$ . Exploiting the cyclic invariance of the trace, we thus can rewrite the last factor in (A20) as  $\text{Tr}\{X B\}$  with  $B := P_m A \rho_n A P_m$ . Since  $B$  is a Hermitian, non-negative operator, it follows that  $\text{Tr}\{X B\} \leq \text{Tr}\{B\}$  and by the same steps as before that  $\text{Tr}\{B\} = \text{Tr}\{\rho_n A P_m A\}$ . Altogether, we finally obtain

$$|\tilde{A}_{mn}|^2 \leq p_m \text{Tr}\{\rho_n A P_m A\}. \quad (\text{A21})$$

## 2. Step 1

In this section, we closely follow the line of reasoning from Ref. [4]. The main result will be (A36). Due to (A6) and (A7), it follows for arbitrary density operators  $\rho$  and observables  $A$  that

$$\text{Tr}\{\rho A\} = \text{Tr}\{(X + Y)\rho(X + Y)A\} = R_1 + R_2 + R_3, \quad (\text{A22})$$

$$R_1 := \text{Tr}\{X \rho X A\}, \quad (\text{A23})$$

$$R_2 := \text{Tr}\{Y \rho (X + Y) A\} = \text{Tr}\{Y \rho A\}, \quad (\text{A24})$$

$$R_3 := \text{Tr}\{X \rho Y A\}. \quad (\text{A25})$$

Exploiting the cyclic invariance of the trace and the definition (A9) yields

$$R_1 = \text{Tr}\{\rho \tilde{A}\}. \quad (\text{A26})$$

By a similar line of reasoning as in the derivation of (A18), we can rewrite (A24) as

$$|R_2|^2 \leq \text{Tr}\{Y \rho Y\} \text{Tr}\{A \rho A\}. \quad (\text{A27})$$

Exploiting that for arbitrary Hermitian, non-negative operators  $B$  and  $C$

$$\text{Tr}\{BC\} \leq \|B\| \text{Tr}\{C\}, \quad (\text{A28})$$

where  $\|B\|$  denotes the standard operator norm (largest eigenvalue), the last term in (A27) can be rewritten as

$$\text{Tr}\{A \rho A\} = \text{Tr}\{\rho A^2\} \leq \|A\|^2 \text{Tr}\{\rho\} = \|A\|^2 < \infty. \quad (\text{A29})$$

The last inequality follows from (4) and (6). Finally, we can conclude from (A7) that

$$\text{Tr}\{Y \rho Y\} = \text{Tr}\{Y \rho\} = \sum_{\gamma=d+1}^D \langle \gamma | \rho | \gamma \rangle \quad (\text{A30})$$

and hence from (A27) that

$$|R_2|^2 \leq \|A\|^2 \sum_{\gamma=d+1}^D \langle \gamma | \rho | \gamma \rangle. \quad (\text{A31})$$

Analogously, one finds for  $R_3$  from (A25) that

$$|R_3|^2 \leq \text{Tr}\{Y \rho Y\} \|A\|^2 \text{Tr}\{X \rho X\} \leq \|A\|^2 \sum_{\gamma=d+1}^D \langle \gamma | \rho | \gamma \rangle. \quad (\text{A32})$$

Introducing (A26), (A31), and (A32) into (A22) finally yields

$$|\text{Tr}\{\rho A\} - \text{Tr}\{\rho \tilde{A}\}| \leq 2\|A\| \left( \sum_{\gamma=d+1}^D \langle \gamma | \rho | \gamma \rangle \right)^{1/2} \quad (\text{A33})$$

for arbitrary density operators  $\rho$ .

Next, we focus on the two specific density operators  $\rho(t)$  and  $\tilde{\rho}$  from Secs. II and III A. With the definition

$$\delta(t) := \sigma(t) - \tilde{\sigma}(t), \quad (\text{A34})$$

it readily follows from (A2), (A16), (A33), and (A34) that

$$\begin{aligned} |\delta(t)| &= |\text{Tr}\{\rho(t)A\} - \text{Tr}\{\bar{\rho}A\} - \text{Tr}\{\rho(t)\tilde{A}\} + \text{Tr}\{\bar{\rho}\tilde{A}\}| \\ &\leq |\text{Tr}\{\rho(t)A\} - \text{Tr}\{\rho(t)\tilde{A}\}| + |\text{Tr}\{\bar{\rho}A\} - \text{Tr}\{\bar{\rho}\tilde{A}\}| \\ &\leq 4\|A\| \left( \sum_{\gamma=d+1}^D \langle \gamma | \bar{\rho} | \gamma \rangle \right)^{1/2}. \end{aligned} \quad (\text{A35})$$

The last step exploited that  $\langle \gamma | \rho(t) | \gamma \rangle = \langle \gamma | \bar{\rho} | \gamma \rangle$  for all  $t$  and  $\gamma$ , as can be verified by choosing  $A = |\gamma\rangle\langle\gamma|$  in (2) and (9).

Observing that  $\|A\|$  is finite [cf. (A29)] and that  $\sum_{\gamma=1}^d \langle \gamma | \bar{\rho} | \gamma \rangle$  is monotonically increasing with  $d$  and bounded from above by  $\text{Tr}\{\bar{\rho}\} = 1$ , it follows from (A35) that for any given  $\epsilon > 0$  there exists a finite  $d$  with

$$\delta^2(t) \leq \epsilon \quad (\text{A36})$$

for all  $t$ . This is the main result of this section.

### 3. Step 2

In this section, we closely follow the line of reasoning from Ref. [11], which in turn amounts to a simplification of the previous approach from Ref. [3]. The main results will be (A45) and (A49).

Denoting the set of unequal label pairs as

$$\mathcal{G} := \{(m, n) : m, n \in \{1, \dots, N\}, m \neq n\} \quad (\text{A37})$$

and defining for any  $\alpha = (m, n) \in \mathcal{G}$

$$G_\alpha := E_m - E_n, v_\alpha := \tilde{A}_{mn}, \quad (\text{A38})$$

it readily follows with (A16) that

$$\tilde{\sigma}^2(t) = \left| \sum_{\alpha \in \mathcal{G}} v_\alpha e^{-iG_\alpha t} \right|^2 = \sum_{\alpha, \beta \in \mathcal{G}} v_\alpha^* v_\beta e^{i(G_\alpha - G_\beta)t} \quad (\text{A39})$$

and hence that

$$\tilde{\sigma}^2(t) = R(t) + S, \quad (\text{A40})$$

$$R(t) := \sum_{\substack{\alpha, \beta \in \mathcal{G} \\ G_\alpha \neq G_\beta}} v_\alpha^* v_\beta e^{i(G_\alpha - G_\beta)t}, \quad (\text{A41})$$

$$S := \sum_{\substack{\alpha, \beta \in \mathcal{G} \\ G_\alpha = G_\beta}} v_\alpha^* v_\beta. \quad (\text{A42})$$

Note that both  $R(t)$  and  $S$  are real numbers and that their sum must be non-negative.

Abbreviating the time average of an arbitrary function  $f(t)$  as

$$\langle f(t) \rangle_T := \int_0^T \frac{dt}{T} f(t), \quad (\text{A43})$$

one readily finds by integrating over the exponential in (A41) that

$$\langle R(t) \rangle_T \leq \frac{1}{T} \sum_{\substack{\alpha, \beta \in \mathcal{G} \\ G_\alpha \neq G_\beta}} |v_\alpha^* v_\beta| \frac{2}{|G_\alpha - G_\beta|}. \quad (\text{A44})$$

Since the number of summands is finite [cf. (A37)], we can conclude from (A40)–(A44) that for any given  $\epsilon > 0$  there

exists a finite  $T_\epsilon$  with

$$\langle \tilde{\sigma}^2(t) \rangle_T \leq \epsilon + S \quad (\text{A45})$$

for all  $T \geq T_\epsilon$ .

Next, we consider subsets  $\mathcal{G}_j$  of  $\mathcal{G}$  from (A37), defined via the property that all elements  $\alpha = (m, n)$  which belong to the same subset  $\mathcal{G}_j$  exhibit identical energy gaps  $G_\alpha := E_m - E_n$  [cf. (A38)], while for any pair  $\alpha \in \mathcal{G}_j, \beta \in \mathcal{G}_k$  with  $j \neq k$  the corresponding energy gaps  $G_\alpha$  and  $G_\beta$  are different. It follows that the number of subsets  $\mathcal{G}_j$  is finite, say  $j = 1, \dots, J$ , that  $\mathcal{G}$  is the disjoint union of all those subsets  $\mathcal{G}_j$ , and that each subset  $\mathcal{G}_j$  contains a finite number of elements, which we denote by  $g_j$ . Recalling that  $g$  from (12) denotes the maximal number of degenerate energy gaps, it follows that

$$g_j \leq g \quad (\text{A46})$$

for all  $j$ . Furthermore, we can rewrite  $S$  from (A42) as

$$S = \sum_{j=1}^J \sum_{\alpha, \beta \in \mathcal{G}_j} v_\alpha^* v_\beta. \quad (\text{A47})$$

Next, we define the scalar product  $\langle B|C \rangle := \sum_{k,l=1}^M B_{kl}^* C_{kl}$  for arbitrary  $M \times M$  matrices  $B$  and  $C$ . For the special choice  $B_{kl} := x_k$  (independent of  $l$ ) and  $C_{kl} := x_l$  (independent of  $k$ ), the Cauchy-Schwarz inequality implies

$$\left| \sum_{k,l} x_k^* x_l \right|^2 \leq \sum_{k,l} |x_k|^2 \sum_{k,l} |x_l|^2 = \left( M \sum_k |x_k|^2 \right)^2 \quad (\text{A48})$$

for arbitrary complex numbers  $x_1, \dots, x_M$ . Observing that the last sum in (A47) is exactly of this structure with  $M = g_j$ , it follows with (A46) that

$$S \leq \sum_{j=1}^J g_j \sum_{\alpha \in \mathcal{G}_j} |v_\alpha|^2 \leq g \sum_{j=1}^J \sum_{\alpha \in \mathcal{G}_j} |v_\alpha|^2 = g \sum_{\alpha \in \mathcal{G}} |v_\alpha|^2.$$

Returning to our original notation via (A37) and (A38), we finally obtain

$$S \leq g \sum_{m \neq n} |\tilde{A}_{mn}|^2. \quad (\text{A49})$$

This relation together with (A45) is the main result of this section.

### 4. Step 3

In this section, we closely follow the line of reasoning from Ref. [4]. The main result will be (A57). Denoting by  $\Sigma_1$  the partial sum on the right hand side of (A49) over all summands with  $n = 1$  implies with (A21) that

$$\Sigma_1 := \sum_{m=2}^N |\tilde{A}_{m1}|^2 \leq \max_{n \geq 2} p_n W_1, \quad (\text{A50})$$

$$W_1 := \sum_{m=2}^N \text{Tr}\{\rho_1 A P_m A\}. \quad (\text{A51})$$



Since  $\rho_n A P_m A$  is a non-negative operator for arbitrary  $m, n$  [see also (A5)], it follows that

$$\begin{aligned} W_1 &\leq \sum_{m,n} \text{Tr}\{\rho_n A P_m A\} \\ &= \text{Tr}\left\{\left(\sum_n \rho_n\right) A \left(\sum_m P_m\right) A\right\}, \end{aligned} \quad (\text{A52})$$

where, similarly as in (1) and (2), the sums run over the full range of admitted  $m$  and  $n$  values. With (7), (A4), and (A50), we thus obtain

$$\Sigma_1 \leq \max_{n \geq 2} p_n \text{Tr}\{\bar{\rho} A^2\}. \quad (\text{A53})$$

From the definition (A11) it readily follows that  $\tilde{A}_{nm} = \tilde{A}_{mn}^*$ . Hence,  $\Sigma_1$  can also be considered as the partial sum on the right hand side of (A49) over all summands with  $m = 1$ . As a consequence, we can rewrite (A49) as

$$S \leq g \Sigma_1 + g \Sigma', \quad (\text{A54})$$

$$\Sigma' := \sum_{m=2}^N \sum_{\substack{n=1 \\ n \neq m}}^N |\tilde{A}_{mn}|^2. \quad (\text{A55})$$

Analogously as in (A50)–(A53), one can conclude that

$$\Sigma' \leq \max_{n \geq 2} p_n \text{Tr}\{\bar{\rho} A^2\}. \quad (\text{A56})$$

For the sake of convenience only, we have so far assumed that the largest energy level population is given by  $p_1$  [see (A12)]. In order to get rid of this convenient but unnecessary special role of  $n = 1$ , we introduce (A13) into (A53) and (A56), yielding with (A54)

$$S \leq 2g \max'_n p_n \text{Tr}\{\bar{\rho} A^2\} \quad (\text{A57})$$

as the main result of this section.

### 5. Final result

We first address the case  $\text{Tr}\{\bar{\rho} A^2\} = 0$ . Since  $A^2$  as well as all the summands on the right hand side on (9) are Hermitian, non-negative operators, it follows that

$$\text{Tr}\{P_n \rho(0) P_n A^2\} = 0 \quad (\text{A58})$$

for all  $n$ . Similarly as in (A18), we can conclude from (3) that

$$\begin{aligned} |A_{mn}|^2 &= \text{Tr}\{(P_m \rho^{1/2})(\rho^{1/2} P_n A)\} \\ &\leq \text{Tr}\{P_m \rho(0) P_m\} \text{Tr}\{P_n \rho(0) P_n A^2\}. \end{aligned} \quad (\text{A59})$$

With (A58) it follows that  $A_{mn} = 0$  for all  $m, n$  and with (2) that  $\text{Tr}\{\rho(t) A\} = 0$  for all  $t$ . Likewise, one finds with (9) that  $\text{Tr}\{\bar{\rho} A\} = \sum_n A_{nn} = 0$ . As a consequence, (A1) is trivially fulfilled.

Next, we turn to the case  $\text{Tr}\{\bar{\rho} A^2\} > 0$  (since  $\bar{\rho}$  and  $A^2$  are non-negative, the case  $\text{Tr}\{\bar{\rho} A^2\} < 0$  is excluded). It follows that

$$\beta := g \max'_n p_n \text{Tr}\{\bar{\rho} A^2\} > 0. \quad (\text{A60})$$

We thus can choose  $d$  in (A36) so that  $\delta^2(t) \leq \beta/20$  for all  $t$  and hence that

$$\langle \delta^2(t) \rangle_T \leq \beta/20 \quad (\text{A61})$$

for all  $T > 0$ . Likewise, we can choose  $\epsilon = \beta/20$  in (A45), implying with (A57) that

$$\langle \bar{\sigma}^2(t) \rangle_T \leq 2.05 \beta \quad (\text{A62})$$

for all sufficiently large  $T$ . In view of (A34), we can conclude that

$$\langle \sigma^2(t) \rangle_T = \langle \bar{\sigma}^2(t) \rangle_T + 2V + \langle \delta^2(t) \rangle_T, \quad (\text{A63})$$

$$V := \langle \bar{\sigma}(t) \delta(t) \rangle_T. \quad (\text{A64})$$

Observing that  $\langle f_1(t) f_2(t) \rangle_T$  represents a well-defined scalar product for arbitrary real valued functions  $f_{1,2}(t)$ , the Cauchy-Schwarz inequality implies

$$|V|^2 \leq \langle \bar{\sigma}^2(t) \rangle_T \langle \delta^2(t) \rangle_T. \quad (\text{A65})$$

With (A61) and (A62) it follows that  $|V| \leq 0.4\beta$ , and with (A63) that

$$\langle \sigma^2(t) \rangle_T \leq 3\beta \quad (\text{A66})$$

for all sufficiently large  $T$ . Due to (A43) and (A60), we thus recover (A1).

## APPENDIX B

In this Appendix, we derive the general bound from Eq. (29) by generalizing the approach of Short in Ref. [2]. We imagine many repetitions of the measurement series considered in Sec. IV. As above Eq. (28), in every repetition, either  $\rho(t)$  or  $\bar{\rho}$  is randomly selected with probability  $\frac{1}{2}$  and then used to randomly generate a measurement outcome  $\vec{s}$  according to the corresponding probability (20) or (21). But, in contrast to Sec. IV, the task is now to guess in every single repetition from the given data  $\vec{s}$  whether  $\rho(t)$  or  $\bar{\rho}$  had been used to generate  $\vec{s}$ .

This decision problem is a generalization of the one considered by Short [2] (see also Sec. III B). It is in many respects also *similar* to those considered in Sec. IV. However, it is crucial to note that it is *not identical* and that quantitative statements in one case do not immediately imply any rigorous conclusions in the other case (see also Sec. III B). Yet, such rigorous conclusions are not impossible, as we will now show.

A key observation is that the above specified problem assigns well defined, objective probabilities (frequencies of occurrence) to each of the two “models”  $\rho(t)$  and  $\bar{\rho}$  (namely,  $\frac{1}{2}$  to each of them). As a consequence, the conventional probabilistic (frequentist) approach happens to coincide with the concepts of Bayesian inference in this specific case.

In other words, in every single repetition we are given the data  $\vec{s}$  and we have at our disposition the full knowledge about  $\rho(t)$  and  $\bar{\rho}$ , but about nothing else. Now, we are forced to produce a decision based on this information. The salient point consists in the observation that for any given  $\vec{s}$ , the only information of use is the pair of probabilities  $p_i(\vec{s})$  and  $\bar{p}_i(\vec{s})$ , following from  $\rho(t)$  and  $\bar{\rho}$  according to (18)–(21). Any other information contained in  $\rho(t)$ ,  $\bar{\rho}$ , and  $\vec{s}$  is of no use for our decision problem. Obviously (or by invoking

Bayesian inference), the best one can do is to opt for  $\rho(t)$  if  $p_t(\vec{s}) > \bar{p}(\vec{s})$  and vice versa [any other way of using the two numbers  $p_t(\vec{s})$  and  $\bar{p}(\vec{s})$  would not lead to a better decision]. In case  $p_t(\vec{s}) = \bar{p}(\vec{s})$  we introduce as a third option the answer “undecided” (alternatively, one could randomly choose one of the two options with probability  $\frac{1}{2}$ ). Counting a correct decision as 1 and a wrong decision as  $-1$ , the success probability (symbol  $P^{\text{succ}}$ ), i.e., the probability of opting by means of the above optimal decision strategy for the correct state minus opting for the wrong state, follows as

$$P_{\text{opt}}^{\text{succ}} = \sum_{\vec{s}} \frac{p_t(\vec{s})}{2} \frac{1 + q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s})}{2} + \sum_{\vec{s}} \frac{\bar{p}(\vec{s})}{2} \frac{1 - q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s})}{2}, \quad (\text{B1})$$

$$\begin{aligned} q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s}) &:= 1 \text{ if } p_t(\vec{s}) > \bar{p}(\vec{s}), \\ q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s}) &:= -1 \text{ if } p_t(\vec{s}) < \bar{p}(\vec{s}), \\ q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s}) &:= 0 \text{ if } p_t(\vec{s}) = \bar{p}(\vec{s}). \end{aligned} \quad (\text{B2})$$

The detailed justification is as follows: The first factor  $p_t(\vec{s})/2$  on the right hand side of (B1) represents the joint probability that the random event  $(\rho(t), \vec{s})$  is realized. The second factor  $[1 + q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s})]/2$  is unity if our guess was right, zero if it was wrong, and  $\frac{1}{2}$  if we were undecided (or randomly picked one of the two options). Similar considerations apply to the second sum in (B1).

Since  $\sum_{\vec{s}} p_t(\vec{s}) = \sum_{\vec{s}} \bar{p}(\vec{s}) = 1$ , it readily follows from (B1) that

$$P_{\text{opt}}^{\text{succ}} = \frac{1}{2} + \sum_{\vec{s}} \frac{p_t(\vec{s}) - \bar{p}(\vec{s})}{4} q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s}). \quad (\text{B3})$$

Without loss of generality, we can restrict the sum to summands with  $p_t(\vec{s}) \neq \bar{p}(\vec{s})$  and rewrite  $q_{\text{opt}}(\rho(t), \vec{\rho}, \vec{s})$  from (B2) for those summands as  $|p_t(\vec{s}) - \bar{p}(\vec{s})|/\{p_t(\vec{s}) - \bar{p}(\vec{s})\}$ , yielding

$$P_{\text{opt}}^{\text{succ}} = \frac{1}{2} + \sum_{\vec{s}} \frac{|p_t(\vec{s}) - \bar{p}(\vec{s})|}{4}. \quad (\text{B4})$$

Next, we consider the very same decision problem, but now by employing any of the  $q$  functions from Sec. IV as follows: If  $q(\rho(t), \vec{\rho}, \vec{s}) \geq 0$  then we opt with probability  $p_+ := q(\rho(t), \vec{\rho}, \vec{s})$  for  $\rho(t)$  and with probability  $1 - p_+$  our answer is “undecided” [randomly pick  $\rho(t)$  or  $\vec{\rho}$ ]. Likewise, if  $q(\rho(t), \vec{\rho}, \vec{s}) < 0$ , then we opt with probability  $p_- := -q(\rho(t), \vec{\rho}, \vec{s})$  for  $\vec{\rho}$  and with probability  $1 - p_-$  we are undecided. Similarly as in (B1), the success probability of this decision strategy now takes the form

$$P^{\text{succ}} = \sum_{\vec{s}} \frac{p_t(\vec{s})}{2} \frac{1 + q(\rho(t), \vec{\rho}, \vec{s})}{2} + \sum_{\vec{s}} \frac{\bar{p}(\vec{s})}{2} \frac{1 - q(\rho(t), \vec{\rho}, \vec{s})}{2} \quad (\text{B5})$$

and, like in (B2), it follows that

$$P^{\text{succ}} = \frac{1}{2} + \sum_{\vec{s}} \frac{p_t(\vec{s}) - \bar{p}(\vec{s})}{4} q(\rho(t), \vec{\rho}, \vec{s}). \quad (\text{B6})$$

On the other hand, subtracting (28) from (27) yields

$$Q(t) = \sum_{\vec{s}} \frac{p_t(\vec{s}) - \bar{p}(\vec{s})}{2} q(\rho(t), \vec{\rho}, \vec{s}). \quad (\text{B7})$$

Upon comparison with (B6) it follows that  $P^{\text{succ}} = [1 + Q(t)]/2$ . Since this success probability cannot exceed the optimal value  $P_{\text{opt}}^{\text{succ}}$  from (B4), we obtain  $[1 + Q(t)]/2 \leq P_{\text{opt}}^{\text{succ}}$ . Likewise, by employing the decision strategy  $-q(\rho(t), \vec{\rho}, \vec{s})$  instead of  $q(\rho(t), \vec{\rho}, \vec{s})$ , one recovers  $[1 - Q(t)]/2 \leq P_{\text{opt}}^{\text{succ}}$ . Combining both inequalities implies  $[1 + |Q(t)|]/2 \leq P_{\text{opt}}^{\text{succ}}$ . Together with (B4) this yields our final result (29).

Note that in order to derive this result, we employed a different decision problem than the one considered in Sec. IV. Yet, the so obtained inequality (29) itself is valid independently of this specific decision problem.

### APPENDIX C

In this appendix, we provide the derivation of (30)–(32). Focusing on any of the projectors  $K_v^{(j)}$  appearing in (18) and (19), one readily finds upon replacing  $A$  by  $K_v^{(j)}$  in (11)–(14) that for any given  $\epsilon_v^{(j)} > 0$ ,

$$T_v^{(j)}/T \leq \alpha \text{Tr}\{\bar{\rho} [K_v^{(j)}]^2\} [\epsilon_v^{(j)}]^{-2} = \alpha \bar{k}_v^{(j)} [\epsilon_v^{(j)}]^{-2} \quad (\text{C1})$$

for all sufficiently large  $T$ , where

$$\alpha := 3 g \max'_n p_n, \quad (\text{C2})$$

$$T_v^{(j)} := |\{0 \leq t \leq T : |\sigma_v^{(j)}(t)| > \epsilon_v^{(j)}\}|, \quad (\text{C3})$$

$$\sigma_v^{(j)}(t) := \langle K_v^{(j)} \rangle_{\rho(t)} - \langle K_v^{(j)} \rangle_{\bar{\rho}} = k_v^{(j)}(t) - \bar{k}_v^{(j)}, \quad (\text{C4})$$

and where we exploited (18), (19), and  $[K_v^{(j)}]^2 = K_v^{(j)}$  in the last equalities in (C1) and (C4).

For any given pair  $(j, v)$  (where  $j \in \{1, \dots, N_{\text{rep}}\}$  and  $v \in \{1, \dots, N_{A_j}\}$ ) and any given  $\epsilon_v^{(j)} > 0$ , the quantity  $T_v^{(j)}$  in (C3) is the Lebesgue measure of all times  $t \in [0, T]$  for which  $|\sigma_v^{(j)}(t)| > \epsilon_v^{(j)}$  holds true. Since the number of pairs  $(j, v)$  is finite, it follows that for any given set of positive  $\epsilon_v^{(j)}$  values, the inequality (C1) applies simultaneously for all pairs  $(j, v)$  provided  $T$  is sufficiently large. Hence, the measure of all times  $t \in [0, T]$  for which  $|\sigma_v^{(j)}(t)| > \epsilon_v^{(j)}$  is true for at least one among all pairs  $(j, v)$  can be estimated from above by

$$T_{\text{tot}} := \sum_{j=1}^{N_{\text{rep}}} \sum_{v=1}^{N_{A_j}} T_v^{(j)} \quad (\text{C5})$$

for all sufficiently large  $T$ . For all other times  $t \in [0, T]$ , it is true that  $|\sigma_v^{(j)}(t)| \leq \epsilon_v^{(j)}$  simultaneously for all pairs  $(j, v)$ . From now on, we exclusively focus on the latter subset of  $[0, T]$ , i.e., on times  $t$  for which

$$|\sigma_v^{(j)}(t)| \leq \epsilon_v^{(j)} \text{ for all } j \in \{1, \dots, N_{\text{rep}}\}, v \in \{1, \dots, N_{A_j}\}. \quad (\text{C6})$$

Thus, the Lebesgue measure of all times  $t \in [0, T]$  for which the subsequently derived implications of (C6) may possibly not apply is bounded by  $T_{\text{tot}}$  from (C5).

A particularly convenient choice of the quantities  $\epsilon_v^{(j)}$  turns out to be

$$\epsilon_v^{(j)} := \bar{k}_v^{(j)} F / N_{\text{rep}} \quad \text{if } \bar{k}_v^{(j)} > k_{th}, \quad (\text{C7})$$

$$\epsilon_v^{(j)} := (k_{th} \bar{k}_v^{(j)})^{1/2} F / N_{\text{rep}} \quad \text{if } k_{th} \geq \bar{k}_v^{(j)} > 0, \quad (\text{C8})$$

$$\epsilon_v^{(j)} := k_{th} F / N_{\text{rep}} \quad \text{if } \bar{k}_v^{(j)} = 0, \quad (\text{C9})$$

where the ‘‘factor’’  $F$  and the ‘‘threshold’’  $k_{th}$  are positive real numbers, whose explicit values will be fixed later. For the moment, we only require that

$$0 < F \leq 1/2. \quad (\text{C10})$$

Introducing (C7)–(C9) into (C1) and (C5) implies for all sufficiently large  $T$  that

$$\frac{T_{\text{tot}}}{T} \leq \sum_{j=1}^{N_{\text{rep}}} \sum_{v=1}^{N_{A_j}} \alpha \frac{N_{\text{rep}}^2}{F^2 k_{th}}. \quad (\text{C11})$$

Exploiting (22), the number of summands in the double sum can be readily bounded from above by  $N_{\text{rep}} N_{\text{obs}}$ , yielding

$$\frac{T_{\text{tot}}}{T} \leq \alpha \frac{N_{\text{obs}} N_{\text{rep}}^3}{F^2 k_{th}} =: \epsilon \quad (\text{C12})$$

for all sufficiently large  $T$ .

Recalling the notation  $\vec{s} := (s_1, \dots, s_{N_{\text{rep}}})$  from below Eq. (19), we divide the set of all possible measurement outcomes

$$S := \{\vec{s} : s_j \in \{1, \dots, N_{A_j}\}, j \in \{1, \dots, N_{\text{rep}}\}\} \quad (\text{C13})$$

into the two subsets

$$S' := \{\vec{s} \in S : \bar{k}_{s_j}^{(j)} > k_{th} \text{ for all } j\}, \quad (\text{C14})$$

$$S'' := S \setminus S'. \quad (\text{C15})$$

Likewise, the sum over all  $\vec{s} \in S$  appearing in (29) is split into two parts according to

$$Q_{\text{max}}(t) = (\Sigma' + \Sigma'')/2, \quad (\text{C16})$$

$$\Sigma' := \sum_{\vec{s} \in S'} |p_t(\vec{s}) - \bar{p}(\vec{s})|, \quad (\text{C17})$$

$$\Sigma'' := \sum_{\vec{s} \in S''} |p_t(\vec{s}) - \bar{p}(\vec{s})|. \quad (\text{C18})$$

To evaluate  $\Sigma'$ , we note that  $\vec{s} \in S'$  implies  $\bar{k}_{s_j}^{(j)} > k_{th}$  for all  $j$  according to (C14) and hence

$$|\sigma_{s_j}^{(j)}(t)| \leq \bar{k}_{s_j}^{(j)} F / N_{\text{rep}} \quad (\text{C19})$$

according to (C6) and (C7). With (C10) and  $N_{\text{rep}} \geq 1$  it follows that  $|\sigma_{s_j}^{(j)}(t)| \leq \bar{k}_{s_j}^{(j)}/2$  and with (C4) that

$$k_{s_j}^{(j)}(t) \geq \bar{k}_{s_j}^{(j)} - |\sigma_{s_j}^{(j)}(t)| \geq \bar{k}_{s_j}^{(j)}/2 \quad (\text{C20})$$

for all  $j$ . Thus, all quantities in Eqs. (20) and (21) are positive real numbers, i.e., we can logarithmize those equations to

obtain

$$x := \ln \left[ \frac{p_t(\vec{s})}{\bar{p}(\vec{s})} \right] = \sum_{j=1}^{N_{\text{rep}}} \ln \left[ \frac{k_{s_j}^{(j)}(t)}{\bar{k}_{s_j}^{(j)}} \right], \quad (\text{C21})$$

$$|p_t(\vec{s}) - \bar{p}(\vec{s})| = |\bar{p}(\vec{s}) (e^x - 1)| = \bar{p}(\vec{s}) |e^x - 1|. \quad (\text{C22})$$

We first focus on the case  $x \geq 0$ . Observing that  $\ln(1+y) \leq y$  for all  $y > -1$ , it follows that  $\ln(a/b) = \ln(1 + [a-b]/b) \leq [a-b]/b$  for all  $a, b > 0$ , and hence with (C21), (C4), and (C19) that

$$0 \leq x \leq \sum_{j=1}^{N_{\text{rep}}} \frac{|\sigma_{s_j}^{(j)}(t)|}{\bar{k}_{s_j}^{(j)}} \leq \sum_{j=1}^{N_{\text{rep}}} \frac{F}{N_{\text{rep}}} = F. \quad (\text{C23})$$

In conclusion,

$$|e^x - 1| \leq e^F - 1 \quad (\text{C24})$$

whenever  $x \geq 0$  in (C22). Turning to  $x < 0$ , we observe that

$$|e^x - 1| = e^x (e^{-x} - 1) < e^{-x} - 1, \quad (\text{C25})$$

$$0 < -x = \sum_{j=1}^{N_{\text{rep}}} \ln \left[ \frac{\bar{k}_{s_j}^{(j)}}{k_{s_j}^{(j)}(t)} \right], \quad (\text{C26})$$

where we exploited (C21) in the last step. Similarly, as in (C23) it follows that

$$-x \leq \sum_{j=1}^{N_{\text{rep}}} \frac{|\sigma_{s_j}^{(j)}(t)|}{k_{s_j}^{(j)}(t)} \leq \sum_{j=1}^{N_{\text{rep}}} \frac{\bar{k}_{s_j}^{(j)}}{k_{s_j}^{(j)}(t)} \frac{F}{N_{\text{rep}}}. \quad (\text{C27})$$

Since  $\bar{k}_{s_j}^{(j)}/k_{s_j}^{(j)}(t) \leq 2$  according to (C20) we can conclude that  $-x \leq 2F$  and with (C25) that  $|e^x - 1| < e^{2F} - 1$  whenever  $x < 0$  in (C22). With (C24), we thus obtain

$$|e^x - 1| < e^{2F} - 1 \quad (\text{C28})$$

for arbitrary  $x$  in (C22). Due to the elementary inequality  $e^z - 1 \leq (e - 1)z \leq 2z$  for all  $z \in [0, 1]$ , it follows with (C10) that  $e^{2F} - 1 \leq 4F$  and hence with (C22) and (C28) that

$$|p_t(\vec{s}) - \bar{p}(\vec{s})| \leq 4F \bar{p}(\vec{s}). \quad (\text{C29})$$

Accordingly,  $\Sigma'$  from (C17) can be estimated as

$$\Sigma' \leq 4F \sum_{\vec{s} \in S'} \bar{p}(\vec{s}) \leq 4F \sum_{\vec{s} \in S} \bar{p}(\vec{s}) = 4F. \quad (\text{C30})$$

Next, we upper bound  $\Sigma''$  in (C18) as

$$\Sigma'' \leq \Sigma_1 + \Sigma_2, \quad (\text{C31})$$

$$\Sigma_1 := \sum_{\vec{s} \in S''} p_t(\vec{s}), \quad (\text{C32})$$

$$\Sigma_2 := \sum_{\vec{s} \in S''} \bar{p}(\vec{s}). \quad (\text{C33})$$

Furthermore, we introduce the following subsets of  $S$  from (C12):

$$S_j := \{\vec{s} \in S : \bar{k}_{s_j}^{(j)} \leq k_{th}\}, \quad (\text{C34})$$

where  $j = 1, \dots, N_{\text{rep}}$ . According to (C14) and (C15) there exists for every  $\vec{s} \in S''$  at least one  $j \in \{1, \dots, N_{\text{rep}}\}$  with the

property that  $\bar{k}_{s_j}^{(j)} \leq k_{th}$ . It follows that the union of all the subsets  $S_j$  from (C34) reproduce  $S''$  and hence that

$$\Sigma_2 \leq \sum_{j=1}^{N_{\text{rep}}} \Sigma_2^{(j)}, \quad (\text{C35})$$

$$\Sigma_2^{(j)} := \sum_{\vec{s} \in S_j} \bar{p}(\vec{s}) = \sum_{\vec{s} \in S_j} \prod_{l=1}^{N_{\text{rep}}} \bar{k}_{s_l}^{(l)}, \quad (\text{C36})$$

where we exploited (21) in the last step. With (C34) it follows that

$$\Sigma_2^{(j)} \leq \sum_{\vec{s} \in S_j} k_{th} \prod_{l \neq j} \bar{k}_{s_l}^{(l)} \leq \sum_{\vec{s} \in S} k_{th} \prod_{l \neq j} \bar{k}_{s_l}^{(l)}, \quad (\text{C37})$$

where the symbol  $l \neq j$  indicates that the  $j$ th factor is omitted and where we exploited that  $S_j \subset S$  in the last step [cf. (C34)]. In view of (C13), we can conclude that

$$\Sigma_2^{(j)} \leq \sum_{s_j=1}^{N_{A_j}} k_{th} \left( \prod_{l \neq j} \sum_{s_l=1}^{N_{A_l}} \bar{k}_{s_l}^{(l)} \right) = k_{th} N_{A_j}, \quad (\text{C38})$$

where we exploited that  $\sum_{s_l=1}^{N_{A_l}} \bar{k}_{s_l}^{(l)} = 1$  for all  $l$ . Taking into account (22) and (C35), we finally obtain

$$\Sigma_2 \leq k_{th} N_{\text{obs}} N_{\text{rep}}. \quad (\text{C39})$$

Similarly as in (C35)–(C37), it follows with (C32) and (20) that

$$\Sigma_1 \leq \sum_{j=1}^{N_{\text{rep}}} \Sigma_1^{(j)}, \quad (\text{C40})$$

$$\begin{aligned} \Sigma_1^{(j)} &:= \sum_{\vec{s} \in S_j} p_t(\vec{s}) = \sum_{\vec{s} \in S_j} \prod_{l=1}^{N_{\text{rep}}} k_{s_l}^{(l)}(t) \\ &\leq \sum_{\vec{s} \in S_j} k_{s_j}^{(j)}(t) \prod_{l \neq j} k_{s_l}^{(l)}(t). \end{aligned} \quad (\text{C41})$$

For all  $s_j$  appearing in the last sum over  $\vec{s} \in S_j$ , Eq. (C34) implies that  $\bar{k}_{s_j}^{(j)} \leq k_{th}$  and hence that  $\epsilon_{s_j}^{(j)} \leq k_{th}$  according to (C8)–(C10). With (C4) and (C6), we thus can infer that

$$k_{s_j}^{(j)}(t) \leq \bar{k}_{s_j}^{(j)} + |\sigma_{s_j}^{(j)}(t)| \leq \bar{k}_{s_j}^{(j)} + \epsilon_{s_j}^{(j)} \leq 2k_{th}. \quad (\text{C42})$$

By combining this result with (C41), one finds exactly as in (C37) and (C38) that

$$\Sigma_1^{(j)} \leq 2 \sum_{\vec{s} \in S_j} k_{th} \prod_{l \neq j}^{N_{\text{rep}}} k_{s_l}^{(l)}(t) \leq 2k_{th} N_{A_j}. \quad (\text{C43})$$

Like in (C39) it follows that  $\Sigma_1 \leq 2k_{th} N_{\text{obs}} N_{\text{rep}}$ , and with (C31) that

$$\Sigma'' \leq 3k_{th} N_{\text{obs}} N_{\text{rep}}. \quad (\text{C44})$$

Introducing (C30) and (C44) into (C16) implies

$$Q_{\text{max}}(t) \leq [4F + 3k_{th} N_{\text{obs}} N_{\text{rep}}]/2, \quad (\text{C45})$$

where  $k_{th} > 0$  and  $F \in (0, 1/2]$  can still be chosen arbitrarily [see below (C9)]. We thus may choose  $k_{th}$  so that the right hand side of (C45) equals  $\epsilon$  from (C12), i.e.,

$$k_{th} = [2\epsilon - 4F]/3N_{\text{obs}} N_{\text{rep}}. \quad (\text{C46})$$

Altogether, Eqs. (C12), (C45), and (C46) imply for all sufficiently large  $T$  that

$$T_{\text{tot}}/T \leq \epsilon, \quad (\text{C47})$$

$$Q_{\text{max}}(t) \leq \epsilon, \quad (\text{C48})$$

$$\epsilon = \frac{3\alpha N_{\text{obs}}^2 N_{\text{rep}}^4}{2F^2[\epsilon - 2F]}. \quad (\text{C49})$$

Finally, we make the choice  $F = \epsilon/3$ , which is obtained by minimizing (C49) with respect to  $F$ . Upon inserting  $\alpha$  from (C2) and  $F = \epsilon/3$  into (C49) and then solving for  $\epsilon$ , one recovers (32).

As announced below (C6), the result (C48) is valid for all  $t \in [0, T]$  apart from a subset of  $[0, T]$ , whose Lebesgue measure is bounded by  $T_{\text{tot}}$ , and provided  $T$  is sufficiently large. It follows that  $T^*$  from (31) cannot exceed  $T_{\text{tot}}$ , i.e.,  $T^* \leq T_{\text{tot}}$ . Upon comparison with (C47), we thus recover (30).

Strictly speaking, the above conclusions are only valid if our choice  $F = \epsilon/3$  [see below (C49)] is self-consistent with the constraint from (C10). Equivalently, this means that  $\epsilon$  must be smaller than  $\frac{3}{2}$ . In the opposite case, i.e., if  $\epsilon$  in (32) should happen to exceed  $\frac{3}{2}$ , then our above arguments no longer apply, but obviously (30) is still trivially fulfilled.

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