Dynamical typicality for initial states with a preset measurement statistics of several commuting observables

Ben N. Balz, Jonas Richter, Jochen Gemmer, Robin Steinigeweg, and Peter Reimann

1Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany
2Department of Physics, University of Osnabrück, 49069 Osnabrück, Germany

We consider all pure or mixed states of a quantum many-body system which exhibit the same, arbitrary but fixed measurement outcome statistics for several commuting observables. Taking those states as initial conditions, which are then propagated by the pertinent Schrödinger or von Neumann equation up to some later time point, and invoking a few additional, fairly weak and realistic assumptions, we show that most of them still entail very similar expectation values for any given observable. This so-called dynamical typicality property thus corroborates the widespread observation that a few macroscopic features are sufficient to ensure the reproducibility of experimental measurements despite many unknown and uncontrollable microscopic details of the system. We also discuss and exemplify the usefulness of our general analytical result as a powerful numerical tool.
INTRODUCTION AND OVERVIEW

Why are macroscopic experiments reproducible, although the molecular details in each repetition of the experiment are largely unknown and not reproducible? A first path breaking step towards answering this question was established by Bartsch and Gemmer [1], putting forward the following so-called dynamical typicality property: The overwhelming majority of all pure states, which exhibit very similar expectation values of a generic observable at some initial time, will yield very similar expectation values for this observable also at any later time point, provided the relevant Hilbert space is of large (but finite) dimension. In proving this statement, a technical assumption is needed, which can strictly speaking only be taken for granted if the given initial expectation value differs sufficiently little from the expectation value in the corresponding microcanonical equilibrium state [1].

Here, we work out a significant extension of the original dynamical typicality scenario from Ref. [1]. Namely, we consider the set of all initial states, which now may be either pure or mixed, and for which all possible measurement outcomes for several commuting observables exhibit certain preset expectation values (projection probabilities). Similarly as in [1], we then show that upon evolving those initial states according to the pertinent Schrödinger or von Neumann equation up to some later time point, the vast majority of them still gives rise to very similar expectation values for any given observable. But unlike in [1], the latter observable may now be different from those which determine the initial conditions, and the dynamics may be governed by an arbitrary, possibly even explicitly time dependent Hamiltonian.

With respect to our analytical explorations, certain partial aspects are also related to numerous previous works, for instance Refs. [2–7]. Yet the main physical conclusions as well as the technical methods are quite different. Concerning the numerical applications, the basic concepts together with the relevant previous literature will be reviewed in the last Section.

Our present topic of dynamical typicality also exhibits certain similarities with non-dynamical typicality phenomena, originally due to Lloyd [8], and independently rediscovered under the labels “canonical typicality” and “concentration of measure effects” in Refs. [9, 10], see also [4, 11–15]. In those non-dynamical typicality explorations, the focus is on all quantum states of a high dimensional Hilbert space, without any further restriction regarding the expectation value of some observable, and without considering the temporal evolution of those states. The key result in this context is that the expectation value of any given observable is for the overwhelming majority of those states extremely close to the pertinent microcanonical (thermal equilibrium) expectation value of the high dimensional Hilbert space under consideration. A first main virtue of the present dynamical typicality approach is to pick out a small subsets of states with distinct non-thermal features, and then to prove typicality properties of their further evolution in time.

Another main virtue of such an approach is to admit statements about the time evolution without actually solving the dynamics. As exemplified by Chaps. 18 and 19, the latter is a very challenging task in itself and is outside the conceptual framework of our present Chapter. On the other hand, our approach goes beyond the scope of Chaps. 18, 19, and 20 in that our systems are in general not even required to exhibit equilibration or thermalization in the long time limit. Moreover, our dynamical typicality based numerical scheme can deal with considerably larger systems than many other methods, such as exact diagonalization.

GENERAL FRAMEWORK

We consider quantum mechanical model systems, which can be described by a Hilbert space $\mathcal{H}$ of large but finite dimension $D$. The initial state of the system will be specified in terms of a set of commuting observables $\{A_n\}$ whose common eigenspaces are denoted as $\mathcal{H}_n$ with $n = 1, \ldots, N$. Hence the projectors $P_n$ onto those subspaces $\mathcal{H}_n$ satisfy $P_n P_m = \delta_{mn} P_n$ and $\sum_{n=1}^{N} P_n = \mathbb{1}_\mathcal{H}$ (identity on $\mathcal{H}$), and the dimensions of the $\mathcal{H}_n$ are given by

$$d_n = \text{Tr}\{P_n\}, \quad (1)$$

with $D = \sum_{n=1}^{N} d_n$.

Denoting by $\rho(0)$ any density operator (pure or mixed system state) at the initial time $t = 0$, and considering the $P_n$’s as observables, the corresponding expectation values (projection probabilities) are

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1 The set of commuting observables is not required to be complete, and even a single observable is admissible.
given by

\[ p_n = \text{Tr}\{\rho(0) P_n\} \]  \hspace{1cm} (2)

with \( p_n \geq 0 \) and \( \sum_{n=1}^{N} p_n = 1 \). At the focus of our present investigation will be the set of all initial states \( \rho(0) \) which satisfy the \( N \) constraints \( \{p_n\}_{n=1}^{N} \).

Physically speaking, we have mainly quantum many-body systems in mind where, following von Neumann \[16\], it seems reasonable to expect that a simultaneous measurement of two or more (almost) commuting observables is indeed feasible. In many cases, some or all of those observables will correspond to microscopic (coarse grained) quantities and one of them will usually be the energy (coarse grained Hamiltonian). Although such an (approximate) commutation of those coarse grained observables is usually rather difficult to justify more rigorously, it is commonly considered as a plausible working hypothesis \[13, 17–22\]. For example, we may be dealing with multiple macroscopic observables, that can be measured simultaneously, or with a single microscopic observable together with the coarse grained Hamiltonian: Indeed, it appears as a decent working hypothesis to assume that the measurement, e.g., of a single particle velocity leaves the (coarse grained) energy distribution of the many-body system practically unaffected. On the other hand multiple microscopic observables are not expected to commute even approximately. It should be emphasized that within this mindest not the exact Hamiltonian, which governs the dynamics, but only its coarse grained counterpart is imagined to (approximately) commute with the coarse grained macroscopic observables. In particular, the observables are not required to be conserved quantities. We also emphasize that this physical interpretation of the considered mathematical setup will never be actually used in our subsequent calculations.

Our next observation is that any real measurement device can only exhibit a limited number of different possible outcomes. For instance, a digital instrument with \( K \) digits can only display \( 10^K \) different measurement values. Hence, we can and will assume that the number \( N \) of common eigenspaces of all the commuting observables at hand respects some reasonable bound, say

\[ N \leq 10^{20}. \]  \hspace{1cm} (3)

Differently speaking, the number of commuting observables as well as their resolution limits are assumed to remain experimentally realistic. In principle, also very low \( N \) values are conceivable and admitted in what follows. In the extreme case, there may be just one observable with two different possible measurement outcomes, implying \( N = 2 \).

On the other hand, for generic macroscopic systems with typically \( f \approx 10^{23} \) degrees of freedom, the dimension \( D \) of the relevant Hilbert space is exponentially large in \( f \). For instance, \( \mathcal{H} \) may be an energy shell, spanned by the eigenvalues of the system Hamiltonian with eigenenergies within an energy interval, which is macroscopically small (well defined macroscopic system energy) but microscopically large (exponentially large \( D \)). As a consequence, at least one of the subspaces \( \mathcal{H}_n \) must be extremely high dimensional. More generally, it appears reasonable to assume that many or even all the \( \mathcal{H}_n \) will exhibit a very large dimensionality \( d_n \), at least as long as peculiarities such as experimentally resolvable gaps in the measurement spectra are absent. Note that even if all \( d_n \)'s are large, some of them may still be very much larger than others.

Compared to the above mentioned previous works (see Introduction), we thus admit the possibility of a relatively detailed knowledge about the initial system state: Not only one single expectation value, but rather the full statistics of all possible measurement outcomes of all the commuting observables is considered to be (approximately) fixed via the preset values of the projection probabilities \( p_n \) in \( \{p_n\} \). Yet, this information is obviously still far from being sufficient to uniquely determine the actual microscopic initial state \( \rho(0) \) of the system.

The time evolution of any given initial state \( \rho(0) \) in \( \{p_n\} \) is governed by the usual Schrödinger or von Neumann equation. For our present purposes it is particularly convenient to adopt the Heisenberg picture of quantum mechanics to express the time-dependent expectation value of any given observable, described by some Hermitian operator \( A \), as

\[ \langle A \rangle_{\rho(t)} := \text{Tr}\{\rho(0) A_t\} \]  \hspace{1cm} (4)

\[ A_t := \mathcal{U}_t^\dagger A \mathcal{U}_t \]  \hspace{1cm} (5)

where \( \mathcal{U}_t \) is the quantum-mechanical time evolution operator. For a time-independent Hamiltonian \( H \), the propagator \( \mathcal{U}_t \) takes the simple form \( \exp\{-iHt/\hbar\} \), but in full generality, also any explicitly time
dependent Hamiltonian $H(t)$ is admitted in (4). In particular, the system is not required to exhibit equilibration or thermalization in the long time limit (see also Chap. 18).

Finally, largely arbitrary observables $A$ are admitted in (5), except for the weak and physically reasonable restriction that the measurement range

$$\Delta_A := a_{\text{max}} - a_{\text{min}},$$

(6)
i.e., the difference between the largest and smallest possible eigenvalues (or measurement outcomes) of $A$ must be finite, and that the maximal resolution $\delta A$ of the considered measurement device must not be unrealistically small compared to $\Delta_A$. For instance, if the measurement device yields at most $K$ relevant digits, then we know that $\Delta_A/\delta A \leq 10^K$. Alternatively, $\delta A$ may also account for the finite precision when solving the considered quantum system by numerical means, or simply for the accuracy with which we actually want or need to know the expectation value in (4). In any case, the natural reference scale for $\delta A$ is the measurement range from (4), i.e., the appropriate quantity to consider is the ratio between resolution and range,

$$R := \delta A/\Delta_A.$$ (7)

**MAIN IDEA AND RESULT**

In essence, our main idea will be as follows: We start by distributing all initial states $\rho(0)$ compatible with (2) into different subsets. Next, we show that the vast majority of all $\rho(0)$’s within any given subset exhibits very similar expectation values in (4) for an arbitrary but fixed $A$. To begin with, we denote by $U_n$ any unitary transformation within the subspace $\mathcal{H}_n$ introduced above Eq. (4), i.e., $U_n : \mathcal{H}_n \to \mathcal{H}_n$ and $U_n^\dagger U_n = \mathbb{1}_{\mathcal{H}_n}$ (identity on $\mathcal{H}_n$). As usual, this operator on $\mathcal{H}_n$ can be readily “lifted” to the full space $\mathcal{H}$, i.e., the same symbol $U_n$ now denotes an operator on $\mathcal{H}$ with the key properties that $U_n^\dagger U_n = P_n$ and $U_n P_m = P_m U_n = 0$ for all $m,n \in \{1,...,N\}$. One thus can infer that

$$U := \sum_{n=1}^N U_n$$ (8)
is a unitary transformation on $\mathcal{H}$, i.e., $U^\dagger U = \mathbb{1}_\mathcal{H}$. The set of unitaries $U$ which can be generated via all possible choices the $U_n$’s in (5) is denoted as $S_U$. One readily confirms that any $U \in S_U$ commutes with all the $P_n$. Furthermore, if $\rho(0)$ satisfies the $N$ constraints (2), then also

$$\rho_U(0) := U^\dagger \rho(0) U$$ (9)

will do so for all $U \in S_U$.

Any given $\rho(0)$ which satisfies (2) thus generates one of the above announced subsets, namely $S_{\rho(0)} := \{\rho_U(0) | U \in S_U\}$. Obviously, many different $\rho(0)$’s which satisfy (2) generate identical subsets $S_{\rho(0)}$. On the other hand, the union of all subsets contains all $\rho(0)$’s which satisfy (2). As an aside we note that all $\rho(0)$’s from the same subset exhibit the same spectrum, but not all $\rho(0)$’s with same spectrum belong to the same subset.

Finally, we assign a probability to the $U \in S_U$ as follows: For any given $n$, the $U_n$’s are assumed to be uniformly distributed (Haar measure with respect to the subspace $\mathcal{H}_n$), i.e., all of them are equally probable and statistically independent of each other for different indices $n$. Accordingly, the probability of $U$ in (5) is defined as the joint probability of all the $U_n$’s appearing on the right hand side, i.e., each combination of $U_n$’s in (5) is realized with equal probability. Averaging any $U$-dependent quantity $X(U)$ over all $U$’s according to this probability measure is henceforth indicated by the symbol $\langle X(U) \rangle_U$.

Intuitively, this choice is extremely natural. Indeed, if it is understood that the probability of any $\rho_U(0)$ within a given set $S_{\rho(0)}$ equals the probability of $U$, then our above choice is the only one which is consistent, i.e., each $\rho(0)$ which generates the same set $S_{\rho(0)}$ also generates the same probability measure on it.
Next we consider $A$ and $t$ in (5) and thus $A_t$ in (6) as arbitrary but fixed. In general, different $\rho(0)$’s which satisfy (2) are expected to entail different expectation values in (4). Focusing on all $\rho(0)$’s which belong to the same, arbitrary but fixed subset $S_t(0)$, one finds for the average and the variance of the expectations values in (4) the following results

$$
\mu_t := \langle \text{Tr}\{\rho_U(0)A_t\} \rangle_U = \sum_{n=1}^N \frac{P_n}{d_n} \text{Tr}\{A_t P_n\},
$$

(10)

$$
\sigma_t^2 := \langle [\text{Tr}\{\rho_U(0)A_t\} - \mu_t]^2 \rangle_U \leq \lambda \Delta_A^2,
$$

(11)

$$
\lambda := 5 \max_n \left( \frac{P_n}{d_n} \right).
$$

(12)

These relations (10)-(12) represent the main result of our present work. However, their detailed derivation is tedious, not very insightful, and hence postponed to the Appendix.

**DISCUSSION**

As announced at the beginning of the previous section, the right hand side of (10) is independent of the actual subset $S_t(0)$, over which the average on the left hand side is performed, and likewise for (11). Hence, the following conclusion, which *a priori* implicitly assumes that the $\rho(0)$’s are randomly sampled from one single subset $S_t(0)$, *de facto* also remains true when randomly sampling $\rho(0)$’s from *any* of those subsets, i.e., for all $\rho(0)$’s which satisfy (2). Taking into account this fact and (11), it follows either obviously or by exploiting the so-called Chebyshev (or Markov) inequality that

$$
\text{Prob}( |\text{Tr}\{\rho(0)A_t\} - \mu_t| > \epsilon ) \leq \lambda (\Delta_A/\epsilon)^2
$$

(13)

for any $\epsilon > 0$, where the probability on the left hand side is understood as the fraction of all $\rho(0)$’s compatible with (2), for which $\text{Tr}\{\rho(0)A_t\}$ differs by more than $\epsilon$ from the mean value $\mu_t$. If we choose for $\epsilon$ the pertinent experimental, numerical, or theoretically required resolution $\delta_A$ in (7), then

$$
\lambda \ll R^2
$$

(14)

implies that $\text{Tr}\{\rho(0)A_t\}$ can be considered as indistinguishable from $\mu_t$ for the vast majority of all $\rho(0)$’s which satisfy (6). In view of (11) and (13) this means that all those $\rho(0)$’s satisfy the approximation

$$
\langle A \rangle_{\rho(t)} = \text{Tr}\{\rho_{\text{gmc}} A_t\}
$$

(15)

for our purposes practically perfectly well, where

$$
\rho_{\text{gmc}} := \sum_{n=1}^N P_n \rho(n),
$$

(16)

$$
\rho(n) := \frac{1}{d_n} P_n.
$$

(17)

With (11) one readily sees that $\rho(n)$ in (17) amounts to a microcanonical density operator on the subspace $\mathcal{H}_n$, hence $\rho_{\text{gmc}}$ in (16) may be viewed as a “generalized microcanonical ensemble”, properly accounting for the preset weight $P_n$ of each subspace in (2).

According to the definitions (1) and (2), the ratio $p_n/d_n$ may be viewed as the (mean) population per eigenstate within any given eigenspace $\mathcal{H}_n$. Recalling that $p_n \geq 0$, $\sum_{n=1}^N p_n = 1$, and that the total number of eigenstates $D$ is unimaginably large, it is obvious that (13) with (7) and (12) will be satisfied under many very common circumstances. For instance, one often expects (see below (3)) that the dimension $d_n$ of every eigenspace $\mathcal{H}_n$ is so large that (14) is automatically fulfilled without any further restriction regarding the $p_n$’s in (12). Moreover, even if certain subspaces $\mathcal{H}_n$ should happen to be relatively low dimensional, it will be sufficient that their “weights” $p_n$ are not unreasonably large (compared to their relatively low dimensions) in order to still guarantee (14). Note that this argument even

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2 More sophisticated distinguishability measures between quantum states than expectation values could in principle be taken into account along similar lines as in Ref. [23].
admits that \( d_n = 1 \) for all \( n \), though such cases seem physically unrealistic according to the considerations below [3].

Finally, it is possible to further generalize our so far results in the following two ways:

First, there may be one exceptional subspace \( \mathcal{H}_n \) of dimension \( d_n = 1 \), for which \( p_n \) is not restricted at all. In other words, one \( n \) with \( d_n = 1 \) may be disregarded when taking the maximum on the right hand side of (12). For instance, this case may be of interest for a system with a non-degenerate ground state, which is energetically separated by a gap from the first excited state and thus may exhibit an exceptionally large (macroscopic) population \( p_n \) compared to all the other level populations \( p_m / d_m \) with \( m \neq n \). The derivation of this generalization amounts to a straightforward combination of the approach in Refs. [23, 24] and in the Appendix below, and is therefore omitted.

Second, not all weights \( p_n \) may be known, but, say, only those with indices \( n \in \{1,...,N'\} \), where \( N' < N \). Accordingly, there are only \( N' \) constraints of the form (2) with \( p_n \geq 0 \) and \( \sum_{n=1}^{N'} p_n \leq 1 \). It follows that the union (direct sum) of all the remaining subspaces \( \mathcal{H} := \mathcal{H}_{N'+1} \oplus \ldots \oplus \mathcal{H}_N \) will be populated with probability \( \bar{p} := 1 - \sum_{n=1}^{N'} p_n \) and that the projector onto this subspace \( \mathcal{H} \) is given by \( 
abla := P_{N'+1} + \ldots + P_N \). Altogether the case at hand can thus be reduced to the original situation with a new "effective" \( N \) value, namely \( N = N' + 1 \), complemented by \( P_N := \bar{P} \) and \( p_N := \bar{p} \).

Taking for granted that condition (14) is satisfied, it follows that the expectation values of \( A \) at time \( t \) on the left hand side of (15) are practically indistinguishable from each other for the vast majority of all initial states \( \rho(0) \) which satisfy the \( N \) constraints (2), i.e., we recover our main dynamical typicality result announced in the first section.

Note that there may still be a small set of "untypical" \( \rho(0) \)'s which satisfy (2) but notably violate the approximation (15). Recalling that \( A \) and \( t \) in (14) and thus \( A_t \) in (4) are still considered as arbitrary but fixed (see above (10)), this set of "untypical" \( \rho(0) \)'s will usually be different for different time points \( t \) and/or different observables \( A \). In this context, it is worth noting that the upper bound in (11) does not depend on \( t \). Since averaging over \( U \) and integrating over \( t \) are commuting operations, we thus can conclude from (11) that

\[
Q := [qv]_{UV} \leq \lambda \Delta X^2,
\]

where

\[
qv := \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \xi_U^2(t) \, dt
\]

and

\[
\xi_U(t) := \text{Tr}\{\rho_U(0)A_t\} - \mu_t
\]

for arbitrary \( t_2 \geq t_1 \geq 0 \). Since \( qv \geq 0 \), one can conclude as before from (14) and (18) that the quantity \( qv \) must be very small for the vast majority of all \( \rho(0) \)'s. For any given such \( \rho(0) \), also the integrand \( \xi_U^2(t) \) in (19) must be very small simultaneously for all \( t \in [t_1,t_2] \), apart from a negligible small fraction of exceptional times \( t \)'s. For sufficiently small \( \lambda \) in (14), those exceptional \( t \)'s become unobservably rare and can be ignored. We thus can conclude that for any given time interval and any given observable \( A \), most \( \rho(0) \)'s which satisfy (2) exhibit very similar expectation values of \( A \) over the entire time interval.

Formally, this typical time evolution is given by the right hand side of (15), but its explicit quantitative evaluation is usually very difficult (see Chaps. 18 and 19) and goes beyond the scope of our present work. In fact, it is exactly one of the main conceptual virtues of such a dynamical typicality approach that interesting predictions can be obtained without actually solving the dynamics. In particular, our present finding helps us to better understand and explain the well established fact that a few macroscopic features are sufficient to ensure the reproducibility of experimental measurements despite many unknown and uncontrollable microscopic details of the system.

**Typicality as Numerical Technique**

As already mentioned at the end of the previous section, the typical time evolution is given by the expression for the ensemble average on the right hand side of (15). The precise quantitative evaluation of this expression can be a challenging task for a specific observable and many-body quantum model and therefore it very often has to be done numerically (see also Chap. 19). In this context, the left hand side of (15) turns out to be very useful in order to establish a powerful numerical technique [4, 25, 32]. This
in the section "Main idea and results" one finds that of expectation values. This scheme is based on (15) with a random sampled initial state of the form much larger Hilbert spaces and thus allows for significant progress in the context of real-time dynamics.

To start with, it is convenient to discuss existing numerical approaches. Within the large variety of different approaches, a straightforward and widely used procedure is the direct evaluation of the ensemble average via

\[
\text{Tr}\{\rho_{\text{gmc}} A_t\} = \sum_{\mu,\nu=1}^{D} \langle \mu | \rho_{\text{gmc}} | \nu \rangle \langle \nu | A | \mu \rangle e^{i(E_\nu - E_\mu) t / \hbar},
\]

(21)

where \(|\mu\rangle, |\nu\rangle\) and \(E_\mu, E_\nu\) are the eigenstates and corresponding eigenenergies of a given many-body Hamiltonian \(H\). In principle, these eigenstates and eigenenergies can be calculated numerically by the exact diagonalization of systems of finite size. However, because the Hilbert-space dimension \(D\) grows exponentially fast in the number of degrees of freedom, exact diagonalization is only feasible for rather small system sizes and finite-size effects can be huge. For a Heisenberg spin-1/2 chain of length \(L\), for example, \(D = 2^L\) and \(L_{\text{max}} \sim 20\) is the maximum length treatable [27–30]. For a Fermi-Hubbard chain with \(L\) sites, as another important example, \(D = 4^L\) and \(L_{\text{max}} \sim 10\) is even much less. Clearly, if the Hamiltonian \(H\) and the observable \(A\) have common and mutually commuting symmetries, such as total magnetization/particle number or translation invariance, it is also possible to exploit these symmetries via

\[
\text{Tr}\{\rho_{\text{gmc}} A_t\} = \sum_{m=1}^{M} \sum_{\mu,\nu=1}^{d_m} \langle m, \mu | \rho_{\text{gmc}} | m, \nu \rangle \langle m, \nu | A | m, \mu \rangle e^{i(E_{m,\nu} - E_{m,\mu}) t / \hbar}.
\]

(22)

However, using these symmetries for the above examples yields a largest subspace with the dimension \(d_m\) being \(d_m \approx (L, L/2)/L\) for the Heisenberg spin-1/2 chain and \(d_m \approx (2L, L)/L\) for the Fermi-Hubbard chain [33], where the bracket \((n,k) := n!/[k!\{n-k\}!]\) denotes the binomial coefficient. In fact, symmetries are already exploited to reach the aforementioned system sizes \(L_{\text{max}}\).

As compared to exact diagonalization (see Chap. 19), a dynamical typicality based scheme can treat much larger Hilbert spaces and thus allows for significant progress in the context of real-time dynamics of expectation values. This scheme is based on (15) with a randomly sampled initial state of the form

\[
\rho(0) := \frac{1}{2 \langle \psi | \rho_{\text{gmc}} | \psi \rangle} (\rho_{\text{gmc}} | \psi \rangle \langle \psi | + \text{h.c.}),
\]

(23)

with the (unnormalized) pure state

\[
|\psi\rangle := \sum_{k=1}^{D} (a_k + ib_k) \ |k\rangle,
\]

(24)

where \(|k\rangle\) is an arbitrary but fixed orthonormal basis, and where the \(a_k\) and \(b_k\) are independent, normally distributed random variables (i.e. Gaussian distributed with zero mean and unit variance). One readily confirms that all statistical properties of the random ensemble of pure states in (23) are independent of the choice of the basis \(|k\rangle\) in (24). In particular, this basis needs not to be the eigenbasis of \(H\). Rather, any numerically convenient basis will do the job. In particular, the basis can be but does not need to be adapted to the symmetries of the specific system under consideration.

It readily follows that \(\rho(0)^\dagger = \rho(0)\) and \(\text{Tr}\{\rho(0)\} = 1\). Moreover, by means of similar calculations as in the section “Main idea and results” one finds that

\[
\langle \psi | P_n \rho_{\text{gmc}} | \psi \rangle = \frac{p_n}{d_n} \langle \psi | P_n | \psi \rangle \approx 2 p_n, \quad \langle \psi | \rho_{\text{gmc}} | \psi \rangle = \sum_{n=1}^{N} \frac{p_n}{d_n} \langle \psi | P_n | \psi \rangle \approx 2
\]

(25)

for sufficiently large subspace dimensions \(d_n\). For the initial state \(\rho(0)\) in (23), these two equations lead to the expectation value \(\text{Tr}\{P_n \rho(0)\} \approx p_n\), i.e., the condition in (2). Therefore, (15) applies to this initial state and yields

\[
\text{Tr}\{\rho_{\text{gmc}} A_t\} \approx \frac{\langle \psi | (\rho_{\text{gmc}} A_t + \text{h.c.}) | \psi \rangle}{2 \langle \psi | \rho_{\text{gmc}} | \psi \rangle} = \frac{\text{Re} \langle \psi | \rho_{\text{gmc}} A_t | \psi \rangle}{\langle \psi | \rho_{\text{gmc}} | \psi \rangle}
\]

(26)
and, using $\langle \psi | \rho_{\text{gmc}} | \psi \rangle \approx 2$ again, as well as $\langle \psi | \psi \rangle \approx 2D$, one obtains the relation

$$\text{Tr}\{\rho_{\text{gmc}} A_1\} \approx D \frac{\text{Re} \langle \psi | \rho_{\text{gmc}} A_1 | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (27)$$

Thus, the trace $\text{Tr}\{\bullet\}$ is essentially replaced by a scalar product $\langle \psi | \bullet | \psi \rangle$ involving a single pure state drawn at random from a Hilbert space of finite but high dimension $D$. This relation can be also written in the form

$$\text{Tr}\{\rho_{\text{gmc}} A_1\} \approx D \frac{\text{Re} \langle \Phi(t) | A | \varphi(t) \rangle}{\langle \varphi(0) | \varphi(0) \rangle} \quad (28)$$

with the two auxiliary pure states

$$|\varphi(t)\rangle := e^{-iHt/\hbar} |\psi\rangle, \quad |\Phi(t)\rangle := e^{-iHt/\hbar} \rho_{\text{gmc}} |\psi\rangle. \quad (29)$$

Note that these pure states look similar but differ from each other because of the additional operator $\rho_{\text{gmc}}$ in the definition of $|\Phi(t)\rangle$.

A central advantage of the relation in (28) is that no time dependence of operators occurs. Instead, the full time dependence appears as a property of pure states only. As a consequence, one does no need to (i) employ exact diagonalization and (ii) store full matrices in computer memory. To see that exact diagonalization can be circumvented, consider the Schrödinger equation

$$\frac{d}{dt} |\varphi(t)\rangle = \frac{i}{\hbar} H |\varphi(t)\rangle \quad (30)$$

for $|\varphi(t)\rangle$. This differential equation and the corresponding equation for $|\Phi(t)\rangle$ can be solved numerically by straightforward iterator schemes like fourth-order Runge-Kutta [27–29] or more sophisticated schemes like Trotter decompositions or Chebyshev polynomials [34, 35]. Still, one has to implement the action of the Hamiltonian on pure states. Since it is possible to carry out these matrix-vector multiplications without storing matrices in computer memory, the memory requirement of the algorithm is set only by the size of vectors, i.e., $O(D)$ or, in case of symmetry reduction, $O(d_m)$. Nevertheless, to reduce the run time of the algorithm, it is convenient to store at least parts of matrices in computer memory. In this respect, one can profit from the fact that the Hamiltonian is usually a few-body operator with a sparse-matrix representation. Thus, the memory requirement essentially remains linear in the relevant Hilbert-space dimension. In this way, for the above example of a Heisenberg spin-1/2 chain, $L_{\text{max}} = 34$ has been reached using medium-sized clusters while $L_{\text{max}} > 34$ is feasible using massive parallelization and supercomputers [30, 36]. As compared to exact diagonalization, the corresponding Hilbert space dimension is larger by several orders of magnitude, e.g., by a factor $2^{34}/2^{20} = O(10^4)$. For such finite but already huge Hilbert spaces, the typicality-related approximation error has been demonstrated to be negligibly small, by a detailed comparison with other state-of-the-art numerical methods including time-dependent density-matrix renormalization group [28] and Lanczos diagonalization [24].

To illustrate the accuracy of the numerical method and the validity of the analytical considerations of the last sections in detail, let us consider the Heisenberg spin-1/2 chain and the specific operators $n_r = S_z^r + 1/2$, where $S_z^r$ is the $z$-component of a spin at site $r$. These $L$ local operators are mutually commuting and can be adjusted independently between 0 and 1. We choose initial conditions $\rho(0)$ with $\langle n_r | \rho(0) \rangle = 1$ at a single site $r$ and $\langle n_r | \rho(0) \rangle = 1/2$ at all other sites $r' \neq r$. This choice corresponds to $\rho_{\text{gmc}} = n_r/2^{L-1}$ and, for the observable $A = n_r$, the ensemble average is then given by the two-point correlation function $\text{Tr}\{\rho_{\text{gmc}} A_1\} = \text{Tr}\{n_r n_r(t)\}/2^{L-1}$ at formally infinite temperature, see Ref. [34]. In Fig. 1 (a) we show this ensemble average, as obtained from exact diagonalization for a finite lattice with $L = 14$ sites. We further depict the approximation in Eq. (28), as obtained from the Runge-Kutta propagation of a random pure state. Clearly, both curves are very close to each other, especially in view of the small $L = 14$. Moreover, an agreement of the same quality is found for another random pure state. In Fig. 1 (c) we compare the approximation in Eq. (28) for two different pure states drawn at random and a substantially larger lattice with $L = 28$ sites. Apparently, the corresponding curves are much closer to each other. This closeness demonstrates the fact that the approximation in Eq. (28) becomes exact in the thermodynamic limit $L \rightarrow \infty$.

Remarkably, typicality also provides the basis of a numerical approach to autocorrelation functions at finite temperatures. This approach is based on the relation

$$\frac{\text{Re} \text{Tr}\{e^{-\beta H} A_1\}}{\text{Tr}\{e^{-\beta H}\}} \approx \frac{\text{Re} \langle \psi | e^{-\beta H} A_1 | \psi \rangle}{\langle \psi | e^{-\beta H} | \psi \rangle}, \quad (31)$$

where $\beta$ is the inverse temperature.
where $\beta = 1/kT$ denotes the inverse temperature and $|\psi\rangle$ is a randomly sampled pure state as defined before. Thus, once again, the trace $\text{Tr}\{\bullet\}$ is replaced by the scalar product $\langle \psi | \bullet | \psi \rangle$. Similar to (28), this relation can be rewritten as

$$\frac{\text{Re} \text{Tr}\{e^{-\beta H} A_k \}}{\text{Tr}\{e^{-\beta H}\}} \approx \frac{\text{Re} \langle \Phi_{\beta}(t) | A | \varphi_{\beta}(t) \rangle}{\langle \varphi_{\beta}(0) | \varphi_{\beta}(0) \rangle}$$

(32)

with the two modified auxiliary pure states

$$|\varphi_{\beta}(t)\rangle := e^{-iHt/\hbar} e^{-\beta H/2} |\psi\rangle, \quad |\Phi(t)\rangle := e^{-iHt/\hbar} A e^{-\beta H/2} |\psi\rangle.$$

(33)

An important difference between these pure states and the ones in (29) is the additional occurrence of the imaginary time $\beta$. As the dependence on real time $t$, this dependence can be obtained from iteratively solving an imaginary-time Schrödinger equation,

$$\frac{d}{d\beta} |\varphi_{\beta}(0)\rangle = -\frac{1}{2} H |\varphi_{\beta}(0)\rangle$$

(34)

for $|\varphi_{\beta}(0)\rangle$ and analogously for $|\Phi_{\beta}(0)\rangle$. Certainly, typicality arguments justify the relation in (32) only, if the dimensions of the relevant energy subspaces are sufficiently large. If the inverse temperature $\beta$ is small, the dominant contribution stems from energy subspaces far from the borders of the spectrum. However, if the inverse temperature $\beta$ is large, the dominant contribution stems from small energy subspaces close to the lower border of the spectrum and typicality arguments cannot be employed any further.

Interestingly, however, this relation does not break down in the limit $\beta \to \infty$ and even becomes exact in this limit. This fact follows from the definition of the two pure states in (33) and whenever the random pure state $|\psi\rangle$ has a finite overlap with the ground state $|\mu_0\rangle$,

$$\langle \mu_0 | \psi \rangle > 0,$$

(35)

even if this overlap is tiny. Then,

$$\lim_{\beta \to \infty} \frac{|\varphi_{\beta}(t)\rangle}{\sqrt{\langle \varphi_{\beta}(0) | \varphi_{\beta}(0) \rangle}} = e^{-iHt/\hbar} |\mu_0\rangle, \quad \lim_{\beta \to \infty} \frac{|\Phi_{\beta}(t)\rangle}{\sqrt{\langle \varphi_{\beta}(0) | \varphi_{\beta}(0) \rangle}} = e^{-iHt/\hbar} A |\mu_0\rangle$$

(36)

and, as a consequence,

$$\lim_{\beta \to \infty} \frac{\text{Re} \langle \Phi_{\beta}(t) | A | \varphi_{\beta}(t) \rangle}{\langle \varphi_{\beta}(0) | \varphi_{\beta}(0) \rangle} = \text{Re} \langle \mu_0 | AA_k | \mu_0 \rangle.$$

(37)

Thus, in conclusion, Eq. (32) also provides a reasonable numerical approach to low temperatures.
APPENDIX

This appendix provides the detailed derivation of the main result (10)–(12) of our present work.

For notational simplicity, we adopt the abbreviations
\[ \rho := \rho(0) \]
\[ B := A_1 , \]
where \( A_t \) is defined in (5). It follows that the eigenvalues of \( B \) are identical to those of \( A \). In particular, the measurement range \( \Delta_B \) of \( B \) will agree with the measurement range \( \Delta_A \) of \( A \) from (4), i.e.,
\[ \Delta_A = \Delta_B . \]  

**Derivation of (10)**

For any given \( n \in \{1, ..., N\} \), we denote by \( \{ |n, a\rangle \}_{a=1}^{d_n} \) an arbitrary but fixed orthonormal basis of \( \mathcal{H}_n \).

The union of all those bases thus amounts to an orthonormal basis of \( \mathcal{H} \), i.e.,
\[ \sum_{n=1}^{N} \sum_{a=1}^{d_n} |n, a\rangle \langle n, a| = \mathbb{1}_\mathcal{H} . \]

Inserting \( \mathbb{1}_\mathcal{H} \) from (12) three times into the definition of \( \mu_t \) in (10) and observing (9) yields
\[ \mu_t = \left[ \sum_{l,j,m,a} \sum_{\alpha,\beta,a,b} (l,\alpha|U^\dagger |m,\alpha) \langle m,\alpha| \rho |n,b\rangle \langle n,b|U|j,\beta\rangle \langle j,\beta|B|l,\alpha\rangle \right]_U \]
\[ = \left[ \sum_{m,n} \sum_{\alpha,\beta,a,b} (m,\alpha|U^\dagger |m,\alpha) \langle m,\alpha| \rho |n,b\rangle \langle n,b|U|n,\beta\rangle \langle n,\beta|B|m,\alpha\rangle \right]_U . \]  

In the last step above we used \( \langle n,b|U|m,\beta\rangle = \delta_{mn} \langle n,b|U|n,\beta\rangle \) since any \( U \in S_U \) commutes with all the \( P_n \)’s as mentioned below (8).

Now, we define the abbreviation for the basis representation of the \( U_n \) introduced above (8) as
\[ U_{n,b\beta} := \langle n,b|U_n|n,\beta\rangle = \langle n,b|U|n,\beta\rangle . \]

This enables us to rewrite equation (43) as
\[ \mu_t = \sum_{m,n} \sum_{\alpha,\beta,a,b} \langle m,\alpha| \rho |n,b\rangle \langle n,\beta|B|m,\alpha\rangle [U_{m,\alpha\alpha} U_{n,b\beta}]_U . \]

To continue evaluating this expression we revert to (37). There, the following is stated for the average over uniformly (Haar) distributed unitaries:\[ \left[ U_{l_1 a_1 b_1} \cdots U_{l_m a_m b_m} U_{l_1 a_1 b_1}^* \cdots U_{l_m a_m b_m}^* \right]_{U_l} = \delta_{m_n} \sum_{\Pi,\Pi'} V_{\Pi,\Pi'} \prod_{j=1}^{n} \delta_{\alpha_j \beta_{j'}} \delta_{\alpha_{j'} a_{j'}} . \]

Quoting verbatim from (37): “the summation is over all permutations \( \Pi \) and \( \Pi' \) of the numbers 1, ..., \( n \). The coefficients \( V_{\Pi,\Pi'} \) depend only on the cycle structure of the permutation \( \Pi^{-1}\Pi' \). Recall that each permutation of 1, ..., \( n \) has a unique factorization in disjoint cyclic permutations (“cycles”) of lengths \( c_1, ..., c_k \) (where \( n = \sum_{j=1}^{k} c_j \)). The statement that \( V_{\Pi,\Pi'} \) depends only on the cycle structure of \( \Pi^{-1}\Pi' \) means that \( V_{\Pi,\Pi'} \) depends only of the lengths \( c_1, ..., c_k \) of the cycles in the factorization of \( \Pi^{-1}\Pi' \). One may therefore write \( V_{c_1, ..., c_k} \) instead of \( V_{\Pi,\Pi'} \).” The factors \( V_{c_1, ..., c_k} \) are given by the columns “CUE” of Tables II and IV in (37).

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\[ ^3 \text{ Averages of this type were analyzed by many authors} \] 11, 15, 12, \textit{often independently. We refer to} 57, \textit{since only there cases up to} \( n \leq 5 \) \textit{are provided, although in the following} \( n \leq 2 \).
As said below (3), the symbol \( \langle \ldots \rangle_U \) indicates an average over all \( U_n \) within each \( \mathcal{H}_n \) according to the Haar measure. Averages over Haar measures in distinct eigenspaces are statistically independent (see below (3)). Thus, by applying (42) to (43) we see that \( m \) has to equal \( n \) or the average vanishes

\[
\mu_t = \sum_{n=1}^{N} \sum_{a,\beta,a,b} \langle n, a | \rho | n, b \rangle \langle n, \beta | B | n, \alpha \rangle \left[ U^*_{a,\alpha,b} U_{n,\beta} \right]_{U_n}
\]

\[
= \sum_{n=1}^{N} \sum_{a,\beta,a,b} \langle n, a | \rho | n, b \rangle \langle n, \beta | B | n, \alpha \rangle V_{n,...,n} \delta_{a\alpha} \delta_{b\beta}.
\]

(47)

(48)

Here, there is only one permutation: namely the identity, denoted by \( \Pi_1 \). In this case \( \Pi^{-1}_1 \Pi_1 = \Pi_1 \) yields only one cycle of length \( c_1 = 1 \). The corresponding \( V_{n,...,n} = V_1 \) can be found, in the Tables II and IV in [37] (column “CUE”, row \( n = 1 \)) as \( V_{n,...,n} = \frac{1}{d_n} \). Plugging this back into the above equation we obtain

\[
\mu_t = \sum_{n=1}^{N} \frac{1}{d_n} \text{Tr} \{ p_{P_n} \} \text{Tr} \{ B P_n \} .
\]

(49)

Observing (2) and (39), we finally recover (10).

Derivation of (11) and (12)

The variance in (11) can be rewritten as

\[
\sigma^2_t = \left[ \text{Tr} \{ p_U B \} \right]_U^2 - \mu^2_t.
\]

(50)

On the right hand side, the last term \( \mu^2_t \) follows from (19) above. Turning to the first term, one finds similarly as in (19) and (20) that

\[
\left[ \text{Tr} \{ p_U B \} \right]_U^2 = \left[ \sum_{l,i} \sum_{\alpha,\beta,a,b} U^*_{l,i,a} U_{j,b} \langle l, a | \rho | j, b \rangle \langle j, \beta | B | l, \alpha \rangle \right. \\
\cdot \left. \sum_{m,n} U^*_{m,c} U_{n,d} \langle m, c | \rho | n, d \rangle \langle n, \omega | B | m, \gamma \rangle \right]_U.
\]

(51)

For the summation indices \( l, j, m, n \) we define the set of quadruples

\[
S := \{ (l, j, m, n) \mid l, j, m, n \in \{ 1, ..., N \} \}.
\]

(52)

If one reverts back to equation (10), one finds the necessity to study three cases for which the average in (51) does not vanish, which amount to the following index subsets of \( S \): \( S_1 : l = j \neq m = n, S_2 : l = j = m = n \) and \( S_3 : l = n \neq m = j \). From now on, the \( S_i \) refer not only to the corresponding index sets but to the associated terms in (51). Thus the following holds

\[
\left[ \text{Tr} \{ p_U B \} \right]_U = [S_1]_U + [S_2]_U + [S_3]_U.
\]

(53)

In the first case, \( S_1 \), the average over \( U \) factorizes into two averages over the eigenspaces labeled by \( l \) and \( m \). Hence, the calculation reduces to the derivation of (10) and we find

\[
[S_1]_U = \sum_{l \neq m} \sum_{\alpha,\beta,a,b} \langle l, a | \rho | l, b \rangle \langle l, \beta | B | l, \alpha \rangle \left[ U^*_{l,a} U_{l,b} \right]_{U_l} \sum_{\gamma,\omega,c,d} \langle m, c | \rho | m, d \rangle \langle m, \omega | B | m, \gamma \rangle \left[ U^*_{m,c} U_{m,d} \right]_{U_m}
\]

\[
= \frac{1}{d_l} \text{Tr} \{ p_P \} \text{Tr} \{ B P \} \frac{1}{d_m} \text{Tr} \{ p_{P_m} \} \text{Tr} \{ B P_m \}.
\]

(54)

In the second case, \( S_2 \), the unitary average is not the same as performed before, but instead:

\[
[S_2]_U = \sum_{l=1}^{N} \sum_{\alpha,\beta,a,b} \langle l, a | \rho | l, b \rangle \langle l, \beta | B | l, \alpha \rangle \sum_{\gamma,\omega,c,d} \langle l, c | \rho | l, d \rangle \langle l, \omega | B | l, \gamma \rangle \left[ U^*_{l,a} U_{l,b} U^*_{l,c} U_{l,d} \right]_{U_l}.
\]

(55)
To further evaluate this expression we make again use of (46), arriving at
\[ [U_{1,b}U_{t,d}V^*_t U^*_c]_{U} = \sum_{i=1}^{N} \frac{1}{d_i (d_i^2 - 1)} \text{Tr} \{ \rho P_1 \}^2 \text{Tr} \{ BP \}^2 + S'_2, \]
\[ S'_2 = \sum_{i=1}^{N} \left[ \frac{1}{d_i (d_i^2 - 1)} \text{Tr} \{ \rho P_1 \}^2 \text{Tr} \{ BP \}^2 - \frac{1}{d_i (d_i^2 - 1)} \sum_{a,b} |(l, a| \rho | l, b) |^2 \text{Tr} \{ BP \}^2 + \frac{1}{d_i^2 - 1} \sum_{a,b} |(l, a| \rho | l, b) |^2 \text{Tr} \{ BP \}^2 \right]. \]

The very first summand of the above expression, \( [S_2]_{U} \), can be used, combined with the first case, \( [S_1]_{U} \), to eliminate the second part of the variance, \( \mu^2 \):
\[ \sigma^2 = ||I_1|_U + |I_2|_U - \mu^2 + |I_3|_U \leq |S'_2| + ||I_3|_U \]. \]

To start estimating an upper bound we notice that there exists a self-adjoint and non-negative operator \( \rho^{1/2} \) which fulfills \( \rho^{1/2} \rho^{1/2} = \rho \). This enables us to use the Cauchy-Schwarz inequality on
\[ \sum_{a,b} |(l, a| \rho | l, b) |^2 \leq \sum_{a,b} (l, a| \rho | l, a) (l, b| \rho | l, b) = \text{Tr} \{ \rho P_1 \}^2. \]

Also, we state that the variance is invariant under a shift \( B \rightarrow B + 1_{4c} \), where \( c \) is an arbitrary real number. We perform this shift such that \( B \) will be positive definite. Then we observe that
\[ \text{Tr} \{ CD \} \leq |D| \text{Tr} \{ C \}, \]
with \( |D| \) denoting the operator norm and with \( C \) as well as \( D \) being self-adjoint and non-negative operators. One readily verifies that \( P_1 \) and \( BP \) are self adjoint and non-negative as well. Applying all this we can bound
\[ |S'_2| \leq \sum_{i=1}^{N} \left( \frac{p_i^2 |B|^2 d_i^2}{d_i (d_i^2 - 1)} + \frac{p_i^2 |B|^2 (d_i + d_i^2)}{d_i (d_i^2 - 1)} + \frac{p_i^2 |B|^2 d_i^4}{d_i^4 - 1} \right) \]
}\]

For \( d \geq 2 \) and the correct choice of \( c \), such that \( |B| = \Delta_B \), we find
\[ |S'_2| \leq 4 \left( \frac{(\Delta_B)^2}{\xi} \right) \max_{n} \left( \frac{p_n}{d_n} \right). \]

This leaves us to evaluate the third case, namely \( S_3 \),
\[ [S_3]_U = \sum_{l \neq j} \sum_{\alpha, \beta, a, b} \langle l, a| \rho | j, b \rangle \langle j, \beta| B | l, \alpha \rangle \sum_{\gamma, \omega, c, d} \langle j, c| \rho | l, d \rangle \langle l, \omega| B | j, \gamma \rangle \cdot [U_{j,b}U_{t,d}V^*_t U^*_c]_{U} \]

(64)
The unitary average here amounts to the same calculation as in equations (48) and (54):
\[
\left[ U_{j,b} U_{l,d} U_{l,a}^* U_{j,c}^* \right]_{U_i} = \left[ U_{l,d} U_{l,a}^* \right]_{U_i} \left[ U_{j,b} U_{j,c}^* \right]_{U_i} = \frac{1}{d_j} \delta_{\omega \delta_{\alpha \beta}} \frac{1}{d_l} \delta_{\omega \delta_{\alpha \beta}},
\]
(65)

implying that
\[
\left| \left[ S_3 \right]_{U_i} \right| = \left| \sum_{l \neq j} \sum_{\alpha, \beta, a, b} \frac{1}{d_j} \langle l, a | \rho | b \rangle \langle j, \beta | B | l, \alpha \rangle \langle j, b | \rho | l, a \rangle \langle l, \alpha | B | j, \beta \rangle \right|
\]
(66)

Now we invoke the Cauchy-Schwarz inequality from (60) again to arrive at
\[
\left| \left[ S_3 \right]_{U_i} \right| \leq \sum_{l=\alpha} \frac{1}{d_j} \text{Tr} \left\{ \rho P_j \right\} \text{Tr} \left\{ P_j B P_j B \right\}
\]
(67)
\[
\leq \max_n \left( \frac{P_n}{d_n} \right) \sum_{j} \frac{1}{d_j} \text{Tr} \left\{ P_j \right\} \text{Tr} \left\{ B \sum_{l} P_l B P_j \right\}
\]
(68)
\[
\leq \max_n \left( \frac{P_n}{d_n} \right) (\Delta B)^2.
\]
(69)

In (68), we noticed that \( \text{Tr} \left\{ B P_j B \right\} \) has to be non-negative since \( B P_j B \) as well as \( P_j \) are non-negative operators. To achieve equation (69), we made use of (61), \( |B|^2 = |B|^2 \) and \( |B| = \Delta \).

Recalling (59) and making use of (63) as well as (69), we obtain the following bound for the variance
\[
\sigma^2_t \leq 5 (\Delta \Delta) \max_n \left( \frac{P_n}{d_n} \right).
\]
(70)

Finally, using (40) we reach (11), (12).

ACKNOWLEDGMENTS: This work was supported by the Deutsche Forschungsgemeinschaft (DFG) under Grants No. RE 1344/10-1, RE 1344/12-1, GE 1657/3-1, STE 2243/3-1 within the Research Unit FOR 2692, and by the Studienstiftung des Deutschen Volkes.

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