IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta

Phys. Scr. **92** (2017) 033001 (17pp) https://doi.org/10.1088/1402-4896/aa5bee

Invited Comment

Loschmidt echo in many-spin systems: a quest for intrinsic decoherence and emergent irreversibility

Pablo R Zangara and Horacio M Pastawski[1]

Instituto de Física Enrique Gaviola (CONICET-UNC) and Facultad de Matemática, Astronomía, Física y Computación (FaMAF), Universidad Nacional de Córdoba, 5000, Córdoba, Argentina

E-mail: horacio@famaf.unc.edu.ar

Received 3 September 2016, revised 22 January 2017
Accepted for publication 25 January 2017
Published 13 February 2017

Abstract

If a magnetic polarization excess is locally injected in a crystal of interacting spins in thermal equilibrium, this 'excitation' would spread as consequence of spin–spin interactions. Such an apparently irreversible process is known as spin diffusion and it can lead the system back to 'equilibrium'. Even so, a unitary quantum dynamics would ensure a precise memory of the non-equilibrium initial condition. Then, if at a certain time, say $t/2$, an experimental protocol reverses the many-body dynamics by changing the sign of the effective Hamiltonian, it would drive the system back to the initial non-equilibrium state at time t. As a matter of fact, the reversal is always perturbed by small experimental imperfections and/or uncontrolled internal or environmental degrees of freedom. This limits the amount of signal $M(t)$ recovered locally at time t. The degradation of $M(t)$ accounts for these perturbations, which can also be seen as the sources of decoherence. This general idea defines the Loschmidt echo (LE), which embodies the various time-reversal procedures implemented in nuclear magnetic resonance. Here, we present an invitation to the study of the LE following the pathway induced by the experiments. With such a purpose, we provide a historical and conceptual overview that briefly revisits selected phenomena that underlie the LE dynamics including chaos, decoherence, localization and equilibration. This guiding thread ultimately leads us to the discussion of decoherence and irreversibility as an emergent phenomenon. In addition, we introduce the LE formalism by means of spin–spin correlation functions in a manner suitable for presentation in a broad scope physics journal. Last, but not least, we present new results that could trigger new experiments and theoretical ideas. In particular, we propose to transform an initially localized excitation into a more complex initial state, enabling a dynamically prepared LE. This induces a global definition of the LE in terms of the raw overlap between many-body wave functions. Our results show that as the complexity of the prepared state increases, it becomes more fragile towards small perturbations.

Keywords: irreversibility, decoherence, Loschmidt echo, non-equilibrium quantum many-body dynamics, emergent phenomena

(Some figures may appear in colour only in the online journal)

[1] Author to whom any correspondence should be addressed

1. Irreversibility and decoherence: a conceptual and historical overview

1.1. On the emergent hierarchical structure of Nature

Our knowledge about the Universe surrounding us is far from being harmoniously unified. Instead, we have a large catalog of almost independent disciplines that constitute, with different degree of success, our comprehension on how Nature works. Quantum Physics, Chemistry, Biology, and their subfields belong to such a hierarchical catalog that could end with Psychology and Sociology. Each of these fields of knowledge provides partial descriptions that correspond to different *levels* of reality [1]. The relation between the basic laws of a discipline in terms of the ones ruling the previous level in the hierarchical tree (usually called *reduction*) is highly nontrivial as the passage from one level to another may involve conceptual and mathematical discontinuities or 'phase transitions' [2–4]. Among these, life and consciousness have proved to be the most elusive, with only a few hints as to when and why they emerge [5, 6].

Within the realm of Physics, these transitions occur between different domains characterized by specific energy, time and length scales. Here, we have reasons to be more optimistic since we have well-developed experimental and mathematical tools. To begin with, let us consider a textbook example which is close to our central problem of irreversibility, namely the derivation of equilibrium Thermodynamics from Classical Statistical Mechanics (SM). The former, one of the driving forces behind the Industrial Revolution, describes the properties of matter in terms of pressure, volume, temperature, among other macroscopic variables. The latter, mainly developed by James C Maxwell, Ludwig Boltzmann and Josiah W Gibbs, provides a probabilistic description of a system composed by N 'atomic' constituents. These elementary entities, and the way in which they interact, are described by means of Classical Mechanics (CM). In fact, Boltzmann [7, 8] considered '*the world as a mechanical system of an enormously large number of constituents, and of an immensely long period of time*' (t), i.e. what we currently call the thermodynamic limit (TL) of $N \to \infty$ and then $t \to \infty$. Then, simple macroscopic relations (thermodynamic equations of state) can be derived from SM by focusing on certain microscopic observables and taking such a limit.

While the previous *reduction* framework works in principle, and to a large extent in practice, it fails when dealing with specific and highly nontrivial physical situations: the critical points. Indeed, a critical point indicates the onset of a phase transition, where the thermodynamic variables, expressed as functions of certain control variable, become non-analytic or even diverge. Here, the reduction paradigm has to be replaced by the *emergence* of qualitatively new phenomena. As stated by Sir Michael Berry [3],

'*Thermodynamics is a continuum theory, so reduction has to show that density fluctuations arising from interatomic forces have a finite (and microscopic) range. This is true everywhere except at the critical point, where there are fluctuations on all scales up to the sample size. Thus, at criticality the continuum limit does not exist, corresponding to a new state of matter. In terms of our general picture, the critical state is a singularity of thermodynamics, at which its smooth reduction to statistical mechanics breaks down; nevertheless, out of this singularity, emerges a large class of new 'critical phenomena', which can be understood by a careful study of the large-N asymptotes.*'

Our everyday experience corresponds to a macroscopically large classical domain, where our falling glass shatters, our cup of coffee cools down, and the ice cube left out of the refrigerator melts. All of these *irreversible* phenomena are manifestations of the well known second law of thermodynamics, i.e. things evolve towards an unavoidable increase of entropy. Indeed, the physical description of such a macroscopic domain involves time-asymmetric equations of motion, such as hydrodynamic and diffusive ones. As already stated, the elementary or microscopic constituents of each macroscopic entity belong to a 'more fundamental' level, whose physical description involves time-symmetric equations of motion, such as Newtonian dynamics or, even better, the Schrödinger equation. In other words, while the microscopic world is reversible, the macroscopic one is not. This paradoxical contrast has fed a recurrent controversy since the end of the nineteenth century to the present day. Our position on this issue relies on the emergence of irreversibility from a microscopically reversible quantum dynamics provided that the TL $N \to \infty$ is appropriately considered.

This article constitutes an invitation to the study of irreversibility as en emergent phenomenon following a pathway much entangled with a series of NMR experiments led by Patricia Levstein and Horacio Pastawski at Córdoba, Argentina [9–11]. In what follows, we discuss and summarize the key concepts on this regard in a manner suitable for a broad readership. Novel results and new insights of interest for specialists are discussed in section 3.

1.2. The irreversibility paradox in the classical world

In his attempt to reconcile the irreversible nature of the second law with the reversible Newtonian laws of motion underlying SM, Boltzmann considered the evolution of a gas composed by colliding particles which is prepared out of equilibrium. Such a complex system was then described according to a kinetic equation that irreversibly leads the system to equilibrium. Here, the time-reversal symmetry is removed through the assumption of 'molecular chaos' or *stosszahl*-ansatz. This hypothesis implies that after each particle collision (characterized by a typical time) the memory of the previous state is lost. Boltzmann's approach finally led him to the celebrated H theorem, which is the first formal justification of the Second Law. At that time, Joseph Loschmidt raised the objection that for every possible trajectory that leads to equilibrium there will be another trajectory, equally possible, that would lead to the initial out-of-equilibrium state. Therefore, it would be possible to revert the velocities of every particle to get again a low entropy state. As an answer, Boltzmann emphasized on the extreme practical difficulty of achieving the time reversed

evolution proposed by Loschmidt, allegedly by saying '*it is you who would invert the velocities!*' [12] .

Boltzmann himself improved his theory transforming it into a probabilistic description. More precisely, the separation between microscopic and macroscopic scales, is exactly what enables us to predict the *typical* evolution of a particular macroscopic system. In fact, this constitutes the modern wisdom that explains the so called 'irreversibility paradox'. As stated by Joel Lebowitz [13] (see also [14, 15]),

'*... several interrelated ingredients which together provide the sharp distinction between microscopic and macroscopic variables required for the emergence of definite time-asymmetric behavior in the evolution of the latter despite the total absence of such asymmetry in the dynamics of individual atoms. They are: (a) the great disparity between microscopic and macroscopic scales, (b) the fact that events are, as put by Boltzmann, determined not only by differential equations, but also by initial conditions, and (c) the use of probabilistic reasoning: it is not every microscopic state of a macroscopic system that will evolve in accordance with the second law, but only the 'majority' of cases—a majority which however becomes so overwhelming when the number of atoms in the system becomes very large that irreversible behavior becomes a near certainty.*'

The key point here is that, already in the classical Boltzmann's approach, the notion of the *emergent* irreversibility depends somehow on the conditions under which the passage from the microscopic to the macroscopic domain is performed. More precisely, the main *qualitative* features of this paradigm have only a slight dependence on the specific details of the underlying microscopic dynamics. However, there exist microscopic properties that do determine the *quantitative* description of the macroscopic evolution [13]. In other words, the derivation of hydrodynamic and diffusive macroscopic equations ultimately depends on the behavior of microscopic trajectories. These microscopic details can include two mutually complementary properties: an extreme sensitivity towards initial conditions, i.e. *chaoticity*, and a tendency towards a uniform distribution of the state in the available phase space, i.e. *mixing*.

Let us explore the two ingredients just mentioned in the context of few-body CM. According to CM, the state of a system, composed by N particles in d-dimensions, is described as a point X in a $(2dN)$-dimensional phase space. If the system is conservative, the energy is the primary conserved quantity, and the phase space is restricted to a hypersurface Ω of $2dN-1$ dimensions usually called *energy shell*. In this scenario, *chaos* implies that two trajectories in Ω, starting from points separated by an arbitrarily small distance δ_0, will separate exponentially as a function of time, $\delta(t) \sim \delta_0 \exp[\lambda t]$. Here, the typical inverse time λ is a Lyapunov characteristic exponent. The *mixing* property implies that the system evolves over time so that any given region contained in Ω eventually overlaps with any other given region in Ω. This can be thought as an 'intertwined' picture of the phase space. None of these properties are satisfied in the case of fully integrable systems, since their solutions are regular and non-dense orbits in Ω. But if integrability is completely broken, chaos and mixing imply that the orbits become irregular and cover Ω densely. This means that an actual trajectory $X(t)$ will be arbitrarily close to every possible configuration within Ω, provided that enough time has elapsed. This last observation embodies the concept of *ergodicity*: an observable can be equivalently evaluated by averaging it for different configurations in Ω or by its time-average along a single trajectory $X(t)$. Such a property is the cornerstone of—classical—SM since it sets the equivalence between the Gibbs' description in terms of ensembles and Boltzmann kinetic approach. Furthermore, we remark that this result does not depend on the limit $N \to \infty$.

By the early 1950s, Enrico Fermi, John Pasta and Stanislaw Ulam (FPU) [16] tried to study when and how the integrability breakdown could lead to an ergodic behavior within a deterministic evolution. They considered a string of harmonic oscillators perturbed by anharmonic forces in order to verify that these nonlinearities can lead to energy equipartition as a manifestation of ergodicity. Even though Ulam himself stated '*The motivation then was to observe the rates of mixing and thermalization...*' [17], the results were not those expected: 'thermalization' dynamics did not show up at all. Instead, the dynamics of the FPU problem, at least for the small number of particles considered, evidenced remarkable recurrences much as those invoked by Henri Poincaré in his famous recurrence theorem [8, 18, 19].

Nowadays, the striking FPU results are understood in terms of the theory of chaos [20]. More precisely, the microscopic instabilities are systematically described by the theory of dynamical chaos developed by Boris Chirikov [21, 22]. In fact, the onset of dynamical chaos can be identified with the transition from non-ergodic to ergodic behavior [23]. A more general criterion for the onset of ergodicity is given by the Kolmogorov–Arnold–Moser (KAM) theorem [24]. It predicts that a weak nonlinear perturbation of an integrable system destroys the constants of motion only locally in the regions of resonances. In other regions of the phase space, islands of quasi-periodic motion persist. Although a direct application of KAM theorem to the FPU model suffers from technical difficulties, it constitutes the main indication that one should not naively expect that weak nonlinear perturbations ensure ergodicity. In addition, it is crucial to remember that real physical systems are neither closed nor finite in a strict sense. Already Boltzmann used this argument to conjure up the peril that cyclic or recurrent motion posed on SM [7, 8]:

'In practice, however, the walls are continuously undergoing perturbations, which will destroy the periodicity resulting from the finite number of molecules.'

Furthermore, the final way out should be found outside the realm of CM, in a description already foreseen by Boltzmann, an emergent from a many-body (quantum) description in the TL $N \to \infty$ [7, 8]:

'Since today it is popular to look forward to the time when our view of Nature will have been completely changed, I will mention the possibility that the fundamental equations for the motion of individual molecules will turn out to be only approximate formulas which give average values, resulting from the probability calculus from the interactions of many

independent moving entities forming the surrounding medium —as for example metheorology laws are valid only on average values obtained by long series of observations using the probability calculus. These entities must be of course so numerous and must act so rapidly that the correct average values are attained in millionths of a second.'

1.3. A coherent quantum world

Is it possible to formulate an straightforward extension of the previous physical picture within Quantum Mechanics (QM)? Any closed and finite quantum system involves a discrete energy spectrum and evolves quasi-periodically in the Hilbert space, which becomes the quantum analog to the classical phase space. As in CM, a closed and finite quantum system is intrinsically reversible due to the unitarity of the evolution operator. However, there exists a crucial difference: while integrability, ergodicity and chaos are well-established concepts within CM, their extensions in QM are much less clear.

The notion of *integrability* in the QM literature may refer to different criteria. Contrary to CM, the existence of '*N* independent (local) conserved mutually commuting linearly independent operators' does not necessarily imply that the system is 'exactly solvable' in the quantum domain [25, 26]. In addition, the concept of *ergodicity* in QM has also generated intense debate, even after the recent rediscovery of the John von Neumann's Quantum Ergodic Theorem [27, 28]. Last, but not least, the classical definition of chaos as the sensitivity to initial conditions does not apply to a wave equation as Schrödinger's. Indeed, we will discuss below that the quantum signature of dynamical chaos had to be found as an instability of a quantum evolution towards perturbations in the Hamiltonian [29].

1.3.1. Decoherence and the theory of open quantum systems.

A phenomenological description of irreversible dynamics within QM can be performed by postulating that the system of interest is in contact with an environment. This implies the removal of the assumption that the system is 'closed'. As stated by Göran Lindblad [30]

'*It seems that the only possibility of introducing an irreversible behavior in a finite system is to avoid the unitary time development altogether by considering non-Hamiltonian systems. One way of doing this is by postulating an interaction of the considered systems S with an external system R like a heat bath or a measuring instrument.*'

The first consequence of the coupling to infinitely many environmental degrees of freedom seems to be the destruction of quantum weirdness within the system. More precisely, this means the attenuation of the interferences evidenced in specific observables and, ultimately, the appearance of classicality [31]. Since this degradation is originated in the loss of phase-coherence between the components of specific quantum superpositions, such a process is called *decoherence*. This automatically implies that the open system dynamics is irreversible.

A theoretical framework, developed in the 1960s by Leo Kadanoff and Gordon Baym [32] and by Leonid Keldysh [33], describes the non-equilibrium SM and it intrinsically deals with open-system dynamics. Such a framework uses the tools of Quantum Field Theory and it ultimately involves the TL. Precisely, this limit may shadow the nature of the approximations involved. A more 'controlled' formalism to describe open-system dynamics had to wait until 1976, when Lindblad's work [30] was independently and simultaneously complemented by Vittorio Gorini, Andrzej Kossakowski, and George Sudarshan [34]. They provide the mathematical structure of the quantum master equations (QME), which in turn can be understood as generalized Liouville-von Neumann differential equations for the reduced density matrix. In this approach, the system under study is finite and specific assumptions are made to describe its environment. These physical hypothesis, which are basically known as the Markovian approximation, were already known and discussed in the 1950s by Felix Bloch [35] and Ugo Fano [36]. As summarized by Karl Blum [37],

'*It is assumed that R has so many degrees of freedom that the effects of the interaction with S dissipate away quickly and will not react back onto S to any significant extent so that R remains described by a thermal equilibrium distribution at constant temperature, irrespective of the amount of energy and polarization diffusing into it from the system S. In other words, it is assumed that the reaction of S on R is neglected and the correlations between S and R, induced by the interaction, are neglected.*'

The QME approach has proved to be operationally successful in describing the dynamics of open systems, as in the case of nuclear magnetic resonance (NMR) [38, 39] and quantum optics [40, 41]. The more prominent model within the theory of open quantum systems is the two-level system in the presence of a structured environment [42]. In particular, the Kadanoff–Baym–Keldysh approach was recently applied to such a model with the specific purpose of describing *quantum dynamical phase transitions* [43]. This novel phenomenon, firstly observed in NMR [44], corresponds to a functional change or non-analyticities in the dynamics of specific observables. More recently, these transitions were also described by means of the QME approach [45]. In any case, the environment is required to be already in the TL, a requisite automatically satisfied in the experimental realm.

1.3.2. Closed quantum systems: to equilibrate or to localize?

As in the original Boltzmann's gas of colliding molecules, let us consider now a closed quantum system composed by a large number N of interacting particles, e.g. fermions or spins in a lattice. We assume that the initial state of the system ($t = 0$) is given by $\hat{\rho}_0$, which does not commute with the time-independent Hamiltonian $\hat{H}$. In other words, $\hat{\rho}_0$ is a non-equilibrium state. Its time evolution is given by

$$\hat{\rho}_t = \exp\left[-\frac{\mathrm{i}}{\hbar}t\hat{H}\right]\hat{\rho}_0 \exp\left[\frac{\mathrm{i}}{\hbar}t\hat{H}\right],$$

which, being dependent on time through quasiperiodic functions, is nearly recurrent and, strictly speaking, it cannot

describe the approach to any 'equilibrium' state. This is merely the result of an unitary dynamics.

Given a specific observable, say $\hat{O}$, the time-evolution of its expectation value is:

$$\langle \hat{O}(t) \rangle = \mathrm{tr}(\hat{\rho}_t \hat{O}).$$

Surprisingly, provided that $\hat{O}$ fulfils certain conditions, *equilibration* can occur for $\langle \hat{O}(t) \rangle$. Here, equilibration means that after some transient behavior, $\langle \hat{O}(t) \rangle$ reaches some 'stationary' value and remains *close* to it for *most* of the time [27, 28]. There exists several theoretical and experimental questions around such idea [46, 47]. For instance, one may naturally ask on the conditions required for $\hat{O}$, $\hat{H}$, and $\hat{\rho}_0$ in order to observe the equilibration of $\langle \hat{O}(t) \rangle$. Indeed, it seems that a key requirement for equilibration is the *locality* of $\hat{O}$. Loosely speaking, this means that $\hat{O}$ involves only a small number of sites or particles. The idea of locality provides for a natural argument in favor of an apparently irreversible behavior of $\langle \hat{O}(t) \rangle$. Indeed, if we 'observe' a local subsystem that involves only a small fraction of the degrees of freedom of the entire system, the coupling to the rest of the system mimics a coupling to an environment. Therefore, as in the above discussion on open system dynamics, the relaxation of $\langle \hat{O}(t) \rangle$ occurs due to the presence of a large environment 'observing' the subsystem. In such a case, the complete system is said to act as its own environment.

Given an interacting many-body system, is it natural to expect that local observables do equilibrate? The answer is no, since there exist striking phenomena in which the equilibration mechanisms are completely inhibited. In fact, a paradigmatic example can be drawn from a very active area in physics: the *quantum localization*. The concept was originally developed by Philip W Anderson [48], who described the absence of diffusion of spin excitations in a disordered system. This phenomenon was observed by George Feher in electron–nuclei double resonance experiments performed in doped semiconductors [49]. While the problem had indeed a many-body nature, Anderson succeed in simplifying it as a system of non-interacting electrons in a d-dimensional disordered lattice. He realized that its dynamics described by Bloch states can change dramatically when a perturbing disordered potential exceeds a critical value. This is known as the extended-to-localized transition or Anderson's localization (AL) [49]. Indeed, if the disorder is small, single-particle states are essentially described in terms of the scattering of Bloch states with some finite lifetime. Precisely, this physical picture was employed by Robert Laughlin to re-examine quantum transport in a random potential as a problem of Quantum Chaos [52]. He proved that the Lyapunov characteristic exponent of the classical electron motion in such a potential can be identified with the collision rate $1/\tau$ appearing in Ohm's law. This constitutes a conceptual link between chaos and diffusive transport. Then, for small disorder, one can generally say that a local excitation is described as a wave packet that ultimately diffuses throughout the system. But AL involves a paradigm shift: when the disorder is large enough, the eigenstates of the system become localized in the real space. Thus, in contrast to the diffusive picture, localization implies that the excitation remains close to its initial location and transport phenomena is no longer possible [50, 51]. In some sense, the same impurities that produce chaos and Lyapunov exponents, which make possible diffusion, dissipative transport and equilibration [52], end up conspiring against them. For dimension $d \leqslant 2$, even a weak disorder ensures the onset of AL.

A step beyond the standard AL problem corresponds to the original problem of localization in interacting systems. As a matter of fact, adding interactions increases the effective dimensionality of the problem, and hence significantly magnifies its complexity. A clean (ordered) system can already evidence a transition into an insulating phase if the interactions are strong enough. This is the case of the Mott-Hubbard transition, whose most paradigmatic case occurs in a crystal with one electron per atomic orbital. John Hubbard showed by means of a Hartree–Fock calculation that for strong local electron–electron repulsion, an otherwise half-filled band of electronic states would split into an occupied band and an unoccupied one [53]. This drives the system from a metallic phase to a insulator one [54, 55], a situation that would persist at fillings where the strong electron-electron Coulomb repulsion forbids the identification of single-particle bands. If the system is disordered, the naive expectation would be that interactions prevent the existence of AL essentially for two reasons. First, collisional dephasing would destroy the specific interferences needed to localize. Second, including interactions automatically implies an exponential increase in the fraction of the Hilbert space required to describe the excitation dynamics. This, in turn, constitutes a more favorable scenario for diffusion, consistent with the fact that a large d prevents localization. Nevertheless, a different kind of transition does occur between extended and localized many-body phases, which is called many-body localization (MBL) [56, 57]. The MBL is a dynamical transition that results when both perturbations to Bloch states, i.e. interactions and Anderson disorder, are present. As in the AL case, an interacting many-body system is said to be localized if the diffusion or transport of excitations becomes frozen, and therefore a memory of the initial conditions is preserved in local observables for long times [58]. However, there is a hierarchical difference between AL and MBL: while the former deals with the eigenstates in a single particle Hilbert space, the latter relies on the properties of the many-body eigenstates in the much bigger Fock space.

The study of localization phenomenon, and particularly the MBL, is extremely attractive from fundamental grounds. Its importance traces back to the FPU problem and the (classical) theoretical framework developed to understand it. As in the attempt by Fermi and collaborators, the current aim is to study simple quantum models that could go parametrically from an ergodic to a non-ergodic quantum dynamics. Moreover, a fundamental question is whether such a transition occurs as a smooth crossover or it has a critical value, a sort of generalized quantum KAM threshold [59]. As a matter of fact, the MBL transition is the promising candidate

in the quantum realm. If the many-body states are extended, then one may expect that the system is ergodic enough to behave as its own environment, and, as stated before, equilibration is enabled. Quite on the contrary, if the many-body states are localized, any initial excitation would remain out-of-equilibrium. In this case, equilibration is precluded. Therefore the MBL would evidence the sought threshold between ergodic and non-ergodic behaviors.

During the last years, the literature dealing with the dynamics of equilibration and thermalization has grown overwhelmingly (see [47, 58]). On the experimental side, an extreme degree of isolation and control has been achieved, such as in the case of ultracold quantum gases [60], trapped ions [61] and also NMR [62]. On the theoretical side, the use of the Hubbard model [53] has proven useful to address the dynamics of strongly interacting many-body systems [63–65]. In addition, for spin systems, numerical studies have provided evidence indicating that the competence between disorder and interactions may lead to highly non-trivial dynamical phase diagrams [115, 116].

1.4. Echoes from the future: NMR comes back

We are now ready to focus on our major question. Namely, to what extent would equilibration, as introduced above, could turn the excitation spreading into an irreversible phenomenon? In order to tackle such a question, we consider specifically a system composed by N quantum spins which is perturbed from a high temperature equilibrium by injecting a local polarization excess. In addition, we assume that the system can indeed equilibrate, i.e. dynamics can lead to a homogeneous distribution of the polarization. Such an equilibration of the polarization is a consequence of a mechanism usually called *spin diffusion* [66, 67]. However, even though a particular observable seems to have reached 'equilibrium', a unitary quantum dynamics would ensure a precise memory of the non-equilibrium initial condition. In other words, the initial state is completely encoded into correlations (eventually non-local) present in the evolved state.

If some experimental protocol could manage to achieve the inverse evolution operator, i.e. to *reverse* the many-body dynamics, then it would drive the system back to the initial non-equilibrium state [68]. This 'echo idea' has remained at the heart of NMR. In fact, the first NMR time-reversal experiments were performed by Erwin Hahn in the 1950s [69]. There, the total polarization, that sums up contributions from individual spins, when lying perpendicular to the external magnetic field, will ideally precess indefinitely. However, each independent spin contributing to the polarization precesses at different velocity due to the local inhomogeneities of the magnetic field. This dephasing produces the decay of the observed polarization. Hahn's procedure involves the inversion of the sign of the Zeeman energy in order to reverse these precessions. If such an inversion is performed at time $t/2$, it will produce the refocusing of the total polarization at time t, which is the well known 'spin echo'. Nevertheless, the sign of the energy scale associated to the spin–spin interactions is not inverted and, accordingly, the echo signal $M(t)$ becomes progressively degraded with t. This decay has a characteristic time scale called T_2, which, in a crystal, characterizes these many-body interactions.

By the early 1970s, Horst Kessemeier, Won-Kyu Rhim, Alex Pines, and John Waugh implemented the reversal of the dynamics induced by the spin–spin dipolar interaction which was missed by the Hahn's procedure [70, 71]. This results in the 'magic echo' signal, which indicates the recovery of a global polarization state. Two decades later, Richard Ernst and collaborators introduced the 'polarization echo' [72]. There, the polarization along the external field is injected *locally* at some labeled spins. As the global polarization is a conserved quantity in this experiment, the local polarization diffuses away for a time $t/2$ due to the spin–spin dipolar interaction. Since it originates in many-spin interactions, this spreading occurs in time scale T_2. By the implementation of a time-reversal procedure involving a change in the sign of the spin–spin energy at time $t/2$, some polarization $M(t)$ is recovered at time t in the same initial spots where it was injected.

While the success of these time reversal echoes unambiguously evidenced the deterministic and quantum nature of spin-dynamics in NMR, it is unavoidable that the reversal results degraded by uncontrolled internal or environmental degrees of freedom, or by imperfections in the pulse sequences. In terms of the theory of open quantum systems, these perturbations would constitute sources of decoherence. Quite often, their precise assessment could only be evidenced through the time reversal experiment [9, 73]. In addition, it was noticed that, since in the 'polarization echo' experiments the total polarization is a conserved quantity, an imperfectly recovered $M(t)$ would be roughly proportional to inverse of the number of spins among which the polarization is distributed. This gives a clear entropic meaning for $-\ln[M(t)]$ [11]. Most importantly, the degradation of $M(t)$ in such experiments, where the many-spin interactions are globally and quite perfectly time-reversed, occurs in a new time scale T_3. Remarkably, the experiments indicate that T_3 seems to be much shorter than any naive estimation of the characteristic time scale of the perturbations, say τ_Σ. Thus, the question is whether the complexity inherent to a large number of correlated spins would enhance the fragility of the procedure under perturbations [9].

1.5. The Loschmidt echo (LE): irreversibility as an emergent phenomenon

The time-reversal procedures just described can be thought as a quantum realization of the gedanken experiment suggested by Loschmidt. As mentioned above, he proposed the reversal of the particles' velocities as a mechanism for undoing the increase of entropy. Actually, the aforementioned NMR time-reversal experiments are specific procedures for backtrace the time evolution [74]. This led Patricia Levstein and Horacio Pastawski to define the *LE* as an idealization which embodies the various, eventually imperfect, time-reversal procedures implemented in NMR [75].

A next generation of experiments in organic crystals [9–11], suggested that the experimental time scale for irreversibility T_3

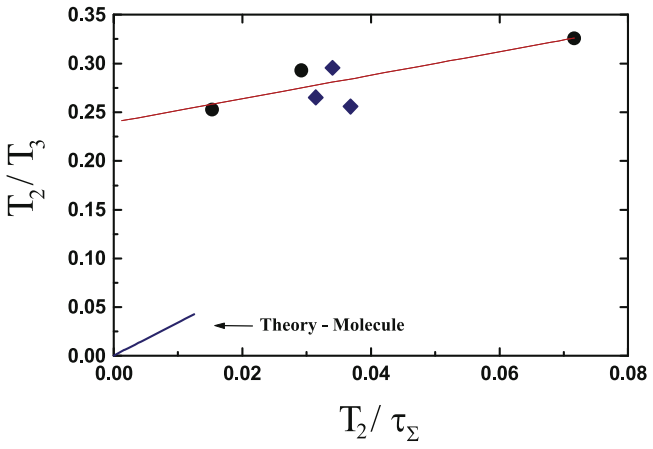

Figure 1. The LE decay rate $1/T_3$ as a function of the perturbation's characteristic rate $1/\tau_\Sigma$. Both quantities are rescaled by the T_2 time scale, which corresponds to the reversible or controlled Hamiltonian. Thus, the vertical axis corresponds to the irreversibility time-scale, while the horizontal one is associated with the strength of the perturbation. In the limit of vanishing perturbation, the irreversibility time-scale saturates at a fraction $\sim\frac{1}{4}$ of the reversible time-scale. This drastically differs from what expected for a single molecule: a perfectly reversible dynamics as the perturbation goes to zero. Adapted from [79].

never exceeds more than a few times T_2, and indeed, it remains tied to it [10, 11]. Thus, it seems that one is left with a sort of unbeatable limit

$$T_2 \lesssim T_3 \ll \tau_\Sigma.$$

The most immediate conclusion would be that there is still an uncontrolled source of decoherence not described by τ_Σ, an explanation that both theoreticians and experimentalists would subscribe to [76]. However, the experiments hinted that this 'perturbation independent decay' (PID) has a much deeper origin, with T_3 acting as a sort of inverse Lyapunov exponent [10]. Since this is in fact an intrinsic property of the system (in the absence of external perturbations), the PID can also be understood as an *intrinsic decoherence* rate. We should stress that until now, this observation holds for LE experiments where polarization is a conserved magnitude. Those of the magic echo type fail to fulfill this requirement [77].

When the decay rate $1/T_3$ (of a LE with polarization conserved) is plotted against the intensity of the most relevant non-inverted term, namely the residual non-secular interaction, it saturates to a finite value: $T_3 \sim 4T_2$. This is explicitly shown in figure 1. This plot resembles a standard resistivity versus temperature plot in an impure metal, where the finite resistivity offset at the zero temperature limit is determined by the impurity scattering [78], i.e. by chaos [52]. Analogously, T_3 in the zero perturbation limit, keeps tied to the time scale that characterizes the reversible many-body interaction. This observation led to postulate the *Central Hypothesis of Irreversibility*: in an infinite many-spin system far away from its ground state, the complex dynamics amplifies the action of any small non-inverted interaction to the degree that such complex (reversible) dynamics provides for the dominant time-scale. Thus, reversible interactions responsible for spin diffusion turn out to be the determinant contribution to the irreversibility rate.

The previous hypothesis triggered the theoretical study of simpler problems in which the LE can be evaluated systematically. In particular, the role of a 'testing bench' was played by single particle systems whose classical counterpart is chaotic. There, the LE is defined as [29]

$$M(t) = \left| \langle\psi| \exp\left[\frac{\mathrm{i}}{\hbar}(\hat{H}_0 + \hat{\Sigma})t\right] \exp\left[-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t\right] |\psi\rangle \right|^2, \quad (1)$$

i.e. the square of the overlap between two one-body wave functions, one of them being evolved by an unperturbed Hamiltonian $\hat{H}_0$ and the other by a perturbed one $\hat{H}_0 + \hat{\Sigma}$. A pioneering prediction by Asher Peres [80] pointed that, if the unperturbed evolution is classically chaotic, the long time limit $M(\infty)$ would yield an evenly spread excitation (not expected for integrable systems). Intermediate times probed a more subtle behavior. Semiclassical calculations showed that at a finite energy ε and small perturbation strengths (but exceeding the spectral discreteness), the LE decay rate $1/T_3$ equals $\Gamma(\Sigma, \varepsilon)$, i.e. the broadening estimated from a Fermi golden rule (FGR) calculation [29, 81]. This lifetime is proportional to the square of the perturbation strength. Exponential decays were soon found for different observables and methods [82, 83]. However, the real surprise was the existence of a regime in which the decay rate of the LE corresponds to the classical Lyapunov exponent [29, 84]. More specifically

$$1/T_3 = \min[\Gamma/\hbar, \lambda].$$

The LE Lyapunov regime is a particular PID that holds for a semiclassical initial state built from a dense spectrum with a perturbation above certain critical threshold Σ_c. Notably, Σ_c falls inversely proportional to the energy ε of the state. Since $\varepsilon \to \infty$ is equivalent to $\hbar \to 0$, we may say that Σ_c vanishes in the classical limit, providing the elusive quantum–classical limit [85].

One should point out that the LE Lyapunov regime may not be fully equivalent with the more natural Lyapunov growth of correlation functions at short times which is, by now, much used to address the so called 'information paradox' of black holes in the context of AdS-CFT [86–91] . In fact, the search for diverging correlations was inspired by the expected growth of the uncertainties of an electron wave packet propagating in a dirty metal [92]. Such an evolution of the correlation functions holds up to the Ehrenfest or 'scrambling' time, when different portions of a spread wave packet are scattered by different impurities. At this point we should remember that the LE Lyapunov regime holds until the much longer Thouless time, when the already scrambled excitation had fully spread through the whole system [84, 93].

The discovery of the PID or Lyapunov regimes in specific LE evaluations was a very big leap that triggered the interest of the Quantum Chaos and Quantum Information communities [94, 95]. Indeed, the mere existence of a PID regime would pose a great challenge on the controllability of quantum devices as it evidences an intrinsic fragility of

quantum dynamics towards minuscule perturbations. The sensitivity to perturbations or fragility of quantum systems [96–98] has become a major problem that transversely affects several fields, e.g. possible chaoticity of quantum computers [99, 100], NMR quantum information processing [101–104], quantum criticality [105, 106] and, more recently, quantum control theory [107]. Nevertheless, the ultimate numerical or analytical proof that would support the above hypothesis, and thus explain the experimental observations, is still lacking. The reason for such a theoretical bottleneck relies on the inherent difficulty in addressing many-body dynamics. Precisely, the association of many-body complexity with a form of chaos [108, 109], could provide a rational for the experimentally observed PID.

An unavoidable starting point for the analysis of PID is the identification of the conditions for the 'perturbation *dependent* decay' that manifests at the relatively short times when exponential decay described by FGR is manifested [110]. As mentioned above, in single-particle systems with a semiclassical excitation, the FGR holds for weak perturbations up to threshold given by the classical Lyapunov exponent that indicates the onset of the PID. So, could a many-body system have a vanishing threshold for the PID? If that is the case, it could show up as a quantum dynamical phase transition in the TL ($N \to \infty$). As a matter of fact, a standard experiment involves a crystalline sample with an infinitely large number of spins. In other words, experiments are 'already in the TL'. In contrast, any numerical approach to assess many-spin dynamics can only cope with a strictly finite N. This is the key point where the original discussion on an emergent irreversibility comes back into scene: an appropriate finite size scaling is required in order to grasp the emergent mechanism that rules irreversibility in the TL. Indeed, one should increase progressively N going from small systems to larger ones with a controlled perturbation. There, the emergent behavior would follow only in a precise order of the limits: first $N \to \infty$ and then $\tau_\Sigma \to \infty$.

Reference [111] constitutes a first attempt to pursue such an ambitious program. The numerical detection of the PID was not achieved and, in fact, it may stay beyond the state-of-the-art numerical techniques [112]. However, an effective FGR regime was reported being consistent with an emergent picture of irreversibility. Keeping in mind the crucial order of the limits stated above, in an infinitely large system, an infinitesimal perturbation is associated to a finite τ_Σ. If a *unitary evolution* keeps the polarization equilibrated during a time $t > \tau_\Sigma$, such an equilibration becomes *irreversible*, and its time-reversal would be completely ineffectual.

In what follows, inspired by the LE experiments in NMR, we provide a framework for theoretical evaluations of LE of the polarization type. We do not consider here LE of the magic echo type, as in this case neither the numerical resolution of small systems [113] nor the actual experiments on scaled Hamiltonians [77] seem to evidence a PID regime. We start by summarizing the LE formulation in spin systems as a local autocorrelation function. Moreover, as introduced in [112], we discuss the local correlation in terms of two global ones. One of these global correlations is defined as the *many-body* LE and resembles the standard one-body LE definition embodied by equation (1). The other is an initially fast growing multi-spin cross correlation that later decays. This formalization leads us to address a fundamental question underlying the LE literature [114]: what is the relation between the LE as defined in one-body systems, i.e. the overlap of wave functions, and the LE as defined in many-body systems, i.e. a spin correlation function? Precisely, we propose and discuss a dynamical preparation protocol to transform the local LE into a global one. Such a dynamically prepared LE (DPLE) can, in turn, lead to a new series of NMR experiments to systematically address the fragility of strongly correlated many-body systems in the presence of small perturbations.

2. The LE formulation

2.1. The local autocorrelation function

Following the early LE experiments [9–11], let us discuss and formalize here the spin system and the time reversal protocol. We consider N spins $1/2$ whose initial condition is described by an infinite temperature state, i.e. a completely depolarized mixture, plus a locally injected polarization

$$\hat{\rho}_0 = \frac{1}{2^N}(\hat{\mathbf{I}} + 2\hat{S}_1^z). \tag{2}$$

Here, the spin 1 is polarized while the others are not, i.e. $\mathrm{tr}[\hat{S}_i^z \hat{\rho}_0] = \frac{1}{2}\delta_{i,1}$.

The polarization, which is initially placed in a single spin, diffuses all around due to the spin–spin interactions. More precisely, a many-spin Hamiltonian $\hat{H}_0$ rules such a *forward* evolution of the system up to a certain time t_R. At that moment, an inversion of the sign of $\hat{H}_0$ is performed, leading to a symmetric *backward* evolution. Typically, $\hat{H}_0$ stands for a truncated dipolar Hamiltonian. Nevertheless, there are unavoidable perturbations, denoted by $\hat{\Sigma}$, that could arise from the incomplete control of the spin Hamiltonian, acting on both periods. The procedure ends up with a local measurement in the same spin that was originally polarized. See figure 2. The evolution operators for each t_R-periods are $\hat{U}_+(t_R) = \exp\left[-\frac{\mathrm{i}}{\hbar}(\hat{H}_0 + \hat{\Sigma})t_R\right]$ and $\hat{U}_-(t_R) = \exp\left[-\frac{\mathrm{i}}{\hbar}(-\hat{H}_0 + \hat{\Sigma})t_R\right]$ respectively. Thus, it is natural to define the LE operator as:

$$\hat{U}_{\mathrm{LE}}(2t_R) = \hat{U}_-(t_R)\hat{U}_+(t_R), \tag{3}$$

which produces an imperfect refocusing at time $2t_R$. The local measurement of the polarization, performed at site 1, defines the local LE:

$$M_{1,1}(t) = 2\mathrm{tr}[\hat{S}_1^z \hat{U}_{\mathrm{LE}}(t)\hat{\rho}_0\hat{U}_{\mathrm{LE}}^\dagger(t)] = 2\mathrm{tr}[\hat{S}_1^z\hat{\rho}_t]. \tag{4}$$

Here, we choose as free variable $t = 2t_R$, the total elapsed time in the presence of the perturbation. The time dependence of $\hat{\rho}_t$ in the Schrödinger picture is

$$\hat{\rho}_t = \hat{U}_{\mathrm{LE}}(t)\hat{\rho}_0\hat{U}_{\mathrm{LE}}^\dagger(t). \tag{5}$$

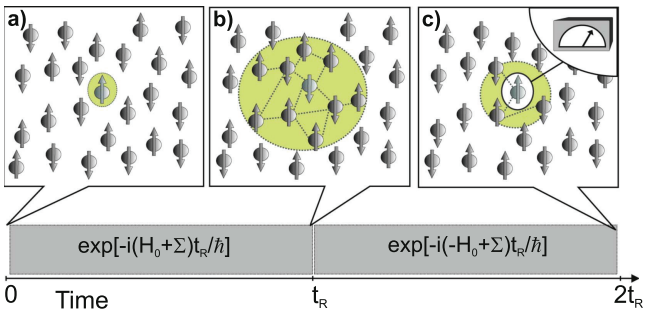

Figure 2. The pictorial scheme of the dynamics involved in $M_{1,1}(t)$. (a) A local excitation in injected in a high temperature spin system. The corresponding state is given by equation (2). The system evolves ruled by the Hamiltonian $\hat{H}_0 + \hat{\Sigma}$. Spin diffusion leads to the spreading of the excitation until a time $t = t_R$ (b). At that time, the sign of $\hat{H}_0$ is inverted. A backward evolution takes place ruled by $-\hat{H}_0 + \hat{\Sigma}$. At time $t = 2t_R$ (c), at the same initial spot, a local measurement is performed.

Using equation (2), and after some algebraic manipulation, the LE can be explicitly written as a correlation function:

$$M_{1,1}(t) = \frac{1}{2^{N-2}}\mathrm{tr}[\hat{U}^{\dagger}_{\mathrm{LE}}(t)\hat{S}^{z}_{1}(0)\hat{U}_{\mathrm{LE}}(t)\hat{S}^{z}_{1}(0)] = \frac{\mathrm{tr}[\hat{S}^{z}_{1}(t)\hat{S}^{z}_{1}(0)]}{\mathrm{tr}[\hat{S}^{z}_{1}(0)\hat{S}^{z}_{1}(0)]}. \quad (6)$$

Here, the time dependence is written according to the Heisenberg picture

$$\hat{S}^{z}_{1}(t) = \hat{U}^{\dagger}_{\mathrm{LE}}(t)\hat{S}^{z}_{1}(0)\hat{U}_{\mathrm{LE}}(t). \quad (7)$$

Notice that equation (6) is an explicit correlation function at the same site but different times, i.e. an *auto*correlation. This correlation has been recently employed to address MBL in spin systems [115, 116].

If we use the identity $\hat{S}^{z}_{1} = \hat{S}^{+}_{1}\hat{S}^{-}_{1} - \frac{1}{2}\hat{\mathbf{I}}$ in equation (6), the invariance of the trace under cyclic permutations ensures that $\mathrm{tr}[\hat{S}^{z}_{1}(t)\hat{S}^{z}_{1}(0)] = \mathrm{tr}[\hat{S}^{-}_{1}(0)\hat{S}^{z}_{1}(t)\hat{S}^{+}_{1}(0)] - \frac{1}{2}\mathrm{tr}[\hat{S}^{z}_{1}(t)]$. Since $\mathrm{tr}[\hat{S}^{z}_{1}(t)] = \mathrm{tr}[\hat{S}^{z}_{1}(0)] = 0$, then:

$$M_{1,1}(t) = 2\sum_{i}\frac{1}{2^{N-1}}\langle i|\hat{S}^{-}_{1}(0)\hat{U}^{\dagger}_{\mathrm{LE}}(t)\hat{S}^{z}_{1}(0)\hat{U}_{\mathrm{LE}}(t)\hat{S}^{+}_{1}(0)|i\rangle = 2\sum_{i\in\mathcal{A}}\frac{1}{2^{N-1}}\langle i|\hat{U}^{\dagger}_{\mathrm{LE}}(t)\hat{S}^{z}_{1}\hat{U}_{\mathrm{LE}}(t)|i\rangle. \quad (8)$$

Here, the states $|i\rangle$ correspond to the computational Ising basis for N spins. In the second line, we restrict the sum to the set $\mathcal{A}$ of numbers i that label basis states which have the 1st spin pointing up, i.e. $i \in \mathcal{A} \Leftrightarrow \hat{S}^{z}_{1}|i\rangle = +\frac{1}{2}|i\rangle$. Equation (8) is indeed an explicit way to rewrite equation (4) in the form of an ensemble average. From the computational point of view, we are left with two possible ways to evaluate, *without any truncation,* the correlation function $M_{1,1}(t)$.

The first (and naive) alternative would be the storage and manipulation of the complete density matrix (whose size scales as $\sim 2^N \times 2^N$). Additionally, the time-dependence represented in equation (5) would eventually require the diagonalization of the Hamiltonian matrix. This strategy has strong limitations due to the memory constraints of any hardware and thus one would hardly achieve systems larger than $N \sim 12$. The second alternative would be the independent (trivially *parallel*) computation of each of the 2^{N-1} expectation values in equation (8). In such a case, one would handle single vectors (whose size scales as $\sim 2^N$). The evolution operators, in turn, can be implemented according to the Trotter–Suzuki formula up to a desired accuracy [117].

Remarkably, there is a *parallel* way to successfully approximate the previous calculation using quantum superpositions. Since $\hat{S}^{z}_{1}$ is a local ('one-body') operator, its evaluation in equation (8) can be replaced by the expectation value in a single superposition state [118]

$$M_{1,1}(t) = 2\langle\Psi_{\mathrm{neq}}|\hat{U}^{\dagger}_{\mathrm{LE}}(t)\hat{S}^{z}_{1}\hat{U}_{\mathrm{LE}}(t)|\Psi_{\mathrm{neq}}\rangle, \quad (9)$$

where:

$$|\Psi_{\mathrm{neq}}\rangle = \sum_{k\in\mathcal{A}}\frac{\exp[-\mathrm{i}\phi_k]}{\sqrt{2^{N-1}}}|k\rangle. \quad (10)$$

Here, $\{\phi_k\}$ are random phases uniformly distributed in $[0, 2\pi)$. As a matter of fact, the state defined in equation ((10) is a random superposition that can successfully mimic the dynamics of ensemble calculations and provides a quadratic speedup of computational efforts [118] (for similar implementations, see also [119, 120]).

2.2. From local to global LE

According to the basis states introduced above, the initial state in equation (2), can be written as

$$\hat{\rho}_0 = \sum_{j\in\mathcal{A}}2^{-(N-1)}|j\rangle\langle j|. \quad (11)$$

Using equations (2), (8) and (11), we can rewrite $M_{1,1}(t)$ as introduced in [121]

$$M_{1,1}(t) = 2\left[\sum_{i\in\mathcal{A}}\sum_{j\in\mathcal{A}}\frac{1}{2^{N-1}}|\langle j|\hat{U}_{\mathrm{LE}}(t)|i\rangle|^2 - \frac{1}{2}\right]. \quad (12)$$

After some manipulation

$$M_{1,1}(t) = 2\left[\sum_{i\in\mathcal{A}}\sum_{j\in\mathcal{A}}\frac{1}{2^{N-1}}|\langle j|\hat{U}_{\mathrm{LE}}(t)|i\rangle|^2 - \frac{1}{2}\right] = \sum_{i\in\mathcal{A}}\frac{1}{2^{N-1}}\left[|\langle i|\hat{U}_{\mathrm{LE}}(t)|i\rangle|^2 + \sum_{j\in\mathcal{A}\ (j\neq i)}\times|\langle j|\hat{U}_{\mathrm{LE}}(t)|i\rangle|^2 - \sum_{j\in\mathcal{B}}|\langle j|\hat{U}_{\mathrm{LE}}(t)|i\rangle|^2\right]. \quad (13)$$

Here, $\mathcal{B}$ stands for the complement of $\mathcal{A}$, i.e. $j \in \mathcal{B} \Leftrightarrow \hat{S}^{z}_{1}|j\rangle = -\frac{1}{2}|j\rangle$. We follow [112] to split the contributions in $M_{1,1}(t)$. Then, the first sum in equation (13) is defined as the many-body or global LE, denoted by $M_{\mathrm{MB}}(t)$

$$M_{\mathrm{MB}}(t) = \sum_{i\in\mathcal{A}}\frac{1}{2^{N-1}}|\langle i|\hat{U}_{\mathrm{LE}}(t)|i\rangle|^2 \quad (14)$$

and stands for the average probability of revival of the many-body states. As a matter of fact, this magnitude resembles the

original LE definition stated in equation (1). Moreover, a widely employed extension of the LE in many-body systems corresponds to single overlaps of specific many-body wave functions, i.e. a specific single term in the sum of equation (14). Such an approach has been performed in many scenarios, such as criticality [105], non-Markovianity in open systems [122, 123], orthogonality catastrophe [124], equilibration dynamics that follows a quantum quench [125–128], MBL [129], among others.

The second sum in equation (13) represents the average probability of changing the configuration of any spin except the 1st. The third sum stands for the average probability that the 1st spin has actually flipped, i.e. of all those processes that do not contribute to $M_{1,1}(t)$. The sum of these terms defines a correlation function $M_X(t)$

$$M_X(t) = \sum_{i\in\mathcal{A}} \frac{1}{2^{N-1}} \left(\sum_{j\in A\ (j\neq i)} |\langle j|\hat{U}_{\rm LE}(t)|i\rangle|^2 - \sum_{j\in B} |\langle j|\hat{U}_{\rm LE}(t)|i\rangle|^2 \right). \quad (15)$$

This balance of probabilities leads to the appropriate asymptotic behavior of $M_{1,1}(t)$ according to the symmetries that constrain the evolution. The decomposition

$$M_{1,1}(t) = M_{\rm MB}(t) + M_X(t) \quad (16)$$

has been recently studied in [112]. The very short-time perturbative behavior of each of these quantities has been specifically quantified: $M_{\rm MB}(t)$ decreases as $1-(N/4)(t/\tau_\Sigma)^2$ and $M_X(t)$ increases initially as $(N/4-1)(t/\tau_\Sigma)^2$. In this specific context, τ_Σ is defined as the characteristic *local* timescale of the perturbation. The precise balance between $M_{\rm MB}(t)$ and $M_X(t)$ provide for the initial decay of $M_{1,1}(t)$, which at very short times is given by $1-(t/\tau_\Sigma)^2$. These expansions indicate an extensivity relation between $M_{\rm MB}(t)$ and $M_{1,1}(t)$ based on the fact that the former decays N times faster than the latter. This has been interpreted [112] as a consequence of statistical independence (at least valid for short-times): the probability of refocusing a complete many-spin state is essentially N times the probability of refocusing a single spin configuration (up or down).

For intermediate times, the experimental evidence indicates that many-body interactions become crucial to provide for decay of $M_{1,1}(t)$. More precisely, reversible interactions in $\hat{H}_0$ are responsible for the observed $M_{1,1}(t)$ decay rates. This experimental observation motivates an analisys of the perturbation series beyond the short-time regime. As already hinted in [112], a general term in these expansions would be proportional to $(t/\tau_\Sigma)^2(t/T_2)^2$, with coefficients that increase rapidly as a function of N. These terms account for the appearance of high order many-body correlations. In the case of $M_X(t)$, it would indicate an increase even faster than the one indicated above. This is fully consistent with the idea of chaos-induced scrambling of quantum information as recently discussed in [130]. Nevertheless, this growth could not persist indefinitely since $M_X(t)$ should ultimately decay, much as in a Multiple Quantum Coherence experiment where two-spin coherences (i.e. correlations) should give place to four-spin coherences and so on [38, 131].

3. Dynamically prepared LE

3.1. Operational ideas

Let us now discuss how to explicitly transform the local LE, i.e. $M_{1,1}(t)$, into a global measure of the reversibility of the many-body dynamics. Here, the strategy is based on dynamical preparation, which provides for an increasing complexity of the initial state in a controllable way. Basically, the procedure consists of a sequence, schematized in figure 3, which is given by: preparation, standard LE, perfect reversal of the preparation and, finally, a local measurement. The preparation results from an evolution, controlled by a Hamiltonian $\hat{H}_p$, that occurs during a time t_p. Then, a standard LE procedure is performed as discussed above, i.e. an imperfect forward–backward evolution. After that, a symmetric t_p backward evolution ruled by $-\hat{H}_p$ unravels the preparation, leading to a local observation. Such a local LE is now denoted by $M_{1,1}(t, t_p)$. The main idea here is that the local measurement, i.e. Figure 3(e), would be equivalent to the overlap between two '*equilibrated*' many-body wave functions that correspond to the states of the system after preparation, i.e. the overlap of the states in figures 3(b) and (d). In this sense, the local autocorrelation $M_{1,1}(t, t_p)$ would take the form of the standard LE definition as in equation (1), but now, in terms of many-body wave functions.

The preparation scheme encodes the local excitation into an extended state. Since the LE procedure is performed after such preparation, the sensitivity under perturbations is evaluated in an initially correlated state. In order to quantify such an observation, let us first consider a single basis state $|j\rangle$, $j\in\mathcal{A}$, that is prepared according to $\hat{U}_p(t_p) = \exp\left[-\frac{\rm i}{\hbar}\hat{H}_p t_p\right]$:

$$\hat{U}_p(t_p)|j\rangle = \sum_k c_k^j(t_p)|k\rangle = |\Psi^{(j)}\rangle. \quad (17)$$

If $\hat{H}_p$ does not exhibit any particular symmetry, dynamics would not be restricted and one should assume that the summation in k effectively runs over the complete Hilbert space. Moreover, the quantum superposition in equation (17) is often assumed to be a sort of 'chaotic' superposition of the basis states $|k\rangle$ [109, 132] . In our case, this observation is particularly true if t_p is larger than the time needed to drive the polarization into an equilibrated value (say, $\tau_{\rm eq}$) [111]. In such an extreme case, the coefficients $c_k^j(t_p)$ fluctuate so randomly as function of the indices j and k that we end up replacing

$$|\Psi^{(i)}\rangle = \sum_k c_k^j(t_p)|k\rangle \longrightarrow \sum_k \frac{\exp[-{\rm i}\phi_k]}{\sqrt{2^N}}|k\rangle = |\Phi\rangle, \quad (18)$$

where, as before, $\{\phi_k\}$ are random phases uniformly distributed in the interval $[0, 2\pi)$. Two different realizations of these random phases, say $\{\phi_k\}$ and $\{\tilde{\phi}_k\}$, lead to two different

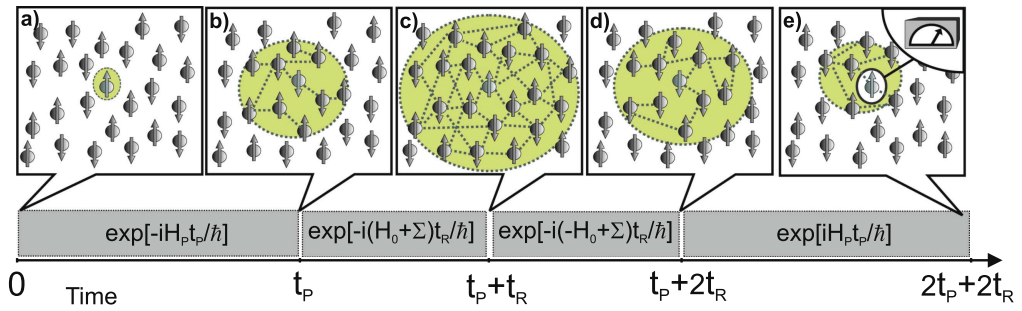

Figure 3. The preparation scheme is included in the protocol shown in figure 2. (a) The initial state given by equation (2) evolves leading to a dynamically correlated state represented in (b). The time reversal procedure is performed afterwards (c)–(d). A 'perfect' reversal of the preparation finally leads to a local measurement in (e).

states

$$|\Phi\rangle = \sum_k \frac{\exp[-\mathrm{i}\phi_k]}{\sqrt{2^N}}|k\rangle,$$
$$|\tilde{\Phi}\rangle = \sum_k \frac{\exp[-\mathrm{i}\tilde{\phi}_k]}{\sqrt{2^N}}|k\rangle,$$

which are typically almost orthogonal:

$$|\langle\tilde{\Phi}|\Phi\rangle|^2 = \left|\sum_k \frac{\exp[-\mathrm{i}(\phi_k - \tilde{\phi}_k)]}{2^N}\right|^2 \sim O(2^{-N}). \quad (19)$$

If we replace $\hat{U}_{\mathrm{LE}}(t)$ by $\hat{U}_p^\dagger(t_p)\hat{U}_{\mathrm{LE}}(t)\hat{U}_p(t_p)$ in equation (15)

$$\begin{aligned} M_X(t, t_p) &= \sum_{i\in\mathcal{A}} \frac{1}{2^{N-1}}\left(\sum_{j\in\mathcal{A}\ (j\neq i)} |\langle j|\hat{U}_p^\dagger(t_p)\hat{U}_{\mathrm{LE}}(t)\hat{U}_p(t_p)|i\rangle|^2 \right.\\ &\quad \left. - \sum_{j\in\mathcal{B}} |\langle j|\hat{U}_p^\dagger(t_p)\hat{U}_{\mathrm{LE}}(t)\hat{U}_p(t_p)|i\rangle|^2\right)\\ &= \sum_{i\in\mathcal{A}} \frac{1}{2^{N-1}}\left(\sum_{j\in\mathcal{A}\ (j\neq i)} |\langle\Psi^{(j)}|\hat{U}_{\mathrm{LE}}(t)|\Psi^{(i)}\rangle|^2 \right.\\ &\quad \left. - \sum_{j\in\mathcal{B}} |\langle\Psi^{(j)}|\hat{U}_{\mathrm{LE}}(t)|\Psi^{(i)}\rangle|^2\right). \end{aligned} \quad (20)$$

Here comes our first specific assumption. Let us replace each of the coherent superpositions states, namely $|\Psi^{(i)}\rangle$ and $|\Psi^{(j)}\rangle$, by incoherent superpositions as in equation (18). Then, the two summations in equation (20) would essentially yield the same outcomes and this leads us to expect that $M_X(t, t_p) \sim O(2^{-N})$. In addition

$$\begin{aligned} &M_{\mathrm{MB}}(t, t_p)\\ &= \sum_{i\in\mathcal{A}} \frac{1}{2^{N-1}} |\langle i|\hat{U}_p^\dagger(t_p)\hat{U}_{LE}(t)\hat{U}_p(t_p)|i\rangle|^2\\ &= \sum_{i\in\mathcal{A}} \frac{1}{2^{N-1}} |\langle\Psi^{(i)}|\hat{U}_{LE}(t)|\Psi^{(i)}\rangle|^2. \end{aligned}$$

Here, the replacement proposed in equation (18) has a practical relevance. Indeed, when replacing $|\Psi^{(i)}\rangle \longrightarrow |\Phi\rangle$, equation (21) consists in the average of 2^{N-1} overlaps, each of them being mathematically equivalent. Then, it is enough to keep just one of these overlaps

$$M_{\mathrm{MB}}(t, t_p) \sim |\langle\Phi|\hat{U}_{\mathrm{LE}}(t)|\Phi\rangle|^2. \quad (21)$$

If our previous observation about $M_X(t, t_p)$ being exponentially small is indeed verified, equation (16) automatically implies that $M_{1,1}(t, t_p) \sim M_{\mathrm{MB}}(t, t_p)$. Then

$$M_{1,1}(t, t_p) \sim |\langle\Phi|\hat{U}_{\mathrm{LE}}(t)|\Phi\rangle|^2. \quad (22)$$

We stress here that the previous expectations, represented by equations (21) and (22), would become valid in the limit of $t_p \gg \tau_{\mathrm{eq}}$. Additionally, we do not expect that these equalities hold for any choice of $\hat{H}_p$. In particular, we need that such a Hamiltonian can create correlations involving a large extent of the Hilbert space $\mathcal{H}$. In practice, this justifies the specific model adopted and described in the following section. Furthermore, the choice is not a purely academic issue, since it is also motivated by a possible experimental realization.

Let us briefly comment on the case in which $\hat{H}_p$ does exhibit a particular symmetry, for instance, the conservation of spin projection $[\hat{H}_p, \sum_{n=1}^N \hat{S}_i^z] = 0$. Such a case naturally induces the decomposition of $\mathcal{H}$ in terms of subspaces $\mathcal{S}_{m_z}$ with definite spin projection quantum number $m_z = \sum_{n=1}^N S_n^z$. Then, the superposition in equation (17), $|\Psi_{[\mathcal{S}_{m_z}]}^{(j)}\rangle$ would be restricted to the specific projection subspace $\mathcal{S}_{m_z}$ according to the initial basis state $|j\rangle$. As a consequence, one should replace in equation (18) the coherent superposition $|\Psi_{[\mathcal{S}_{m_z}]}^{(j)}\rangle$ by a random one also defined in such a subspace $|\Phi_{[\mathcal{S}_{m_z}]}\rangle$. The reasoning is analogous as before but one has to average each of the subspaces

$$\begin{aligned} M_{1,1}(t, t_p) &\sim (1 - M_\infty)\sum_{m_z} D_{m_z}\\ &\quad \times |\langle\Phi_{[\mathcal{S}_{m_z}]}|\hat{U}_{\mathrm{LE}}(t)|\Phi_{[\mathcal{S}_{m_z}]}\rangle|^2 + M_\infty. \end{aligned} \quad (23)$$

Here, D_{m_z} stands for the statistical weight of the subspace $\mathcal{S}_{m_z}$ and M_∞ is the corresponding asymptotic value of the LE. If the total spin projection in the z direction is conserved (i.e. m_z is good quantum number), then one should expect that $M_\infty \sim N^{-1}$. This last asymptotic behavior occurs when the dynamics is sufficiently complex to distribute the polarization homogeneously among the spins in the system, as reported in [110].

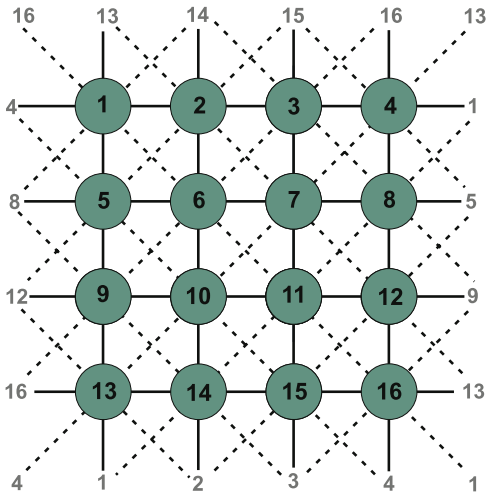

Figure 4. Square lattice with periodic boundary conditions, $N = 16$. Solid lines correspond to the spin pairs $\langle i, j\rangle_{\square}$ in equation (24), and dashed lines to the pairs $\langle i, j\rangle_{\diamond}$ in equation (25).

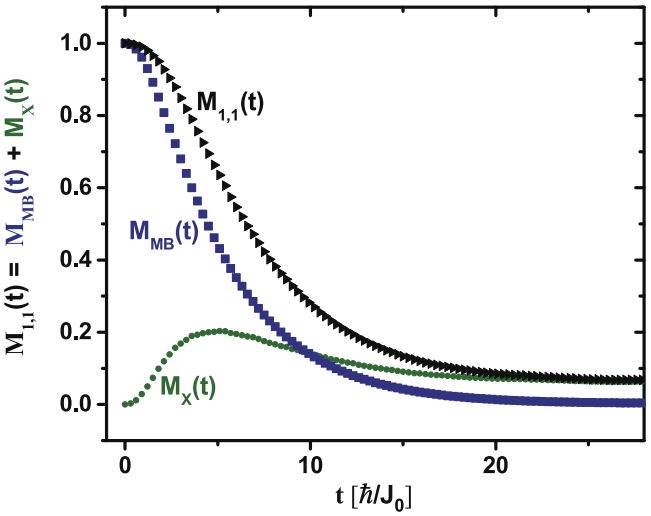

Figure 5. The local autocorrelation function or local LE $M_{1,1}(t)$ (black triangles), and its two non-local contributions: $M_{\mathrm{MB}}(t)$ (blue squares) and $M_X(t)$ (green circles). On the one hand, $M_{\mathrm{MB}}(t)$ exhibits a fast decay (roughly N times faster than that of $M_{1,1}(t)$) and it asymptotically goes to zero. On the other hand, $M_X(t)$ exhibits a rapid growth until it reaches a maximum, and afterwards it decays. Precisely, this decay of $M_X(t)$ determines the intermediate and long-time decay of $M_{1,1}(t)$ and its asymptotic value. As discussed in the text, the case considered ($N = 16$) is still too small to emphasize these observations. The features in the dynamics of these correlation functions will become more prominent as N increases, which may be beyond the state-of-the-art numerical techniques.

3.2. The many-spin model with non-secular interactions

In order to try out the previous expectations, we address the evaluation of the LE in a specific spin system. As in the experiments [9–11], we consider a truncated dipolar Hamiltonian

$$\hat{H}_{\mathrm{dip}}^{\square} = \sum_{\langle i,j\rangle_{\square}}^{N} J_0[2\hat{S}_i^z\hat{S}_j^z - (\hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y)], \tag{24}$$

where the superscript $\square$ in $\hat{H}_{\mathrm{dip}}^{\square}$ corresponds to the summation $\langle i, j\rangle_{\square}$ of first nearest neighbors in a square lattice with periodic boundary conditions, as depicted in figure 4 with solid lines. Additionally, J_0 stands for the appropriate energy units. In analogy, the dipolar coupling between next nearest neighbors in the square lattice is given by

$$\hat{H}_{\mathrm{dip}}^{\diamond} = \sum_{\langle i,j\rangle_{\diamond}}^{N} J_0[2\hat{S}_i^z\hat{S}_j^z - (\hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y)], \tag{25}$$

where, accordingly, $\langle i, j\rangle_{\diamond}$ stands for the pairs of spins connected by dashed lines in figure 4. Then, our LE procedure is defined according to the following choice:

$$\begin{aligned}\hat{H}_0 &= \hat{H}_{\mathrm{dip}}^{\square},\\ \hat{\Sigma} &= \lambda\hat{H}_{\mathrm{dip}}^{\diamond},\end{aligned} \tag{26}$$

where we fix the coefficient $\lambda = 0.1$.

In addition, we consider also the double-quantum (DQ) Hamiltonian [133, 134]

$$\hat{H}_{\mathrm{dq}}^{\square} = \sum_{\langle i,j\rangle_{\square}}^{N} J_0(\hat{S}_i^x\hat{S}_j^x - \hat{S}_i^y\hat{S}_j^y), \tag{27}$$

$$\hat{H}_{\mathrm{dq}}^{\diamond} = \sum_{\langle i,j\rangle_{\diamond}}^{N} J_0(\hat{S}_i^x\hat{S}_j^x - \hat{S}_i^y\hat{S}_j^y), \tag{28}$$

with the same convention as above. This interaction, being proportional to $\hat{S}_i^+\hat{S}_j^+ + \hat{S}_i^-\hat{S}_j^-$, does not conserve spin projection in the z direction since it mixes subspaces with $\delta m_z = 2$.

Given the remarkable degree of control that can be achieved in NMR quantum simulators, in the last years the DQ Hamiltonian has been intensively employed to study the interplay between decoherence and correlations in large spin arrays [101–104, 131]. In addition, it has also been employed to address localization phenomena [135, 136]. Indeed, the DQ Hamiltonian can be used to create, in a controllable way, clusters of correlated spins that can serve as initial states for more sophisticated protocols. This motivates the choice

$$\hat{H}_p = \frac{\hat{H}_{\mathrm{dq}}^{\square} + \hat{H}_{\mathrm{dq}}^{\diamond}}{\sqrt{2}},$$

which provides for the preparation dynamics.

3.3. LE numerical evaluation

We show in figure 5 the evaluation of the correlation functions $M_{1,1}(t)$, $M_{\mathrm{MB}}(t)$ and $M_X(t)$, according to equation (26). One may expect that $M_{1,1}(t)$ and $M_{\mathrm{MB}}(t)$ differ radically since the latter should decay, as stated above, $\sim N$ times faster than the former. Strictly speaking, as discussed in [112], $M_{1,1}^{\eta} \simeq M_{\mathrm{MB}}$, with $\eta \simeq N/4$, which for the case considered ($N = 16$) corresponds to $\eta \simeq 4$. Such a small exponent is basically the reason why the two correlation functions do not separate each other considerably. An ideal finite size scaling would involve a progression of systems satisfying $\eta \gg 1$. In short, our $N = 16$ is still too small. This observation indicates that, within the state-of-the-art numerical techniques, finding numerical evidence of an emerging PID remains a major challenge [111, 112].

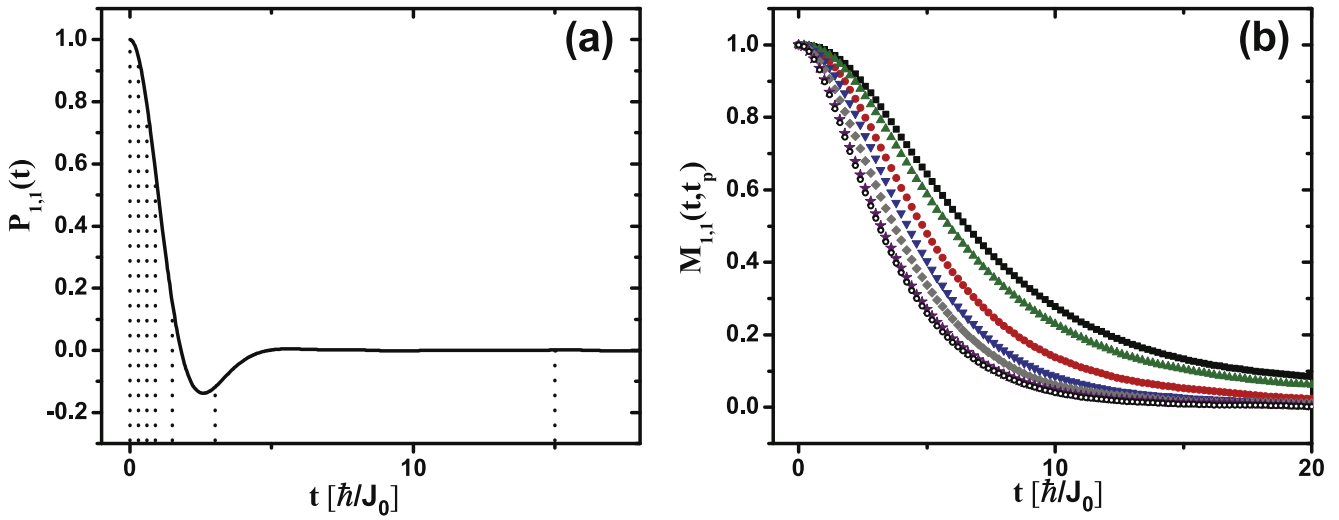

Figure 6. (a) Forward (local) autocorrelation function $P_{1,1}(t)$ defined as in equation (29). Vertical dotted lines indicate the evolution times chosen to play the role of t_p (preparation time in the DPLE protocol). The corresponding DPLE, $M_{1,1}(t, t_p)$, are shown in (b). In particular, $t_p = 0\hbar/J_0$ (black squares); $t_p = 0.3\hbar/J_0$ (green upper triangles); $t_p = 0.6\hbar/J_0$ (red circles); $t_p = 0.9\hbar/J_0$ (blue down triangles); $t_p = 1.5\hbar/J_0$ (gray diamonds); $t_p = 3\hbar/J_0$ (purple stars); $t_p = 15\hbar/J_0$ (open circles).

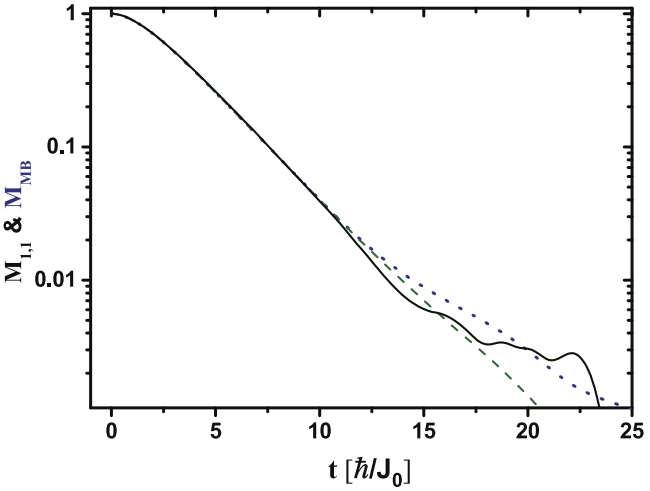

Figure 7. The DPLE. $M_{1,1}(t, t_p = 6\hbar/J_0)$, solid black line, and $M_{MB}(t, t_p = 6\hbar/J_0)$, blue dotted line. The overlap of random superposition states $|\langle\Phi|\hat{U}_{LE}(t)|\Phi\rangle|^2$ is plotted with a green dashed line.

We address the evaluation of the DPLE in figure 6. In particular, figure 6(a) shows a forward autocorrelation function that corresponds to the dynamical preparation, i.e.

$$P_{1,1}(t) = 2\langle\Psi_{neq}|\hat{U}_p^\dagger(t_p)\hat{S}_1^z\hat{U}_p(t_p)|\Psi_{neq}\rangle. \quad (29)$$

The time-evolution of the local polarization at site 1 is monitored and it is observed that it stabilizes near zero within the characteristic time of equilibration $\tau_{eq} \sim 5\hbar/J_0$. This leads us to choose specific preparation times $t_p \lesssim \tau_{eq}$ and $t_p \gg \tau_{eq}$. Accordingly, figure 6(b) shows $M_{1,1}(t, t_p)$ for such choices of preparation times. If $t_p \lesssim \tau_{eq}$, the larger the t_p, the faster the decay of $M_{1,1}(t, t_p)$. When t_p exceeds τ_{eq}, a saturation regime is observed, in which $M_{1,1}(t, t_p)$ becomes independent of t_p. In fact, figure 6(b) shows that $M_{1,1}(t, t_p = 3\hbar/J_0) \simeq M_{1,1}(t, t_p = 15\hbar/J_0)$ (purple stars and open circles, respectively). In general, all the curves representing $M_{1,1}(t, t_p)$, for $t_p > \tau_{eq}$, collapse into a single one.

The fact that $M_{1,1}(t, t_p)$ no longer depends on the precise value of t_p (provided that it exceeds τ_{eq}) indicates that the specific phases in the state $\hat{U}_p(t_p)|\Psi_{neq}\rangle$ have become non-relevant for the dynamics of the polarization. This idea can be generalized to say that outcome of a local measurement is independent of many non-local correlations present in an evolved many-body state. These 'irrelevant' correlations are, in turn, responsible for encoding the precise memory of the initial state, i.e. the evolution is still unitary.

In order to address the saturation aforementioned ($t_p > \tau_{eq}$), we compare $M_{1,1}(t, t_p)$ and $M_{MB}(t, t_p)$ for $t_p = 6\hbar/J_0$ in figure 7. In addition, as stated in equations (21) and (22), we include the overlap $|\langle\Phi|\hat{U}_{LE}(t)|\Phi\rangle|^2$, being $|\Phi\rangle$ the random superposition state defined in equation (18). The coincidence between these three curves is remarkable. It is also worthwhile to notice the clear exponential nature of the decay.

The previous observation essentially states the equivalence $M_{1,1}(t, t_p) \simeq M_{MB}(t, t_p)$ in the regime where $t_p > \tau_{eq}$. Moreover, it identifies such saturation as the overlap between two random superposition states that evolve ruled by perturbed and unperturbed Hamiltonians. This is essentially the many-body extension of the semiclassical LE definition [29]. Then, when the dynamical preparation creates a sufficiently complex state, a given perturbation yields a local LE that is same as a global one for the same perturbation.

The mentioned saturation is relevant for the picture of equilibration discussed in section 1.3.2. When the preparation dynamics equilibrates the polarization, the state $\hat{U}_p(t_p)|\Psi_{neq}\rangle$ can be replaced by the '*equilibrated*' state $|\Phi\rangle$, as far as the evaluation of polarization is concerned. The random phases in $|\Phi\rangle$ correspond to the fact that equilibration of a local

observable is reached when the global correlations are irrelevant or at least redundant for such observable. A similar argument has already been discussed precisely in the context of the LE [111], and it provides a hint for theoretical investigations on the onset of equilibration for local observables in closed many-body systems.

Our observations here may also provide new strategies to understand the experimental results discussed in section 1.5. Since the LE decay accelerates as a function of t_p, the fragility of the reversal procedure in the presence of perturbations can be systematically quantified as a function of t_p. More precisely, this indicates that the preparation dynamics contributes to the time-scale of the LE decay. According to the experimental hints, this contribution would ultimately be the dominant term in the time-scale of LE decay. Of course, this last scenario corresponds to the TL, and thus an appropriate finite size scaling would be needed to confirm it.

4. Conclusions

Starting from a conceptual and historical discussion on the microscopic foundations of the second law of thermodynamics as an emergent of CM, we have introduced and motivated the study of the LE as tool that could help us to reveal the origin of irreversibility in a Quantum Mechanical framework. In particular, we discussed the LE as defined for spin systems, which corresponds to the original NMR polarization echo experiments where the global polarization is a conserved observable. Such experimental LE evaluations have supported an emergent, and quite paradoxical, picture for irreversibility, here embodied by our *Central Hypothesis of Irreversibility*: in an infinite many-spin system in a highly mixed state, any arbitrarily small perturbation is amplified by the progressively increased complexity resulting from the many-body dynamics, which then becomes the dominant time-scale. Thus, the reversal procedure would ultimately be degraded within a time scale determined by such complex, but reversible, many-body interactions.

By formulating the LE in spin systems as a local autocorrelation function, we were able to define the non-local or global LE, and we proposed a protocol to transform the local LE into a global one. This means that a local LE can be employed to measure a global overlap between many-body states. This modified LE procedure introduces a dynamical preparation of the initial state, which creates correlations by means of an (ideally reversible) evolution. In practice, our numerical results confirm that the more correlated the state is, the more fragile under perturbations it becomes, which is manifested in much shorter, perturbation dependent, time scales. Moreover, the decay saturates at a specific time-scale that corresponds to the global LE of random superposition states. This occurs precisely when the preparation time t_p exceeds the equilibration time $\tau_{\text{eq.}}$ of the polarization. Such a saturation indicates that the local LE no longer depends on the precise value of t_p. In other words, a local observation of the polarization does not depend on the specific phases encoded in the many-body evolved state.

Our observations provide for a possible way to understand the experimentally observed PID. Indeed, we showed that reversible dynamics transforms the original local excitation state into a more complex and sensitive one, which in turn is shown to be much more likely to be affected by any small residual perturbation. The time scale at which complexity is being generated could then appear as the dominant time-scale. This dynamical regime, however, has not yet been reached in numerical simulations, as the number of involved spins does not seem to be large enough. Thus, while we are not yet in a position to present a definite numerical test for the Central Hypothesis of Irreversibility, it is worthwhile to mention that the state preparation scheme discussed here can be implemented in a variety of actual NMR experiments. Its application to finite and infinite systems in the form of LE of the polarization- and magic echo types, could shed further light on their strikingly different behaviors, and moreover, into the elusive reversibility paradox.

Acknowledgments

We thank Fernando Pastawski for his careful and critical reading of the manuscript. HMP acknowledges Alexei Kitaev for his hospitality and fruitful discussions at Caltech, and Arturo López Dávalos and Francisco de la Cruz for early inspiring lectures on irreversibility and dissipation. We acknowledge financial support from CONICET, ANPCyT, SeCyT-UNC and MinCyT-Cor. This work used Mendieta Cluster from CCAD at UNC, that is part of SNCAD-MinCyT, Argentina.

References

[1] Chibbaro S, Rondoni L and Vulpiani A 2014 *Reductionism, Emergence and Levels of Reality* (Berlin: Springer)
[2] Anderson P W 1972 More is different *Science* **177** 393–6
[3] Berry M 1994 Asymptotics, singularities and the reduction of theories *Proc. 9th Int. Congress of Logic, Methodoly, and Philosophy of Science* pp 597–607
[4] Primas H 1998 Emergence in exact natural science *Acta Polytech. Sc. Ma.* **91** 83–98
[5] Koch C 2012 *Consciousness: Confessions of a Romantic Reductionist* (Cambridge, MA: MIT Press)
[6] Hofstadter D R 2013 *I am a Strange Loop* (New York: Basic Books)
[7] Boltzmann L 1898 *Vol 2: Vorlesungen über Gastheorie* Leipzig, Barth
[8] Brush S G 1965 *Kinetic Theory* vol 2 (Oxford/New York: Pergamon)
[9] Levstein P R, Usaj G and Pastawski H M 1998 Attenuation of polarization echoes in nuclear magnetic resonance: a study of the emergence of dynamical irreversibility in many-body quantum systems *J. Chem. Phys.* **108** 2718–24
[10] Pastawski H M, Levstein P R, Usaj G, Raya J and Hirschinger J 2000 A nuclear magnetic resonance answer to the Boltzmann–Loschmidt controversy? *Physica* A **283** 166–70
[11] Usaj G, Pastawski H M and Levstein P R 1998 Gaussian to exponential crossover in the attenuation of polarization echoes in NMR *Mol. Phys.* **95** 1229–36

[12] Kuhn T S 1978 *Black-Body Theory and the Quantum Discontinuity 1894–1912* (Chicage, IL: University of Chicago Press)
[13] Lebowitz J L 1999 Statistical mechanics: a selective review of two central issues *Rev. Mod. Phys. Suppl.* **71** 346
[14] Lebowitz J L 1993 Boltzmann's entropy and time's arrow *Phys. Today* **46** 32–8
[15] Lebowitz J L 2008 Time's arrow and Boltzmann's entropy *Scholarpedia* **3** 3448
[16] Fermi E, Pasta J and Ulam S 1955 Studies of nonlinear problems *LANL Report* LA-1940 Los Alamos National Laboratory pp 977–88
[17] Fermi E 1965 *Collected Papers: United States 1939–1954* vol 2 (Chicage, IL: University of Chicago Press)
[18] Poincaré H 1890 Sur le probleme des trois corps et les équations de la dynamique *Acta Math.* **13** A3–270
[19] Zermelo E 1896 On the mechanical explanation of irreversible processes *Ann. Phys.* **57** 485
Zermelo E 1896 *Ann. Phys.* **59** 793
[20] Berman G P and Izrailev F M 2005 The Fermi–Pasta–Ulam problem: fifty years of progress *Chaos* **15** 015104
[21] Chirikov B V 1960 Resonance processes in magnetic traps *J. Nucl. Energy* C **1** 253
[22] Izrailev F M and Chirikov B V 1966 Statistical properties of a nonlinear string *Sov. Phys. Dokl.* **11** 30
[23] Zaslavsky G M 1999 Chaotic dynamics and the origin of statistical laws *Phys. Today* **52** 39–45
[24] Chierchia L and Mather J N 2010 Kolmogorov–Arnold–Moser theory *Scholarpedia* **5** 2123
[25] Caux J S and Mossel J 2011 Remarks on the notion of quantum integrability *J. Stat. Mech.* E P02023
[26] Gogolin C, Müller M P and Eisert J 2011 Absence of thermalization in nonintegrable systems *Phys. Rev. Lett.* **106** 040401
[27] von Neumann J 2010 Proof of the ergodic theorem and the H-theorem in quantum mechanics. Translation of: Beweis des Ergodensatzes und des *H*-Theorems in der neuen *Mechanik. Eur. Phys. J.* H **35** 201–37
[28] Goldstein S, Lebowitz J L, Tumulka R and Zanghì N 2010 Long-time behavior of macroscopic quantum systems. Commentary accompanying the English translation of John von Neumann's 1929 article on the quantum ergodic theorem *Eur. Phys. J.* H **35** 173–200
[29] Jalabert R A and Pastawski H M 2001 Environment-independent decoherence rate in classically chaotic systems *Phys. Rev. Lett.* **86** 2490–3
[30] Lindblad G 1976 On the generators of quantum dynamical semigroups *Commun. Math. Phys.* **48** 119–30
[31] Zurek W H 2003 Decoherence, einselection, and the quantum origins of the classical *Rev. Mod. Phys.* **75** 715–75
[32] Kadanoff L P and Baym G 1962 *Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems* (New York: Benjamin)
[33] Keldysh L V 1964 Diagram technique for nonequilibrium processes *Zh. Eksp. Teor. Fiz.* **47** 1515–27
Keldysh L V 1965 *Sov. Phys.—JEPT* **20** 1018
[34] Gorini V, Kossakowski A and Sudarshan E C G 1976 Completely positive dynamical semigroups of *N* level systems *J. Math. Phys.* **17** 821–5
[35] Wangsness R K and Bloch F 1953 The dynamical theory of nuclear induction *Phys. Rev.* **89** 728–39
[36] Fano U 1957 Description of states in quantum mechanics by density matrix and operator techniques *Rev. Mod. Phys.* **29** 74–93
[37] Blum K 1996 Density matrix theory and applications *Physics of Atoms and Molecules* (New York: Plenum)
[38] Munowitz M 1988 *Coherence and NMR* (New York: Wiley)
[39] Ernst R R, Bodenhausen G and Wokaun A 2004 *Principles of Nuclear Magnetic Resonance in One and Two Dimensions* (Oxford: Clarendon)
[40] Gardiner C and Zoller P 2004 *Quantum Noise: A Handbook of Markovian and Non-Markovian Quantum Stochastic Methods with Applications to Quantum Optics* vol 56 (Berlin: Springer)
[41] Petruccione F and Breuer H P 2002 *The Theory of Open Quantum Systems* (Plenum: Oxford University Press)
[42] Leggett A J, Chakravarty S, Dorsey A T, Fisher M P A, Garg A and Zwerger W 1987 Dynamics of the dissipative two-state system *Rev. Mod. Phys.* **59** 1–85
[43] Pastawski H M 2007 Revisiting the Fermi golden rule: quantum dynamical phase transition as a paradigm shift *Physica* B **398** 278–86
[44] Álvarez G A, Danieli E P, Levstein P R and Pastawski H M 2006 Environmentally induced quantum dynamical phase transition in the spin swapping operation *J. Chem. Phys.* **124**
[45] Horstmann B, Cirac J I and Giedke G 2013 Noise-driven dynamics and phase transitions in fermionic systems *Phys. Rev.* A **87** 012108
[46] Eisert J, Friesdorf M and Gogolin C 2015 Quantum many-body systems out of equilibrium *Nat. Phys.* **11** 124–30
[47] Gogolin C and Eisert J 2016 Equilibration, thermalisation, and the emergence of statistical mechanics in closed quantum systems *Rep. Prog. Phys.* **79** 056001
[48] Anderson P W 1958 Absence of diffusion in certain random lattices *Phys. Rev.* **109** 1492–505
[49] Anderson P W 1978 Local moments and localized states *Rev. Mod. Phys.* **50** 191–201
[50] Kramer B and MacKinnon A 1993 Localization: theory and experiment *Rep. Prog. Phys.* **56** 1469–564
[51] Pastawski H M, Slutzky C M and Weisz J F 1985 Localization as a breakdown of extended states *Phys. Rev.* B **32** 3642–53
[52] Laughlin R B 1987 Electrical resistivity as quantum chaos *Nucl. Phys.* B **2** 213–24
[53] Hubbard J 1963 Electron correlations in narrow energy bands *Proc. R. Soc.* A **276** 238–57
[54] Mott N F 1968 Metal–insulator transition *Rev. Mod. Phys.* **40** 677–83
[55] Madelung O 1996 *Introduction to Solid-State Theory* (*Springer Series in Solid-State Sciences*) (New York: Springer)
[56] Basko D M, Aleiner I L and Altshuler B L 2006 Metal insulator transition in a weakly interacting many-electron system with localized single-particle states *Ann. Phys., NY* **321** 1126–205
[57] Aleiner I L, Altshuler B L and Shlyapnikov G V 2010 A finite-temperature phase transition for disordered weakly interacting bosons in one-dimension *Nat. Phys.* **6** 900–4
[58] Huse D and Nandkishore R 2015 Many-body localization and thermalization in quantum statistical mechanics *Annu. Rev. Condens. Matter Phys.* **6** 15–38
[59] Polkovnikov A, Sengupta K, Silva A and Vengalattore M 2011 *Colloquium*: nonequilibrium dynamics of closed interacting quantum systems *Rev. Mod. Phys.* **83** 863–83
[60] Bloch I, Dalibard J and Nascimbène S 2012 Quantum simulations with ultracold quantum gases *Nat. Phys.* **8** 267–76
[61] Blatt R and Roos C F 2012 Quantum simulations with trapped ions *Nat. Phys.* **8** 277–84
[62] Suter D and Álvarez G A 2016 *Colloquium*: protecting quantum information against environmental noise *Rev. Mod. Phys.* **88** 041001
[63] Tomadin A, Mannella R and Wimberger S 2007 Many-body interband tunneling as a witness of complex dynamics in the Bose–Hubbard model *Phys. Rev. Lett.* **98** 130402

[64] Buonsante P and Wimberger S 2008 Engineering many-body quantum dynamics by disorder *Phys. Rev.* A **77** 041606
[65] Schlagheck P and Shepelyansky D L 2016 Dynamical thermalization in Bose–Hubbard systems *Phys. Rev.* E **93** 012126
[66] Blume M and Hubbard J 1970 Spin correlation functions at high temperatures *Phys. Rev.* B **1** 3815–30
[67] Forster D 1975 *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions* vol 47 (New York: Benjamin)
[68] Brewer R G and Hahn E L 1984 Atomic memory *Sci. Am.* **251** 50–7
[69] Hahn E L 1950 Spin echoes *Phys. Rev.* **80** 580
[70] Rhim W K and Kessemeier H 1971 Transverse-magnetization recovery in the rotating frame *Phys. Rev.* B **3** 3655–61
[71] Rhim W K, Pines A and Waugh J S 1971 Time-reversal experiments in dipolar-coupled spin systems *Phys. Rev.* B **3** 684–96
[72] Zhang S, Meier B H and Ernst R R 1992 Polarization echoes in NMR *Phys. Rev. Lett.* **69** 2149–51
[73] Pastawski H M, Usaj G, Iglesias R A and Levstein P R 1998 Surgimiento de irreversibilidad dinámica en sistemas cuánticos de muchos cuerpos: Una prueba usando resonancia magnética nuclear *Rev. Mex. Fis.* **44** 1–6
[74] Waugh J S, Rhim W K and Pines A 1972 Spin echoes and Loschmidt's paradox *Pure Appl. Chem.* **32** 317–24
[75] Goussev A, Jalabert R A, Pastawski H M and Wisniacki D 2012 Loschmidt echo *Scholarpedia* **7** 11687
[76] Zurek W H, Cucchietti F M and Paz J P 2007 Gaussian decoherence and gaussian echo from spin environments *Acta Phys. Pol.* B **38** 1685
[77] Buljubasich L, Sánchez C M, Dente A D, Levstein P R, Chattah A K and Pastawski H M 2015 Experimental quantification of decoherence via the Loschmidt echo in a many spin system with scaled dipolar hamiltonians *J. Chem. Phys.* **143** 164308
[78] Doniach S and Sondheimer E H 1974 *Green's Functions for Solid State Physicists* (New York: Benjamin-Cummings)
[79] Usaj G 1999 Mesoscopic echoes and polarization echoes in NMR: a study about the spin excitation dynamics in interacting systems *PhD Thesis* Universidad Nacional de Córdoba, Argentina
[80] Peres A 1984 Stability of quantum motion in chaotic and regular systems *Phys. Rev.* A **30** 1610–5
[81] Jacquod P, Silvestrov P G and Beenakker C W J 2001 Golden rule decay versus Lyapunov decay of the quantum Loschmidt echo *Phys. Rev.* E **64** 055203
[82] Prosen T 2002 General relation between quantum ergodicity and fidelity of quantum dynamics *Phys. Rev.* E **65** 036208
[83] Cerruti N R and Tomsovic S 2002 Sensitivity of wave field evolution and manifold stability in chaotic systems *Phys. Rev. Lett.* **88** 054103
[84] Cucchietti F M, Pastawski H M and Jalabert R A 2004 Universality of the Lyapunov regime for the Loschmidt echo *Phys. Rev.* B **70** 035311
[85] Cucchietti F M, Dalvit D A R, Paz J P and Zurek W H 2003 Decoherence and the Loschmidt echo *Phys. Rev. Lett.* **91** 210403
[86] Sekino Y and Susskind L 2008 Fast scramblers *J. High Energy Phys.* JHEP10(2008)065
[87] Shenker S H and Stanford D 2014 Black holes and the butterfly effect *J. High Energy Phys.* JHEP03(2014)067
[88] Roberts D A, Stanford D and Susskind L 2015 Localized shocks *J. High Energy Phys.* **2015** 51JHEP03(2015)
[89] Maldacena J, Shenker S H and Stanford D 2016 A bound on chaos *J. High Energ. Phys.* **106**
[90] Kitaev A 2014 Hidden correlations in the Hawking radiation and thermal noise *Talk Given at Fundamental Physics Prize Symp. November 10 (11 November–18 December)* Stanford SITP Seminars
[91] Swingle B, Bentsen G, Schleier-Smith M and Hayden P 2016 Measuring the scrambling of quantum information *Phys. Rev.* A **94** 040302
[92] Larkin A I and Ovchinnikov Y N 1969 Quasiclassical method in the theory of superconductivity *J. Exp. Theor. Phys.* **28** 1200
[93] Cucchietti F M 2004 The Loschmidt echo in classically chaotic systems: quantum chaos, irreversibility and decoherence *PhD Thesis* Universidad Nacional de Córdoba, Argentina https://arxiv.org/abs/quant-ph/0410121
[94] Gorin T, Prosen T, Seligman T H and Znidaric M 2006 Dynamics of Loschmidt echoes and fidelity decay *Phys. Rep.* **435** 33–156
[95] Jacquod P and Petitjean C 2009 Decoherence, entanglement and irreversibility in quantum dynamical systems with few degrees of freedom *Adv. Phys.* **58** 67–196
[96] Jacquod P, Adagideli I and Beenakker C W J 2002 Decay of the Loschmidt echo for quantum states with sub-Planck-scale structures *Phys. Rev. Lett.* **89** 154103
[97] Karkuszewski Z P, Jarzynski C and Zurek W H 2002 Quantum chaotic environments, the butterfly effect, and decoherence *Phys. Rev. Lett.* **89** 170405
[98] Bendersky D, Zangara P R and Pastawski H M 2013 Fragility of superposition states evaluated by the Loschmidt echo *Phys. Rev.* A **88** 032102
[99] Georgeot B and Shepelyansky D L 2000 Quantum chaos border for quantum computing *Phys. Rev.* E **62** 3504
[100] Flambaum V V 2000 Time dynamics in chaotic many-body systems: can chaos destroy a quantum computer? *Aust. J. Phys.* **53** 489–97
[101] Krojanski H G and Suter D 2004 Scaling of decoherence in wide NMR quantum registers *Phys. Rev. Lett.* **93** 090501
[102] Morgan S W, Oganesyan V and Boutis G S 2012 Multispin correlations and pseudothermalization of the transient density matrix in solid-state NMR: free induction decay and magic echo *Phys. Rev.* B **86** 214410
[103] Kaur G, Ajoy A and Cappellaro P 2013 Decay of spin coherences in one-dimensional spin systems *New J. Phys.* **15** 093035
[104] Sánchez C M, Acosta R H, Levstein P R, Pastawski H M and Chattah A K 2014 Clustering and decoherence of correlated spins under double quantum dynamics *Phys. Rev.* A **90** 042122
[105] Quan H, Song Z, Liu X, Zanardi P and Sun C 2006 Decay of Loschmidt echo enhanced by quantum criticality *Phys. Rev. Lett.* **96** 140604
[106] Silva A 2008 Statistics of the work done on a quantum critical system by quenching a control parameter *Phys. Rev. Lett.* **101** 120603
[107] Caneva T, Silva A, Fazio R, Lloyd S, Calarco T and Montangero S 2014 Complexity of controlling quantum many-body dynamics *Phys. Rev.* A **89** 042322
[108] Flambaum V V and Izrailev F M 2000 Excited eigenstates and strength functions for isolated systems of interacting particles *Phys. Rev.* E **61** 2539–42
[109] Flambaum V V and Izrailev F M 2001 Entropy production and wave packet dynamics in the Fock space of closed chaotic many-body systems *Phys. Rev.* E **64** 036220
[110] Zangara P R, Dente A D, Levstein P R and Pastawski H M 2012 Loschmidt echo as a robust decoherence quantifier for many-body systems *Phys. Rev.* A **86** 012322
[111] Zangara P R, Bendersky D and Pastawski H M 2015 Proliferation of effective interactions: decoherence-induced equilibration in a closed many-body system *Phys. Rev.* A **91** 042112
[112] Zangara P R, Bendersky D, Levstein P R and Pastawski H M 2016 Loschmidt echo in many-spin systems: contrasting time scales of local and global measurements *Phil. Trans. R. Soc.* A **374** 20150163

[113] Fine B V, Elsayed T A, Kropf C M and de Wijn A S 2014 Absence of exponential sensitivity to small perturbations in nonintegrable systems of spins 1/2 *Phys. Rev.* E **89** 012923
[114] Goussev A, Jalabert R A, Pastawski H M and Wisniacki D A 2016 Loschmidt echo and time reversal in complex systems *Phil. Trans. R. Soc.* A **374** 20150383
[115] Zangara P R, Dente A D, Iucci A, Levstein P R and Pastawski H M 2013 Interaction-disorder competition in a spin system evaluated through the Loschmidt echo *Phys. Rev.* B **88** 195106
[116] Zangara P R, Levstein P R and Pastawski H M 2015 Role of energy uncertainties in ergodicity breaking induced by competing interactions and disorder. A dynamical assessment through the Loschmidt echo *Papers Phys.* **7** 070012
[117] Dente A D, Bederián C S, Zangara P R and H M Pastawski 2013 GPU accelerated Trotter–Suzuki solver for quantum spin dynamics arXiv:1305.0036
[118] Álvarez G A, Danieli E P, Levstein P R and Pastawski H M 2008 Quantum parallelism as a tool for ensemble spin dynamics calculations *Phys. Rev. Lett.* **101** 120503
[119] Elsayed T A and Fine B V 2013 Regression relation for pure quantum states and its implications for efficient computing *Phys. Rev. Lett.* **110** 070404
[120] Pineda C, Prosen T and Villaseñor E 2014 Two-dimensional kicked quantum Ising model: dynamical phase transitions *New J. Phys.* **16** 123044
[121] Pastawski H M, Levstein P R and Usaj G 1995 Quantum dynamical echoes in the spin diffusion in mesoscopic systems *Phys. Rev. Lett.* **75** 4310–3
[122] Haikka P, Goold J, McEndoo S, Plastina F and Maniscalco S 2012 Non-Markovianity, Loschmidt echo, and criticality: a unified picture *Phys. Rev.* A **85** 060101
[123] García-Mata I, Pineda C and Wisniacki D 2012 Non-Markovian quantum dynamics and classical chaos *Phys. Rev.* A **86** 022114
[124] Dóra B, Pollmann F, Fortágh J and Zaránd G 2013 Loschmidt echo and the many-body orthogonality catastrophe in a qubit-coupled Luttinger liquid *Phys. Rev. Lett.* **111** 046402
[125] Torres-Herrera E J, Vyas M and Santos L F 2014 General features of the relaxation dynamics of interacting quantum systems *New J. Phys.* **16** 063010
[126] Torres-Herrera E J and Santos L F 2014 Quench dynamics of isolated many-body quantum systems *Phys. Rev.* A **89** 043620
[127] Torres-Herrera E J and Santos L F 2014 Nonexponential fidelity decay in isolated interacting quantum systems *Phys. Rev.* A **90** 033623
[128] Torres-Herrera E J, Kollmar D and Santos L F 2015 Relaxation and thermalization of isolated many-body quantum systems *Phys. Scr.* **T165** 014018
[129] Torres-Herrera E J and Santos L F 2015 Dynamics at the many-body localization transition *Phys. Rev.* B **92** 014208
[130] Kurchan J 2016 Quantum bound to chaos and the semiclassical limit arXiv:1612.01278
[131] Sánchez C M, Levstein P R, Buljubasich L, Pastawski H M and Chattah A K 2016 Quantum dynamics of excitations and decoherence in many-spin systems detected with Loschmidt echoes: its relation to their spreading through the Hilbert space *Phil. Trans. R. Soc.* A **374** 20150155
[132] Flambaum V V and Izrailev F M 1997 Statistical theory of finite Fermi systems based on the structure of chaotic eigenstates *Phys. Rev.* E **56** 5144
[133] Baum J, Munowitz M, Garroway A N and Pines A 1985 Multiple quantum dynamics in solid state NMR *J. Chem. Phys.* **83** 2015–25
[134] Munowitz M, Pines A and Mehring M 1987 Multiple quantum dynamics in NMR: a directed walk through Liouville space *J. Chem. Phys.* **86** 3172–82
[135] Álvarez G A and Suter D 2010 NMR quantum simulation of localization effects induced by decoherence *Phys. Rev. Lett.* **104** 230403
[136] Álvarez G A, Suter D and Kaiser R 2015 Localization-delocalization transition in the dynamics of dipolar-coupled nuclear spins *Science* **349** 846–8