Eigenstate thermalization within isolated spin-chain systems

R. Steinigeweg\textsuperscript{1}, J. Herbrich\textsuperscript{1}, and P. Prelovšek\textsuperscript{1,2}

\textsuperscript{1}J. Stefan Institute, SI-1000 Ljubljana, Slovenia and
\textsuperscript{2}Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

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The thermalization phenomenon and many-body quantum statistical properties are studied on the example of several observables in isolated spin-chain systems, both integrable and generic non-integrable ones. While diagonal matrix elements for non-integrable models comply with the eigenstate thermalization hypothesis (ETH), the integrable systems show evident deviations and similarity to properties of noninteracting many-fermion models. The finite-size scaling reveals that the crossover between two regimes is given by a scale closely related to the scattering length. Low-frequency off-diagonal matrix elements related to d.c. transport quantities in a generic system also follow the behavior analogous to the ETH, however unrelated to the one of diagonal elements.

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Many-body quantum (MBQ) systems and models have been extensively studied in the last decades in connection with novel materials, offering a fresh view on the fundamentals and the interpretation of statistical mechanics. The systematic analysis of the phenomena of thermalization and the limitations of a statistical treatment within isolated MBQ systems have been recently motivated by experiments on cold atoms in optical lattices, revealing very slow relaxation to thermal equilibrium [1, 2], but as well by prototype integrable MBQ systems as the one-dimensional Heisenberg model realized in real materials [3].

Specific for lattice MBQ systems discussed in the above connection is (in contrast to single-body quantum systems) the exponential growth of the Hilbert space and the number of eigenstates $N_L$ with the lattice size $L$. Here, one of the fundamental questions is to what extent even a single eigenstate or a single chosen initial wave-function could be the representative of the canonical ensemble average within the given system, both for static and dynamical quantities. For generic MBQ systems one of the central statements is the eigenstate thermalization hypothesis (ETH) [4, 5] that for a few-body observable $A$ diagonal matrix elements (ME) $A_{\alpha\alpha}$ at a given energy show only exponentially (in $L$) small deviations from the average, being a smooth function of the energy only. Since at the same time the off-diagonal ME are as well exponentially small, the time-average of the observable is determined by diagonal terms only. Therefore for any initial wave-function $|\psi_0\rangle$ with a small energy uncertainty the long-time average is also equal to the thermal average, this being the general condition for the quantum thermalization process [6]. We note that such a hypothesis is also underlying some numerical methods for the calculation of finite-temperature properties, in particular the microcanonical Lanczos method (MCLM) [7, 8] for $T > 0$ static and dynamical properties of MBQ lattice systems. It seems also evident that the ETH is intimately related to general properties of eigenenergy spectra, i.e. level statistics and dynamics in generic MBQ systems, which reveal Wigner-Dyson level statistics with the origin in level repulsion and analogy to random matrix spectra [9, 10].

The deviations from the ETH and normal thermalization have been detected is several directions. The hypothesis is not obeyed in integrable MBQ systems [6, 11–14], although some observables can still thermalize, i.e., approach the equilibrium (canonical ensemble average) value, in particular if the Gibbs statistical ensemble is generalized to include all local conserved quantities in this case [11, 14]. The thermalization can become very slow and the validity of ETH can become restricted if an initial state is far from equilibrium [12, 15–17] as relevant for sudden quenches in cold-atom systems. The latter question is intimately related to the deviation from integrability [13] and the size of isolated MBQ systems [6, 15, 17]. On the other hand, the ETH does not resolve the question of the relation to off-diagonal ME (even in generic non-integrable systems) which are, e.g., relevant for transport properties and dissipation in the d.c. limit [18–20].

In this Letter we study the validity of the ETH and thermalization within a quantum spin-chain system in one dimension (1D), i.e., the antiferromagnetic and anisotropic $S = 1/2$ Heisenberg model (AHM), including integrable (I) and non-integrable (NI) cases. While we confirm in the generic NI case the ETH for diagonal ME of several local observables, we find large deviations and fluctuations for the I case. In particular, we show that the spread of diagonal ME can be qualitatively and even quantitatively understood from the XX model equivalent to the model of noninteracting fermions. With the aim to resolve the problem of the breakdown of the ETH in finite systems we perform the finite-size scaling in NI systems revealing that the crossover from the I regime to the ETH-consistent behavior is determined by a single scale $L_\ast$, coinciding with the transport scattering length. Another finding is that the low-frequency off-diagonal and diagonal ME are not universally related even in NI systems, hence the ETH does not directly address the low-$\omega$ dynamics and the d.c. transport quantities, and the generalization of the ETH is necessary.

As the prototype model we study in the following the anisotropic $S = 1/2$ Heisenberg model on a chain with $L$ sites and periodic boundary conditions,

$$H = J \sum_{i} \left( S_i^x S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z + \Delta_2 S_i^z S_{i+2}^z \right),$$

(1)
where $S^\alpha_i$ ($\alpha = x, y, z$) are spin $S = 1/2$ operators at site $i$ and $\Delta$ represents the anisotropy. The nearest-neighbor XXZ model is an integrable one and we introduce the next-nearest-neighbor $z$-interaction with $\Delta_2 \neq 0$ in order to break its integrability. It should be reminded that the Hamiltonian (1) can be mapped on a $t$-$V$-$W$ model of interacting spinless fermions. A consequence of the integrability at $\Delta_2 = 0$ is the existence of a macroscopic number of conserved local quantities and operators $Q_n, n = 1 - L$ commuting with the Hamiltonian, $[Q_n, H] = 0$. For the 1D AHM a nontrivial example is $Q_3 = J^2$ representing the energy current and leading directly to its non-decaying behavior [21, 22] and dissipationless thermal conductivity [3].

In order to study eigenstate and ME properties of the AHM we choose some simple local (but $q = 0$) quantities involving only few sites. Evident candidates are nontrivial quantities involving $n = 2$ sites, where we consider the “kinetic” energy $H_{\text{kin}}$ containing the first two terms in Eq. (1) and the spin current $J^s$, while for a representative of $n = 3$ operators we consider the energy-current $J^E$ (not including the $\Delta_2$ term),

$$J^s = J \sum_i (S^x_i S^y_{i+1} - S^y_i S^x_{i+1}),$$

$$J^E = J^2 \sum_i [(S^y_i S^y_{i+2} - S^y_i S^y_{i-2}) S^x_{i+1}
- \Delta(S^x_i S^y_{i+1} - S^y_i S^x_{i+1})(S^x_{i-1} + S^x_{i+2})].$$

The choice is motivated by different properties of the considered operators. While $J^E$ is a strictly conserved quantity for the I case, $J^s$ is not, but still leads to dissipationless (non-decaying) spin transport. Both are current operators with ME distributed around the ensemble average $\langle J_{nm}^{s,E} \rangle = 0$. On the other hand, $H_{\text{kin}}$ has not such a specific property. In the following we present results reachable via the exact diagonalization of the model, Eq. (1), on chains up to $L = 20$. The total spin $S_{\text{tot}} = M$ is fixed to $M = -1$ (in order to avoid “particle-hole” symmetry) while we consider both, the representative sector with wavevector $k = 2\pi/L$ and the whole $k$-average as well.

First, we present results for the distribution of diagonal ME, i.e., $J_{nn}^{s}, J_{nn}^{E}$, and $H_{\text{kin}}^{\text{nn}}$ as they arise varying eigenenergies $E = E_n$. In Fig. 1 we show corresponding 2D plots obtained within the gapless regime ($\Delta = 0.5$) and for the magnetization $M = -1$ (due to “particle-hole” symmetry $J_{nn}^{s,E}$ vanishes at $M = 0$). Figure 1 reveals an evident difference between the NI example with $\Delta_2 = 0.5$ and the I case with $\Delta_2 = 0$. All quantities show for the NI example a narrow distribution around the average $\langle J_{nn}^{s,E} \rangle = \langle A_{nn} \rangle (E)$ with the width $(\sigma_{A}^2(E)) = (\langle A_{nn}^2 \rangle - \langle A_{nn} \rangle^2)$. On the system size $L$.

On contrary, for the I case distributions are much wider with a weaker size dependence, clearly not obeying the ETH. The distribution for $J^s$ and $J^E$ is intimately related to the anomalous $T > 0$ spin and energy-current stiffness (without degeneracies), respectively, for the I model [18, 19, 22],

$$D_{nn}^{s,E}(T) = \frac{\tilde{\beta}_s^{s,E}}{L^2} \sum_n e^{-\beta E_n} |J_{nn}^{s,E}|^2,$$

where $\tilde{\beta}_s = \beta, \tilde{\beta}_E = \beta^2$ with $\beta = 1/T$. It is evident that the existence of $D_{nn}^{s,E}(T > 0) > 0$ implies that currents as $J^{s,E}$ do not thermalize to their thermal average $\langle J^{s,E} \rangle = 0$. In particular, their correlation functions do not decay to zero, $\langle J^{s,E}(t \rightarrow \infty) J^{s,E}(0) \rangle \neq 0$, and their time evolution depends crucially on the ensemble of initial states. The same appears to be the case for $H_{\text{kin}}^\text{nn}$ although a physical interpretation is less familiar. With values of $D_{nn}^{s,E}(T)$ known from the Bethe Ansatz [21], and moreover for the energy-current stiffness $D_{nn}^{E}(T \rightarrow \infty)$ obtained easily via the high-$T$ expansion, one can evaluate the distribution widths $\sigma_{E}^s(E) \propto \sqrt{L}$.

Since analogous quantities to stiffness are not known in general, one can use in the gapless regime $(\Delta < 1)$ as a semi-quantitative guide results for the $\Delta = 0$ XX model. The latter can be mapped to the model of non-interacting fermions, $H = \sum_k \epsilon_k n_k$, $\epsilon_k = J \cos k$, being trivially integrable with all $n_k = 0, 1$ as constants of motion, with corresponding currents $J^{s,E}_k = \sum_k (1, \epsilon_k) v_k n_k$. The calculation of $\sigma_{E}^s(E)$ at fixed magnetization $M = \sum_k (n_k - 1/2)$ averaged over energies $E$ is for $L \rightarrow \infty$ equivalent to the grand-canonical averaging in the limit $\beta \rightarrow 0$ yielding for the unpolarized case $N = L/2$: $\sigma_{E}^s = J^2 \sqrt{L}/\sqrt{8}$ and $\sigma_{E}^s = J^2 \sqrt{L}/\sqrt{2}$. On the other hand, instead of $H_{\text{kin}}$ (being within the XY limit equal to $H$) one can treat in an analogous way the complementary potential term $H_{\Delta}$ with the result $\sigma_{E}^s = J \Delta \sqrt{L}/4$ [23]. We note that the above estimates for the widths $\sigma_{E}^s$ represent well the numerical results in Fig. 1 for the I case with $\Delta > 0$.

Next we investigate the crossover from an I to a NI system obeying the ETH. In a finite system fluctuations $\sigma_{E}^s = \sqrt{D_{nn}^{s,E}(T \rightarrow \infty)}$ are $\propto \sqrt{L}$ as well, and the stiffness $\sigma_{E}^s(E)$ is exponentially large at $E \approx E_n$.
\[ \sigma_d^2 / \sqrt{L} \] with \( \alpha = (s, E, \text{kin}) \) are expected to decrease by introducing the NI perturbation \( \Delta_2 \neq 0 \). In Fig. 2 we present corresponding results obtained for different \( \Delta_2 = 0 - 0.5 \) and sizes \( L = 8 - 20 \). In order to reduce the influence of the energy window, we evaluate the fluctuations \( \sigma_d^2 \) in the range \( E = [-1, 1] \) and average over all \( k \)-sectors. For the I case \( \Delta_2 = 0 \) the \( 1/L \)-scaling indicates finite values \( \sigma_d^2 \) (\( L \to \infty \)). This coincides with the well-defined and nontrivial sum rule \( D^E(T \to \infty) / \beta^E \) and \( \sigma_d^2 \) can be related to the high-\( T \) sum rule \( (\sigma_{d^2})^2 = (1 + 2\Delta^2) / 32 \) [21]. This is, however, not the case for the NI case \( \Delta_2 \neq 0 \). Here, there is an evident decrease with \( L \) and crossover to an exponential decrease with \( L \), i.e., ETH-consistent behavior above the crossover scale \( L > L^* \). \( L^* \) crucially depends on the perturbation strength \( \Delta_2 \) but apparently is quite universal for all quantities, at least for those considered here.

In the case of currents the “thermalization length” \( L^* \) may be plausibly interpreted in terms of the transport mean free path. The latter can be determined by a standard hydrodynamic relation, \( 1/(q^2D) \gg 1/\gamma \) [24], involving the diffusion constant \( D \) and the current scattering rate \( \gamma \). Identifying the mean free path as \( L^* = \pi / q \) then yields

\[ L^* = \pi \sqrt{D/\gamma}. \]  \hspace{1cm} (4)

In the case of the spin current, using for \( \Delta = \Delta_2 = 0.5 \) the known quantitative values \( D^s = 2.1 \) and \( \gamma^s = 0.23 \) at \( \beta \to 0 \) [20], one finds \( L^* \approx 10 \). This value turns out to agree well with the scale observed in the inset of Fig. 2. Moreover, \( \gamma^s \to 0 \) as \( \Delta_2 \to 0 \) is consistent with a diverging \( L^* \).

Finally, let us address the relation between off-diagonal and diagonal ME. Since for the I system the behavior can be very singular [20], we concentrate on the generic NI cases satisfying the ETH. In Fig. 3 we present the probability distribution of off-diagonal ME Re \( J_{nm} \) and Re \( H_{nm} \), evaluated for \( \Delta = 0.5 \) and \( \Delta_2 = 0.5 \) in the energy window \( E = [-\delta E/2, \delta E/2] \) with various \( \delta E \). Resulting distributions do clearly not depend on \( \delta E \) and appear to be Gaussian with the width \( \sigma_{ad}^2 \), again in analogy to ETH exponentially decreasing with \( L \). It is a nontrivial observation that both off-diagonal and diagonal ME follow the same scaling with \( L \), as shown in the inset of Fig. 4. It is therefore important and well defined to investigate the ratio of off-diagonal and diagonal ME fluctuations

\[ r^\alpha (E) = \sigma_{ad}^2 (E) / \sigma_{ad}^2 (E). \]  \hspace{1cm} (5)

Results for the spin and energy current are presented in Fig. 4, shown vs. \( E \) for \( \Delta_2 = 0.5 \) and \( \Delta = 0.5, 1.0 \). They indicate that \( r^\alpha (E) \) is not universal (depends on \( \alpha \) and model parameters) and smoothly varies with \( E \), but most important is the independence of \( L \). We can conclude that for the cases considered here \( r^\alpha \) are quite far from the predictions of the random-matrix theory [9, 19] implying generally \( r = 2 \). On the other hand, the ratio still remains within an order of magnitude in contrast to the I case where in the gapless regime the...
ratio appears to vanish leaving finite only diagonal ME [20].

The above observation becomes relevant in the evaluation of d.c. transport quantities, which are within linear response theory related to the low-ω absorption [29], e.g., the spin conductivity (diffusivity) and thermal conductivity, respectively, are in analogy to Eq. (3),

$$C^\alpha(\omega) = \frac{\tilde{\beta}^{3/2} \rho}{LZ} \sum_{m \neq n} e^{-\beta E_n} |J_{mn}^{\alpha}|^2 \delta(\omega - E_m + E_n),$$

where the d.c. limit should be considered as $C^\alpha_0 = C^\alpha(\omega \to 0)$ and can be expressed as

$$C^\alpha_0 = \frac{\tilde{\beta}^{3/2} \rho}{Z} \int e^{-\beta E} \rho(E) |\tilde{\sigma}_d^\alpha(E)|^2 dE,$$

where $\rho(E)$ is the MBQ density of states. From our analysis it follows that in general $\tilde{\sigma}_d^\alpha(E)$ cannot be represented by diagonal $\tilde{\sigma}_d^\alpha(E)$, although the qualitative behavior appears closely related. Note that for the case of $J^s$ diagonal ME can be also expressed as the sensitivity of many-body levels to a fictitious flux $\phi$ (or boundary conditions), i.e. $J_{mn}^s \propto \partial E_n / \partial \phi$, and the latter relation has been previously employed to evaluate the d.c. transport in, e.g., disordered systems [54].

Let us in conclusion summarize our results, which appear to be generic beyond spin-chain systems. The behavior of the considered NI systems we find consistent with the ETH for all considered quantities. If we consider the time evolution of an observable, it can be in terms of (finite-system) eigenstates represented as

$$\bar{A}(t) = \langle \Psi(t) | A | \Psi(t) \rangle = \sum_n c_n^2 A_{nn} + \sum_{n \neq m} r_n^m c_m e^{i(E_n - E_m)t} A_{nm}.$$

In a system obeying ETH, the off-diagonal contribution vanishes for long times $t \to \infty$, due to the exponential smallness of off-diagonal ME as well due to dephasing [6]. If the initial state $|\Psi_0\rangle$ is a microcanonical one with a narrow distribution $\delta E$ [with $(\delta E)^2 = \sum_n |c_n|^2 (E_n - \bar{E})^2$], and due to ETH $A_{nn} \sim \langle A \rangle(\bar{E})$, the first term leads to the microcanonical average $\bar{A}(t) = \langle A \rangle(\bar{E})$ in a large system coinciding with the canonical thermodynamical average at a finite $T > 0$, where $E(T) = \bar{E}$. Such a scenario is then consistent with the “normal” quantum thermalization.

In an IS spin chain the distribution of diagonal ME is large, the long-time average [still neglecting off-diagonal terms in Eq. (8)] in general depends on $|\Psi_0\rangle$ and corresponding $c_n$, even for a small energy uncertainty $\delta E$. In order to satisfy $\bar{A}(t \to \infty) = \langle A \rangle$ one needs assumptions on the distribution of coefficients $c_n$, E.g., in a large enough system randomly chosen $c_n$ would plausibly be adequate. In fact, the numerical MCLM method for the evaluation of $T > 0$ properties [7, 8], based on the microcanonical states and the Lanczos procedure, contains such a choice achieved by random sampling. Hence, a random microcanonical state in a large MBQ system would mostly obey the thermalization process. Still, this is not at all the case for particular states as, e.g., reached by (strong) quenching in an IS system, but as well not in a generic system [13, 17] since the initial state after the quench is not necessarily the microcanonical one with small $\delta E$.

Analyzing the extent of the validity of the ETH and thermalization in a finite-size MBQ system, we find effectively that perturbed IS systems beyond the crossover length $L^* \approx 4$ behave as generic NI ones. Since in a “normal” spin system only total spin and energy are conserved, one can design two relevant diffusion scales and plausibly the largest would determine $L^*$, which then appears to dominate the scaling of all quantities, as shown in Fig. 3. The understanding and the determination of $L^*$ is evidently an important theoretical goal, relevant also for experiments dealing with systems close to integrability [3, 27].

The ETH addresses thermalization and statistical description of static quantities in MBQ systems, with the behavior determined by diagonal ME. On the other hand, d.c. transport quantities and low-ω dynamics involve only off-diagonal ME. We note that in a generic system, properties analogous to the ETH can be defined for off-diagonal ME close in energy, in particular obeying the Gaussian distribution and exponential dependence on size. Also, the relation between diagonal and off-diagonal ME is independent of size $L$, but still the ratio is not universal. In this sense, our results show that for such considerations the generalization of the ETH is needed but also is straightforward, and it can include the response to weak external fields and dissipation phenomena in MBQ systems.

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