Eigenstate thermalization within isolated spin-chain systems

R. Steinigeweg,[1] J. Herbrych,[1] and P. Prelovšek[1,2]
[1] *J. Stefan Institute, SI-1000 Ljubljana, Slovenia*
[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 nonintegrable. While diagonal matrix elements for nonintegrable models comply with the eigenstate thermalization hypothesis, the integrable systems show evident deviations and similarity to properties of noninteracting many-fermion models. The finite-size scaling reveals that the crossover between the two regimes is given by a scale closely related to the scattering length. Low-frequency off-diagonal matrix elements related to dc transport quantities also follow in a generic system a behavior analogous to the eigenstate thermalization hypothesis, however, unrelated to one of the diagonal matrix elements.

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I. INTRODUCTION

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

Specific for lattice many-body quantum 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 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, for both static and dynamical quantities. For generic many-body quantum systems, one of the central statements is the eigenstate thermalization hypothesis (ETH) [4,5], whereby, for a few-body observable A, diagonal matrix elements A_{nn} 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 matrix elements are as well exponentially small, the time average of the observable is determined by diagonal terms only. Therefore, for any initial wave function 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 [7,8] for $T > 0$ static and dynamical properties of lattice many-body quantum 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 many-body quantum 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 in several directions. The hypothesis is not obeyed in integrable many-body quantum 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 many-body quantum systems [6,15,17]. On the other hand, the ETH does not resolve the question of the relation to off-diagonal matrix elements (even in generic nonintegrable systems) which are, e.g., relevant for transport properties and dissipation in the dc limit [18–20].

In this paper we study the validity of the ETH and thermalization within a quantum spin-chain system in one dimension, i.e., the antiferromagnetic and anisotropic $S = 1/2$ Heisenberg model, including integrable and nonintegrable cases. While we confirm in the generic nonintegrable case the ETH for diagonal matrix elements of several local observables, we find large deviations and fluctuations for the integrable case. In particular, we show that the spread of diagonal matrix elements can be qualitatively and even quantitatively understood from 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 nonintegrable systems, revealing that the crossover from the integrable regime to the ETH-consistent behavior is determined by a single scale L^*, coinciding with a transport scattering length. Another finding is that the off-diagonal matrix elements at low frequency (small difference of corresponding eigenenergies) and diagonal matrix elements are not universally related even in nonintegrable systems; hence, the ETH does not directly address the low-frequency dynamics and the dc transport quantities, and the generalization of the ETH is necessary.

The paper is organized as follows: In Sec. II we introduce the model and the considered observables, i.e., "kinetic" energy, spin current, and energy current. In Sec. III we analyze the distribution of diagonal matrix elements for integrable and nonintegrable cases. We particularly present a systematic analysis of the distribution widths as a function of system size and observe in the nonintegrable cases a crossover to ETH-consistent behavior at a certain length scale, which we connect quantitatively to a transport mean free path. Section IV is devoted to the relation between off-diagonal and diagonal matrix elements as well as the impact of this relation on low-frequency dynamics and dc transport quantities. In Sec. V we finally summarize our results.

II. MODEL AND OBSERVABLES

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,

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

where S_i^α ($\alpha = x,y,z$) are spin $S = 1/2$ operators at site i and Δ represents the anisotropy. The nearest-neighbor model is an integrable one and we introduce the next-nearest-neighbor zz interaction with $\Delta_2 \neq 0$ in order to break its integrability. It should be noted that via the Jordan-Wigner transformation [21] the Hamiltonian (1) can be mapped on the t-V-W model of interacting spinless fermions with the hopping $t = J/2$, the nearest-neighbor interaction $V = J\Delta$, and the next-nearest-neighbor interaction $W = J\Delta_2$. A consequence of the integrability at $\Delta_2 = 0$ is the existence of a macroscopic number of conserved local quantities and operators $Q_n, n = 1,\dots,L$ commuting with the Hamiltonian, $[Q_n, H] = 0$. A nontrivial example is $Q_3 = J^E$ representing the energy current and leading directly to its nondecaying behavior [22,23] and dissipationless thermal conductivity [3].

In order to study matrix elements properties, we choose some simple local operators involving only few neighboring sites, however, being still a sum over the whole chain. Evident candidates are nontrivial quantities involving $n = 2$ sites, where we consider the "kinetic" energy

$$H^{\mathrm{kin}} = J \sum_{i=1}^{L} \big(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \big), \tag{2}$$

containing the first two terms in Eq. (1), as well as the spin current

$$J^s = J \sum_{i=1}^{L} \big(S_i^x S_{i+1}^y - S_i^y S_{i+1}^x \big). \tag{3}$$

For a representative of $n = 3$ operators we consider the energy current

$$J^E = J^2 \sum_{i=1}^{L} \big[\big(S_i^x S_{i+2}^y - S_i^y S_{i+2}^x \big) S_{i+1}^z - \Delta \big(S_i^x S_{i+1}^y - S_i^y S_{i+1}^x \big)\big(S_{i-1}^z + S_{i+2}^z \big) \big], \tag{4}$$

not including the Δ_2 term. The choice is motivated by different properties of the considered operators. While J^E is a strictly conserved quantity for the integrable case, J^s is not, but still leads to dissipationless (nondecaying) spin transport. Both are current operators with matrix elements distributed around the ensemble average $\langle J_{nm}^{s,E} \rangle = 0$. On the other hand, H^{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 $S_{\mathrm{tot}}^z = M$ is fixed to $M = -1$ (in order to avoid "particle-hole" symmetry) while we consider both the representative sector with wave vector $k = 2\pi/L$ and the whole k average as well.

III. DISTRIBUTION OF DIAGONAL MATRIX ELEMENTS

First, we present results for the distribution of diagonal matrix elements, i.e., J_{nn}^s, J_{nn}^E, and H_{nn}^{kin}, 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 vanishes at $M = 0$). Figure 1 reveals an evident difference between the nonintegrable example with $\Delta_2 = 0.5$ and the integrable case with $\Delta_2 = 0$. All quantities show for the nonintegrable example a narrow distribution around the average $\langle A_{nn}(E) \rangle$ with the (diagonal) width

$$\big(\sigma_{\mathrm{d}}^A\big)^2(E) = \langle A_{nn}(E)^2 \rangle - \langle A_{nn}(E) \rangle^2 \tag{5}$$

exponentially dependent on the system size L [6], as later demonstrated in detail.

On contrary, for the integrable 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 (Drude weight) for the integrable model [18,19,23], being within linear response the ballistic contribution to spin and energy

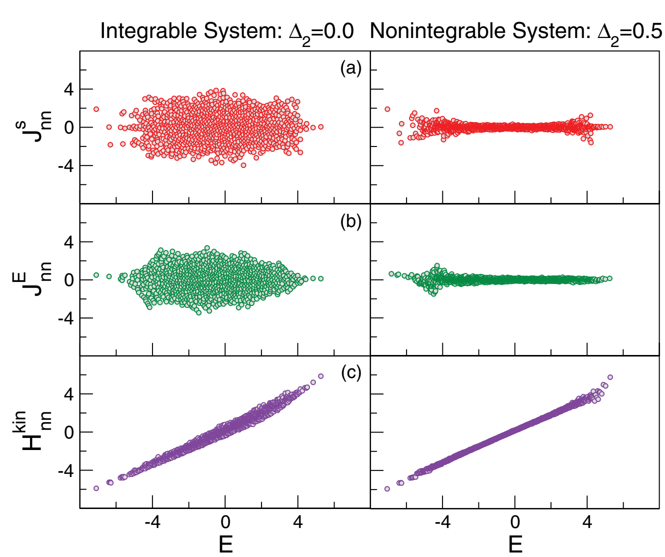

FIG. 1. (Color online) Distribution of diagonal matrix elements of (a) spin current J^s, (b) energy current J^E, and (c) kinetic energy H^{kin} vs energy E for the integrable model $\Delta_2 = 0$ (left-hand side) and the nonintegrable model $\Delta_2 = 0.5$ (right-hand side). In all cases, $\Delta = 0.5$, $L = 20$, $M = -1$, and $k = 2\pi/L$.

conductivity,

$$D^{s,E}(T) = \frac{\tilde{\beta}^{s,E}}{LZ} \sum_n \mathrm{e}^{-\beta E_n} \left| J^{s,E}_{nn} \right|^2, \tag{6}$$

where $\tilde{\beta}^s = \beta, \tilde{\beta}^E = \beta^2$ with $\beta = 1/T$. It is evident that the existence of $D^{s,E}(T > 0) > 0$ 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, $\langle J^{s,E}(t \to \infty) J^{s,E} \rangle \neq 0$, and their time evolution depends crucially on the ensemble of initial states. The same appears to be the case for H^{kin}, although a physical interpretation is less familiar. With values of $D^{s,E}(T)$ known from the Bethe ansatz [22], and, moreover, for the energy-current stiffness $D^E(T \to \infty)$ obtained easily via the high-T expansion, one can evaluate the distribution widths $\sigma_{\mathrm{d}}^{s,E}(E) \propto \sqrt{L}$.

Since analogous quantities to stiffness are not known in general, one can use results for the $\Delta = 0$ model in the gapless regime ($\Delta < 1$) as a semiquantitative guide. The latter can be mapped to the model of noninteracting fermions,

$$H = \sum_k \epsilon_k n_k, \quad \epsilon_k = J \cos k, \tag{7}$$

being trivially integrable with all $n_k = 0,1$ as constants of motion, with corresponding currents

$$J^s = \sum_k \frac{\partial \epsilon_k}{\partial k} n_k, \quad J^E = \sum_k \epsilon_k \frac{\partial \epsilon_k}{\partial k} n_k. \tag{8}$$

The calculation of $\sigma_{\mathrm{d}}^{s,E}(E)$ at fixed magnetization $M = \sum_k (n_k - 1/2)$ averaged over energies E is for $L \to \infty$ equivalent to the grand-canonical averaging in the limit $\beta \to 0$, yielding, for the unpolarized case, $N = L/2$: $\sigma_{\mathrm{d}}^s = J\sqrt{L}/\sqrt{8}$ and $\sigma_{\mathrm{d}}^E = J^2\sqrt{L}/\sqrt{32}$. On the other hand, instead of H^{kin} (being within the $\Delta = 0$ limit equal to H), one can treat in an analogous way the complementary potential term H^Δ with the result $\sigma_{\mathrm{d}}^\Delta = J\Delta\sqrt{L}/4$ [24]. We note that the above estimates for the widths $\sigma_{\mathrm{d}}^\alpha$ represent well the numerical results in Fig. 1 for the integrable case with $\Delta > 0$.

Next we investigate the crossover from an integrable to a nonintegrable system obeying the ETH. In a finite system, fluctuations $\tilde{\sigma}_{\mathrm{d}}^\alpha = \sigma_{\mathrm{d}}^\alpha/\sqrt{L}$ with $\alpha = (s,E,\mathrm{kin})$ are expected to decrease by introducing the nonintegrable perturbation $\Delta_2 \neq 0$. In Fig. 2 we present corresponding results obtained for different $\Delta_2 = 0,\ldots,0.5$ and sizes $L = 8,\ldots,20$. In order to reduce the influence of the energy window, we evaluate the fluctuations $\sigma_{\mathrm{d}}^\alpha$ in the range $E = [-1,1]$ and average over all k sectors. For the integrable case $\Delta_2 = 0$ the $1/L$-scaling indicates finite values $\tilde{\sigma}_{\mathrm{d}}^\alpha(L \to \infty)$. This coincides with the well-defined and nontrivial $D^{s,E}(T \to \infty)$. In particular, $D^E(T \to \infty)/\tilde{\beta}^{s,E}$ and $\tilde{\sigma}_{\mathrm{d}}^E$ can be related to the high-T sum rule $(\tilde{\sigma}_{\mathrm{d}}^E)^2 = (1 + 2\Delta^2)/32$ [22]. This is, however, not the case for the nonintegrable 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 Δ_2 but apparently is roughly the same for all considered quantities.

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, $1/(q^2\mathcal{D}) \gg 1/\gamma$ [25], involving the diffusion constant $\mathcal{D}$ and the current scattering rate γ. Identifying the mean free path as $L^* \approx \pi/q$ then yields

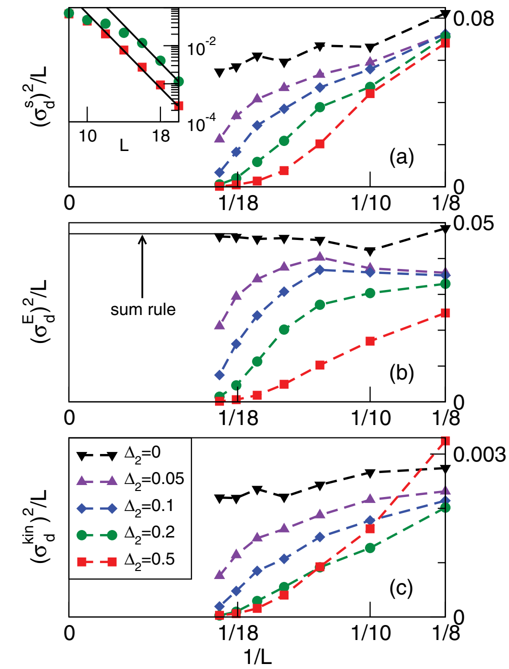

FIG. 2. (Color online) Finite-size dependence of the diagonal matrix elements fluctuations of J^s, J^E, and H^{kin}, respectively, for $\Delta = 0.5$, $M = -1$, and different Δ_2. Fluctuations are evaluated within $E = [-1,1]$. In (b) the exact sum rule is indicated (solid line). Inset in (a): Curves for $\Delta_2 = 0.2$ and 0.5, illustrating the onset of an exponential decrease with L.

$$L^* \approx \pi \sqrt{\frac{\mathcal{D}}{\gamma}}. \tag{9}$$

For instance, in the case of the spin current, using for $\Delta = 0.5$ and $\Delta_2 = 0.2[0.5]$ the known quantitative values [20] $\mathcal{D}^s = 2.1[3.6]$ and $\gamma^s = 0.23[0.13]$ at $\beta \to 0$, one finds $L^* \approx 10[16]$. 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^*.

IV. RELATION BETWEEN OFF-DIAGONAL AND DIAGONAL MATRIX ELEMENTS

Finally, let us address the relation between off-diagonal and diagonal matrix elements. Since for the integrable system the behavior can be very singular [20], we concentrate on the generic nonintegrable cases satisfying the ETH. In Fig. 3 we present the probability distribution of off-diagonal matrix elements, e.g., $\mathrm{Re}J^{s,E}_{nm}$ and $\mathrm{Re}H^{\mathrm{kin}}_{nm}$, evaluated for $\Delta = 0.5$, $\Delta_2 = 0.5$ in the energy window $E_n, E_m = [-\delta E/2, \delta E/2]$ with various $\delta E \ll J$. Using a small δE respects the topology of a banded random matrix [26] with a band width on the order of the exchange coupling constant J. Resulting distributions do clearly not depend on δE and appear to be Gaussian with zero mean.

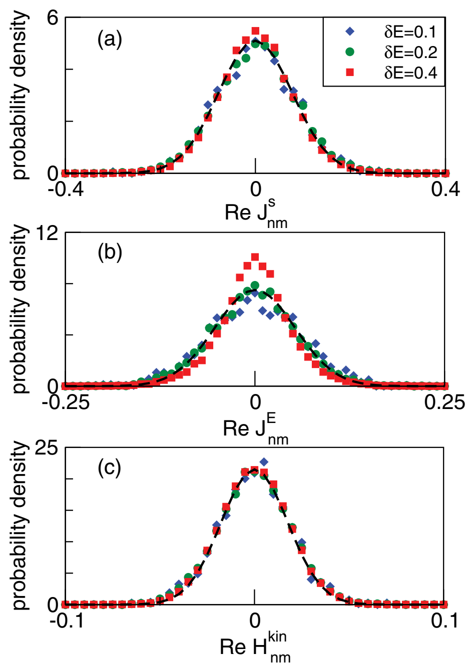

FIG. 3. (Color online) Probability distribution for the real part of the off-diagonal matrix elements of J^s, J^E, and H^{kin}, respectively, for a nonintegrable model with $\Delta = \Delta_2 = 0.5$, $L = 18$, and $M = -1$. For comparison, Gaussian functions are indicated (dashed curves).

It is a nontrivial question whether the fluctuations of off-diagonal and diagonal matrix elements follow the same scaling with L. It is, therefore, important to investigate the ratio of off-diagonal and diagonal matrix elements fluctuations,

$$r^\alpha(E) = \frac{(\sigma_{\mathrm{od}}^\alpha)^2(E)}{(\sigma_{\mathrm{d}}^\alpha)^2(E)}, \quad (\sigma_{\mathrm{od}})^2(E) = \langle |A_{mn}(E)|^2 \rangle. \tag{10}$$

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 α and model

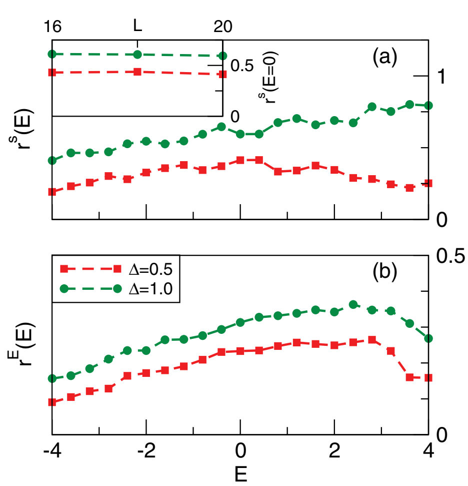

FIG. 4. (Color online) Ratio between off-diagonal and diagonal matrix elements fluctuations for J^s and J^E, respectively, for a nonintegrable model with $\Delta = 0.5, 1$, $\Delta_2 = 0.5$, $L = 20$, $M = -1$, and k average. Inset in (a): Finite-size dependence of $r^s(E = 0)$.

parameters) and smoothly varies with E, but, most importantly, is the independence of L. We can conclude that for the cases considered here r^α are not following relations within the random-matrix theory [9,19] implying generally $r = 1/2$ for the Gaussian orthogonal ensemble (and $r = 1$ for the Gaussian unitary ensemble). On the other hand, the ratio still remains within an order of magnitude, in contrast to the integrable case where, in the gapless regime, the ratio appears to vanish, leaving finite only diagonal matrix elements [20].

The above observation becomes relevant in the evaluation of dc transport quantities, which are within linear response theory related to the low-ω absorption [27], e.g., the spin conductivity (diffusivity) and thermal conductivity, respectively, are in analogy to Eq. (6),

$$C^\alpha(\omega) = \frac{\tilde{\beta}^\alpha \pi}{LZ} \sum_{m \neq n} \mathrm{e}^{-\beta E_n} \left| J_{mn}^\alpha \right|^2 \delta(\omega - E_m + E_n), \tag{11}$$

where the dc limit should be considered as $C_0^\alpha = C^\alpha(\omega \to 0)$ and can be expressed as

$$C_0^\alpha = \frac{\tilde{\beta}^\alpha \pi}{Z} \int e^{-\beta E} \rho^2(E) \left(\tilde{\sigma}_{\mathrm{od}}^\alpha\right)^2(E) dE, \tag{12}$$

where $\rho(E)$ is the many-body quantum density of states. From our analysis it follows that, in general, $\tilde{\sigma}_{\mathrm{od}}^\alpha(E)$ cannot be represented by diagonal $\tilde{\sigma}_{\mathrm{d}}^\alpha(E)$, although the qualitative behavior appears closely related [and even quantitative for C_0^s as evident from Fig. 4(a)]. Note that for the case of J^s diagonal matrix elements can be also expressed as the sensitivity of many-body levels to a fictitious flux ϕ (or boundary conditions), i.e., $J_{nn}^s \propto \partial E_n / \partial \phi$, and the latter relation has been previously employed to evaluate the dc transport in, e.g., disordered systems [10,28].

V. CONCLUSIONS

Let us, in conclusion, summarize our results, which may be generic beyond spin-chain systems. We find the behavior of the considered nonintegrable systems 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

$$\begin{aligned} A(t) = \langle \Psi(t)|A|\Psi(t)\rangle &= \sum_n |c_n|^2 A_{nn} \\ &+ \sum_{n \neq m} c_n^* c_m \mathrm{e}^{\iota(E_n - E_m)t} A_{nm}. \end{aligned} \tag{13}$$

In a system obeying ETH, the off-diagonal contribution vanishes for long times $t \to \infty$, due to the exponential smallness of off-diagonal matrix elements (compare insets of Fig. 2 and Fig. 4) as well due to dephasing [6]. If the initial state $|\Psi_0\rangle$ is a microcanonical one with a narrow distribution δE [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 $A(t) = \langle A \rangle(\bar{E})$ 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 integrable spin chain the distribution of diagonal matrix elements is large, the long-time average [still neglecting off-diagonal terms in Eq. (13)] in general depends on $|\Psi_0\rangle$ and corresponding c_n, even for a small energy uncertainty δE. In order to satisfy $A(t \to \infty) = \langle A\rangle$ one needs assumptions on the distribution of coefficients c_n. For example, in a large-enough system randomly chosen c_n would plausibly be adequate. In fact, the microcanonical Lanczos 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 many-body quantum 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 integrable 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 δE.

Analyzing the extent of the validity of the ETH and thermalization in a finite-size many-body quantum system, we find effectively that perturbed integrable systems beyond the crossover length L^* behave as generic nonintegrable 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 [3,29].

The ETH addresses thermalization and statistical description of static quantities in many-body quantum systems, with the behavior determined by diagonal matrix elements . On the other hand, dc transport quantities and low-ω dynamics involve only off-diagonal matrix elements. We note that in a generic system, properties analogous to the ETH can be defined for off-diagonal matrix elements close in energy, in particular obeying the Gaussian distribution and exponential dependence on size. Also, the relation between diagonal and off-diagonal matrix elements 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 many-body quantum systems.

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