Does thermalization occur in an isolated system after a global quantum quench?

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We consider the question of thermalization for isolated quantum systems after a sudden parameter change, a so-called quantum quench. In particular we investigate the pre-requisites for thermalization focusing on the statistical properties of the time-averaged density matrix and of the expectation values of observables in the final eigenstates. We find that eigenstates, which are rare compared to the typical ones sampled by the micro-canonical distribution, are responsible for the absence of thermalization of some infinite integrable models and play an important role for some finite size non-integrable systems, such as the Bose-Hubbard model. We stress the importance of finite size effects for the thermalization of isolated quantum systems and propose a condition, relying on the Kullback-Leibler entropy, to obtain thermalization.

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The microscopic description of many particle systems is very involved. In many situations, in particular at equilibrium, one can rely on statistical ensembles that provide a framework to compute time-averaged observables and obtain general results like fluctuation-dissipation relations. The use of statistical ensembles relies on the hypothesis that on long timescales physical systems thermalize. In the context of classical statistical physics a very good understanding of the issue of thermalization was reached in the last century [1]: under certain chaoticity conditions, an isolated system thermalizes at long times within the micro-canonical ensemble. Furthermore, a large single portion of a (much larger) isolated system thermalizes within the grand-canonical ensemble.

Instead for quantum systems, it is fair to state that the comprehension of thermalization and its pre-requisites are still open problems [2, 3], except for important results obtained in the semi-classical limit [4, 6] or under the assumption of the coupling to a thermal bath [7] [27]. And this is the case despite a lot of effort especially in the mathematical physics literature starting from the Quantum Ergodic Theorem of von Neumann [8] (see [3] for a very recent account and new results).

The interest in these fundamental questions revived recently due to their direct relevance for experiments in ultracold atomic gases [9]. The almost perfect decoupling of these gases from their environment enables the investigation of the quantum dynamics of isolated systems. In a fascinating experiment by Kinoshita et al. [10] it was observed that two counter-oscillating clouds of bosonic atoms confined in a one-dimensional harmonic trapping potential relax to a state different from the thermal one.

Up to now the absence of thermalization to Gibbs ensembles [28] has been mainly attributed to the presence of infinitely many conserved quantities, i.e. to the integrability of the system (see [11] and references therein). For non-integrable isolated models the presence of thermalization after a global quench, i.e. a sudden global parameter change, is still debated [12, 13, 14, 15, 16, 17]. The origin of thermalization after a global quench was proposed to stem from statistical properties of the time averaged density matrix and the so-called 'eigenstate-thermalization hypothesis' (ETH) [4, 18, 19, 20] which we state later on. In our work we will reconsider these claims both for integrable and non-integrable models with short-range interactions and show that although some of them are indeed valid, the underlying pre-requisite for thermalization is more subtle than what was surmised in Ref. [19, 20]. We will do so by considering a sudden parameter change of the Hamiltonian at time $t = 0$ for a system that is in the ground state for $t < 0$. The following time-evolution of any observable $\mathcal{O}$ can be expressed as

$$\langle \mathcal{O} \rangle(t) = \sum_{\alpha,\beta} c_\alpha c_\beta^* e^{-it(E_\alpha - E_\beta)} \langle \beta | \mathcal{O} | \alpha \rangle.$$

Here $|\alpha\rangle$ are the eigenvectors of the Hamiltonian at $t = 0^+$ with corresponding eigenvalues E_α (we use $\hbar = 1$). The overlap $c_\alpha = \langle \alpha | \psi_0 \rangle$ is taken between the eigenstate $|\alpha\rangle$ and the ground state $|\psi_0\rangle$ of the initial Hamiltonian ($t = 0^-$). The typical time behavior of $\langle \mathcal{O} \rangle(t)$ consists in damped or overdamped oscillations that converge towards a constant average value at long times. Assuming no degeneracy in eigenenergies, the long-time value of $\langle \mathcal{O} \rangle(t)$ can be computed using the time averaged density matrix, $\rho = \sum_\alpha |c_\alpha|^2 |\alpha\rangle\langle\alpha|$ [8] [29]. Following the terminology of [19] we will call "diagonal ensemble averages" all averages with respect to ρ and we will use the notation $\langle \mathcal{O} \rangle_D = Tr(\rho \mathcal{O}) = \sum_\alpha \mathcal{O}_\alpha |c_\alpha|^2$ with $\mathcal{O}_\alpha = \langle \alpha | \mathcal{O} | \alpha \rangle$.

An important property of the diagonal ensemble is that under very general conditions [19] the energy per particle has vanishing fluctuations:

$$\Delta e := \frac{\sqrt{\langle E^2 \rangle_D - \langle E \rangle_D^2}}{L} \to 0 \quad \text{for} \quad L \to \infty. \tag{1}$$

Here L denotes the number of sites and the thermodynamic limit is taken at constant particle density N/L. From a statistical point of view, property (1) means that the distribution of intensive eigenenergies with weights $|c_\alpha|^2$ is peaked for large system sizes.

In [19] it was argued, based on previous work on semiclassical quantum systems [4, 18], that for generic non-integrable interacting many body systems the matrix elements $\mathcal{O}_\alpha$ of a few body observable with respect to any eigenstate $|\alpha\rangle$ with eigenenergy E_α equals the microcanonical ensemble average taken at that energy E_α, the so-called "eigenstate thermalization hypothesis". Were this true, an immediate consequence of property (1) would be that averages in the diagonal ensembles coincide with averages in the microcanonical ensemble at the same energy per particle. This was the explanation of thermalization for generic non-integrable systems of finite size [19]. In contrast a finite width distribution for specific observables was found numerically for a finite size integrable system and claimed to be at the origin of the absence of thermalization for this model.

Actually, one can prove a general property that resembles, at first sight, ETH: the matrix elements $\mathcal{O}_\alpha$ of intensive local few body Hermitian operator (or observable) have vanishing fluctuations over eigenstates close in energy [30]:

$$(\Delta\mathcal{O}_e)^2 = \frac{\sum_e \mathcal{O}_\alpha^2}{\sum_e} - \left(\frac{\sum_e \mathcal{O}_\alpha}{\sum_e}\right)^2 \to 0 \text{ for } L \to \infty. \quad (2)$$

Here the sum $\sum_e$ is taken over eigenstates $|\alpha\rangle$ with eigenenergies $E_\alpha/L \in [e-\epsilon; e+\epsilon]$ where e is the considered energy per particle and ϵ is a small number that can be taken to zero after the thermodynamic limit. The detailed proof of this property will be presented in a longer version of this work [25] but the main steps are easy to grasp: using the Cauchy-Schwarz inequality $(O^2)_\alpha \geq (O_\alpha)^2$ one finds that $(\Delta\mathcal{O}_e)^2$ is bounded from above by the fluctuations of $\mathcal{O}$ within the micro-canonical ensemble characterized by the same intensive energy. Using the general thermodynamic result, valid both for non-integrable and integrable finite dimensional systems, that an intensive local observable $\mathcal{O}$ has vanishing fluctuations in the micro-canonical ensemble one obtains $(\Delta\mathcal{O}_e)^2 \to 0$.

Even though property (2) resembles ETH, it is actually different in a subtle way: a state $|\alpha\rangle$ taken at random between all states with the same energy per particle will have with probability one (approaching one in the thermodynamic limit) a value of $\mathcal{O}_\alpha$ equal to its microcanonical average. However, states with different values $\mathcal{O}_\alpha$ may and actually do exist, as we shall show in the following. They are just rare compared to the other ones. This is not a minor fact and shows that the reason of thermalization (or its absence) is more subtle than what surmised in [19]. Indeed, if the $|c_\alpha|^2$s distribution gives an important weight to these rare states, the diagonal ensemble averages will be different from the micro-canonical one. In this case thermalization will not take place, despite the fact that the overall majority of states is characterized by a value of $\mathcal{O}_\alpha$ equal to the microcanonical average. In the following we shall show, in concrete examples, that this is indeed what happens in some integrable infinite systems and in some *finite size* non-integrable models, such as the Bose Hubbard one. Conjectures on thermalization of infinite size non-integrable models are discussed in the conclusion.

Our first example is a chain of L harmonic oscillators characterized by a mass m and coupling strength ω described by the Hamiltonian

$$H = \frac{1}{2}\sum_x \left[\pi_x^2 + m^2\phi_x^2 + \sum_{y=\pm1}\omega^2(\phi_{x+y}-\phi_x)^2\right].$$

We assume periodic boundary conditions and the usual commutation relations between the operators π_x and ϕ_y given by $[\phi_x, \pi_y] = i\delta_{x,y}$. Using a suitable standard transformation one can rewrite the Hamiltonian as $H = \sum_{k=0}^{(L-1)/2}\Omega_k(R_k^\dagger R_k + I_k^\dagger I_k)$ with the new creation and annihilation operators $R_k, R_k^\dagger$ and $I_k, I_k^\dagger$ and $\Omega_k^2 = m^2 + 2\omega^2(1-\cos(2\pi k/L))$. As a consequence the eigenstates of the Hamiltonian at $t = 0^+$ are characterized by occupation numbers $\{n_k^I\}, \{n_k^R\}$ for the I and R operators. Following Calabrese and Cardy [11], we consider now a quantum quench where the system is in the ground state at a certain initial value of $m = m_i$ that we switch instantaneously to the final value m_f, i.e. $\Omega_k^i \to \Omega_k^f$. In order to discuss thermalization and property (2), we focus on the coupling between next-nearest neighbour R-oscillators which reads $\mathcal{G}_2 = \frac{1}{N}\sum_k g(k)R_k^\dagger R_k$ with $g(k) = \cos(4\pi k/N)$. The diagonal matrix element for a state $\alpha = \{n_k^I, n_k^R\}$ is simply $(\mathcal{G}_2)_\alpha = \frac{1}{N}\sum_k g(k)n_k^R$. In the large system size limit the number of eigenstates with $(\mathcal{G}_2)_\alpha$ and E_α/L respectively between $\mathcal{G}_2$ and $\mathcal{G}_2 + d\mathcal{G}_2$ and e and $e + de$ has the form of a large deviation function, i.e. it is proportional to $\exp(LS_e(\mathcal{G}_2))ded\mathcal{G}_2$. The explicit expression of $S_e(\mathcal{G}_2)$ will be shown elsewhere [25]. Physically S_e is just related to the entropy of the system with intensive energy e and an average coupling between next-nearest neighbour equal to $\mathcal{G}_2$. Thus we find that although the distribution of $\mathcal{G}_2$ is strongly peaked (with a width of the order $1/\sqrt{L}$) rare states do exist, but they are exponentially less numerous than the typical ones. For this simple integrable models all the weights $|c_\alpha|^2$ can also be computed exactly. Using that the modes k are decoupled before and after the quench and that n_k^R, n_k^I and all their powers are conserved quantities, we find that the diagonal ensemble is characterized by weights that read $\prod_k P_k(n_k^I)P_k(n_k^R)$ for the state $\{n_k^I, n_k^R\}$. $P_k(n_k)$ is equal to the square of the overlap between the ground state of the k-mode harmonic oscillator before the quench and the quantum state after the quench with occupation n_k. We computed this scalar product by using its integral expression in terms of Hermite polynomials. Our result reads:

$$P_k(n_k) = \left(\frac{\Omega_k^i}{\Omega_k^f}\right)^{1/2}\frac{1}{A2^{n_k}}\frac{n_k!}{(n_k/2)!^2}(-1+1/A)^{n_k}E_{n_k} \quad (3)$$

where $E_{n_k} = 1$ for n_k even and 0 otherwise and $A = (1 + \Omega_k^i/\Omega_k^f)/2$. This distribution decreases exponentially in n_k for any k. It is interesting to remark that the exact distribution (3) is very different from the one assumed to hold for integrable systems within the Generalized Gibbs Ensemble approach [21]. The expression of the weights,

$\prod_k P_k(n_k^I)P_k(n_k^R)$, makes clear that their typical value is exponentially small in the size of the system and hence they can bias significantly the micro-canonical distribution. This is indeed what happens as it can be explicitly checked by computing the average value of $\mathcal{G}_2$ in the diagonal ensemble: $\langle \mathcal{G}_2 \rangle_D = \frac{1}{N}\sum_k f(k)\langle n_k\rangle_D$. We find, in agreement with [11], that the distributions of $(\mathcal{G}_2)_\alpha$ in the two ensembles become infinitely peaked but around two different values. A general way to understand this phenomenon is to rewrite the average of an observable $\mathcal{O}$ as:

$$\sum_\alpha |c_\alpha|^2 \mathcal{O}_\alpha = \int do \mathcal{N}(o) Z_D(o) o$$

where $Z_D(o) = \sum_\alpha |c_\alpha|^2 \delta(\mathcal{O}_\alpha - o)/\mathcal{N}(o)$ and $\mathcal{N}(o) dode$ is the number of states $|\alpha\rangle$ with a value of $\mathcal{O}_\alpha$ between o and $o+do$ and intensive energy between the micro-canonical average e and $e+de$. As discussed previously in the case of $\mathcal{G}_2$, $\mathcal{N}(o)$ is exponentially large in the size of the system, i.e. it is proportional to $\exp(LS_e(o)))$ where $S_e(o)$ is an entropy like function. As a consequence, the micro-canonical distribution of $\mathcal{O}_\alpha$ is peaked around the value that maximizes S_e and has $1/\sqrt{L}$ fluctuations around it. However, $Z_D(o)$ is exponentially small in the system size and proportional to $\exp(-LC_e(o))$, as it can be checked explicitly [25]. This leads to a diagonal ensemble distribution for $\mathcal{O}_\alpha$ which is peaked at the value that maximizes $S_e(o) - C_e(o)$ and it has a width of the order $1/\sqrt{L}$.

The other example we focus on is the one-dimensional extended Bose-Hubbard model with one particle per site:

$$H = -\sum_{j,d=1,2} J_d \left(b_j^\dagger b_{j+d} + h.c.\right) + \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1),$$

where $b_j^\dagger$ and b_j are the bosonic creation and annihilation operators, and $\hat{n}_j = b_j^\dagger b_j$ the number operators on site j. For $J_2 = 0$ and most values of U and J_1, this model has been shown to be non-integrable [22]. Only in special points, e.g. $(U = 0)$ and $(J_1 = J_2 = 0)$, this model is integrable. At the integrable point $U = 0$ one can obtain results similar to the previous example by quenching the value of J_2 and show that a non-thermal steady state is reached due to the occupation of rare states. Furthermore, one can also study how these results change going away from integrability by increasing U. The details will be published elsewhere [25] and here we focus directly on the non-integrable situations $U_f/J_1 = 10$ and $J_2 = 0$. In Fig. 1 (upper panel) we show the correlations $(\mathcal{G}_1)_\alpha = \sum_j \langle\alpha|b_j^\dagger b_{j+1}|\alpha\rangle/L$ versus energy E_α/L.

At low energies an (overlapping) bandstructure is seen. The center of the bands are separated by the interaction energy U/L and have a width proportional to J_1/L. Within these low energy bands $(\mathcal{G}_1)_\alpha$s decay almost linearly. For intermediate energies a mixing of these energy bands starts to show up (cf. Fig. 1 upper panel $E_\alpha/L \approx 5$) which is weak for small systems and becomes stronger for larger system sizes (cf. already $L = 11$). In most fixed energy intervals the values of the correlations $(\mathcal{G}_1)_\alpha$ are spread considerably.

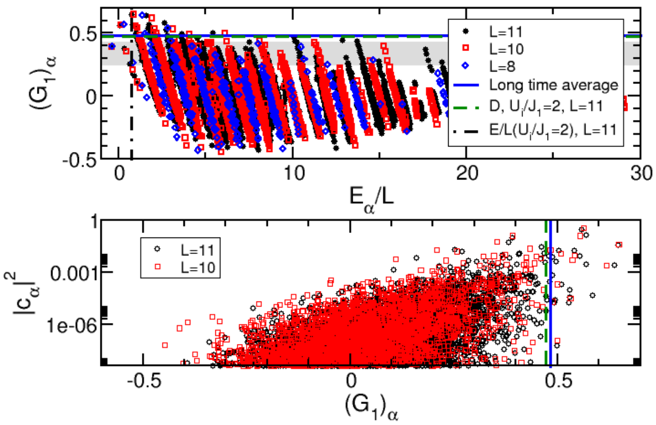

FIG. 1: Full diagonalization results of $(\mathcal{G}_1)_\alpha$ versus energy E_α in the even parity, $k = 0$ momentum sector for the final Hamiltonian characterized by $J_2 = 0$ and $U_f/J_1 = 10$ (upper panel) and correlation of $|c_\alpha|$ versus $(\mathcal{G}_1)_\alpha$ for a quench from $U_i/J = 2$ (lower panel). Additionally the average energy (dashed-dotted line) after the quench and the average value of $\mathcal{G}_1$ obtained from the t-DMRG time-evolution ($L = 100$) (solid line) and the diagonal ensemble for $L = 11$ (dashed line) are shown. The t-DMRG calculations are performed as detailed in Ref. [12]

Let us considered a quench from the superfluid state $U_i/J_1 = 2$ to the interaction strength $U_f/J_1 = 10$. For this quench a non-thermal steady state has been found [12, 16]. In Fig. 1 we compare the longtime value extracted from the time-evolution of $\mathcal{G}_1(t)$ after the quench in systems between 10 to 100 sites (solid horizontal line) and the average taken in the diagonal ensemble ($L = 11$, dashed horizontal line). These two values agree astonishingly well which supports strongly that – at least for the small system sizes – the long-time steady state has been reached. Additionally the average energy after the quench is marked by a vertical line. The microcanonical average around this energy value (shaded region [31]) deviates from the long-time average for $U_f/J_1 = 10$. This supports the previous finding [12, 16] that the long-time correlation functions after the quench to $U_f/J_1 = 10$ cannot be described by a thermal average.

As shown in the lower panel of Fig. 1, the weight of the initial state on the final eigenstates is strongly correlated with the values of the $(\mathcal{G}_1)_\alpha$. The weights are much larger for larger values of $(\mathcal{G}_1)_\alpha$, which correspond to higher values of $|c_\alpha|$ at the lower energy band edges [16]. A general decay of the weights towards lower values of the correlations is evident. All that leads to a larger long-time correlation $(\mathcal{G}_1)_\alpha$ than the one expected from the microcanonical distribution (shaded region). Concerning finite size effects, we note that the long time average which we calculated up to 100 sites is almost system size independent on the time-scales considered (beside finite size revivals). We expect that for the larger sizes the eigenstate with considerable weight will be spread over tens of energy bands and not only over the lowest few ones as it is the case for $L = 8, 10, 11$.

As a conclusion, we find that the absence of thermalization for finite size systems can be attributed to two sources: First, the distribution of the weights $|c_\alpha|^2$ versus energy E_α and the distribution of $\mathcal{O}_\alpha$ in a restricted energy interval may be very broad. Second, 'rare' states characterized by a value of $\mathcal{O}_\alpha$ different from the micro-canonical value may have a considerable weight $|c_\alpha|^2$ and play an important role. All these phenomena clearly are at play for the (finite size) Bose Hubbard model investigated above. The thermodynamic limit will cure the first origin of non-thermalization— the distributions will eventually become infinitely peaked—but not necessarily the second one, which in fact can be seen as the reason of non-thermalization for at least some integrable models (it would be interesting to investigate whether this conclusion holds for more complicated ones). What happens for non-integrable systems and what is the correct requirement on the $|c_\alpha|^2$s in order to have thermalization in the thermodynamic limit is an open question. Rare states leading to $\mathcal{O}_\alpha$s different from the micro-canonical value are expected to persist even for infinite system sizes. Perturbation theory around integrable models [25] and mathematical physics results obtained in the semi-classical limit [5, 6] support this conclusion (how rare are these rare states and whether a large deviation function exist also in this case are interesting questions worth further investigation). As a consequence, in order to justify thermalization after a quantum quench, one has to explain why in physically relevant situations the $|c_\alpha|^2$s do not bias too much the micro-canonical distribution toward these rare states. Since the only apriori distinction between rare and typical states is that the latter are overwhelming more numerous, a plausible (but not necessary) assumption, leading to thermalization on a general basis, is that the $|c_\alpha|^2$s sample rather uniformly states. In order to quantify and check this assumption, one can use the (von Neumann) Kullback-Leibler (KL) entropy S_{KL} [23] of the Gibbs distribution with respect to the diagonal ensemble [32]. A 'rather uniform sampling' would correspond to a zero intensive S_{KL} in the thermodynamic limit. Whether and under which conditions this happens is an open question.

We conclude stressing that thermalization after a quantum quench appears to be a property that emerge for large enough system sizes. Understanding the physics behind this "finite size thermalization length" and estimating its value in concrete cases is a very interesting problem worth investigating in the future, specially because some cold atomic systems formed by hundred of sites may well be below this thermalization threshold.

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[27] The coupling to a thermalized bath is not satisfactory to explain thermalization from a fundamental point of view because one has then to justify why the reservoir is thermalized in the first place.
[28] By thermalization we mean that all the long-time averages of local few body observables coincide with Gibbs averages corresponding to the same intensive energy and particle density.
[29] Counterexamples where no dephasing occurs are often related to special properties of the energy spectra or of the considered observable $\mathcal{O}$, see e.g. Ref. [24].
[30] $\mathcal{O}$ is an intensive local observable if it can be written as $\sum_i \mathcal{O}_i/L$, where $\mathcal{O}_i$ is a local (meaning not infinite range) operator and the sum is over homogeneously distributed spatial positions.
[31] The microcanonical average in these small system is depending on the exact energy interval taken. Therefore several intervals of width $(2, 5, 10, 15, 20)J/L$ have been chosen. The minimum and maximum value obtained define the shaded region.
[32] The Kullback-Leibler (KL) entropy of a probability measure ρ_{II} with respect to the probability measure ρ_I is an information theory tool that measures the dissimilarity between the two distributions [23]: $S_{KL}(\rho_I|\rho_{II}) = \sum_{\mathcal{C}} \rho_I(\mathcal{C}) \log(\rho_I(\mathcal{C})/\rho_{II}(\mathcal{C}))$. S_{KL} is zero if and only if the two distributions are the same except for sets of zero measures [23]. Remarkably, S_{KL} appears to be a measure of the distance from thermal equilibrium also in other contexts, such as non-equilibrium impurity models driven out of equilibrium [26].