Effect of Rare Fluctuations on the Thermalization of Isolated Quantum Systems

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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 prerequisites 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 microcanonical distribution, are responsible for the absence of thermalization of some infinite integrable models and play an important role for some nonintegrable systems of finite size, such as the Bose-Hubbard model. We stress the importance of finite size effects for the thermalization of isolated quantum systems and discuss two scenarios for 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 time scales physical systems thermalize. In classical statistical physics, a very good understanding of thermalization was reached in the last century [1]: Under certain chaoticity conditions, an isolated system thermalizes at long times within the microcanonical 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 prerequisites are still open problems [2,3], except for important results obtained in the semiclassical limit [4,5] or for the coupling to a thermal bath [6,7]. 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 very recent results).

The interest in these fundamental questions has 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 [10], it was observed that two counteroscillating clouds of bosonic atoms confined in a one-dimensional harmonic trap relax to a state different from the thermal one. Up to now, the absence of thermalization [11] has been mainly attributed to the presence of infinitely many conserved quantities, i.e., to the integrability of the system (see [12] and references therein). For nonintegrable isolated models, the presence of thermalization after a global quench, i.e., a sudden global parameter change, is still debated [13–19]. The origin of thermalization (and its absence) 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) [4,19–21]. The ETH, roughly speaking, says that all eigenstates with the same intensive energies are thermal, meaning that expectation values of all local observables within the eigenstate coincide with the ones in the corresponding Gibbs ensemble.

The aim of our work is to understand to what extent the ETH is a necessary and sufficient condition for thermalization. The ETH can be interpreted in two different ways: a weak one, which we show to be verified even for integrable models and which states that the fraction of the nonthermal states vanishes in the thermodynamic limit, and a strong one, which states that nonthermal states completely disappear in the thermodynamic limit. The former interpretation does not imply thermalization. The reason is the possible existence of rare nonthermal states that can have a high overlap with the initial condition. We shall show that this is the origin of nonthermalization of some, and maybe all, integrable models and of some nonintegrable systems of finite size, such as the Bose-Hubbard model. Our results reveal the crucial importance of finite size effects in the study of thermalization and allow us to point out two alternative routes for thermalization.

The initial condition for the dynamics at $t = 0$ is given by the density matrix $\hat{\rho}^0$. The time evolution of any observable $\mathcal{O}$ can be expressed as $\langle \mathcal{O} \rangle(t) = \sum_{\alpha,\beta} \rho^0_{\alpha\beta} e^{-it(E_\alpha - E_\beta)} \langle \beta | \mathcal{O} | \alpha \rangle$. Here $|\alpha\rangle$ are the eigenvectors of the Hamiltonian with corresponding eigenvalues E_α (we use $\hbar = 1$). In order to be concrete we will focus on a sudden parameter change of the Hamiltonian at time $t = 0$ for a system that is in the ground state for $t < 0$. In this case, $\rho_{\alpha\beta} = c_\alpha c^*_\beta$, where $c_\alpha = \langle \alpha | \psi_0 \rangle$ is the overlap between the eigenstate $|\alpha\rangle$ of the Hamiltonian after the quench and the ground state $|\psi_0\rangle$ of the Hamiltonian before the quench ($t = 0^-$). Our results can be generalized straightforwardly to a general ρ^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 by using the time-averaged density matrix: $\rho = \sum_\alpha |c_\alpha|^2 |\alpha\rangle\langle\alpha|$ [8,22]. Following Ref. [21] we call "diagonal ensemble averages" all averages with respect to ρ and we use $\langle \mathcal{O}\rangle_D = \mathrm{Tr}(\rho\mathcal{O}) = \sum_\alpha \mathcal{O}_\alpha |c_\alpha|^2$ with $\mathcal{O}_\alpha = \langle\alpha|\mathcal{O}|\alpha\rangle$. An important property of the diagonal ensemble is that under very general conditions [21] the energy per particle has vanishing fluctuations:

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

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

As already anticipated in the introduction, the eigenstate-thermalization hypothesis says for generic nonintegrable interacting many-body systems that 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. This was first conjectured based on studies of semiclassical systems [4,20] and recently shown numerically to hold for a specific nonintegrable system of finite size [21]. Were this hypothesis 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 given for generic nonintegrable systems and demonstrated for a specific example [21]. 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. Note, however, that for a finite system there are always finite fluctuations of $\mathcal{O}_\alpha$, whether the system is integrable or not. It follows that a precise characterization of the ETH has to involve statements about the evolution of the distribution of $\mathcal{O}_\alpha$ upon approaching the thermodynamic limit. Generically, the width of the distribution of $\mathcal{O}_\alpha$ vanishes as

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

where $\mathcal{O}$ is an intensive local few-body Hermitian operator (or observable); 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. Our proof (see Ref. [24]) is based on the vanishing of the fluctuations in the microcanonical ensemble [25]. Note that Eq. (2) implies that the fraction of states characterized by a value of $\mathcal{O}_\alpha$ different from the microcanonical average vanishes in the thermodynamic limit. 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, since if the $|c_\alpha|^2$'s distribution gives an important weight to these rare states, the diagonal ensemble averages will be different from the microcanonical one. They keep a memory of the initial state. As a consequence, an interpretation of the ETH stating that the *fraction* of thermal states has to vanish would not guarantee thermalization. Instead, the stronger interpretation of the ETH, stating that the *support* of the distribution of the $\mathcal{O}_\alpha$ shrinks around the thermal microcanonical value in the thermodynamic limit, does so because states leading to nonthermal averages disappear. In the following, we shall show, in concrete examples, that these rare states indeed do exist and prevent thermalization in some integrable infinite systems and in some *finite size* nonintegrable models, such as the Bose-Hubbard one.

Our first example is a chain of L harmonic oscillators with a mass m and coupling strength ω described by $H = \frac{1}{2}\sum_x[\pi_x^2 + m^2\phi_x^2 + \sum_{y=\pm1}\omega^2(\phi_{x+y} - \phi_x)^2]$. We assume periodic boundary conditions and the usual commutation relations between the operators π_x and ϕ_y given by $[\phi_x, \pi_y] = i\delta_{x,y}$. 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 $\{n_k^I\}$ and $\{n_k^R\}$ for the I and R operators, respectively. Following Calabrese and Cardy [12], 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., $\Omega_k^i \to \Omega_k^f$. We focus on the coupling between next-nearest neighbor R oscillators which reads $\mathcal{G}_2 = \frac{1}{L}\sum_k g(k) R_k^\dagger R_k$ with $g(k) = \cos(4\pi k/L)$ [26]. The diagonal matrix element for a state $\alpha = \{n_k^I, n_k^R\}$ is $(\mathcal{G}_2)_\alpha = \frac{1}{L}\sum_k g(k) n_k^R$. 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 $\exp[LS_e(\mathcal{G}_2)]ded\mathcal{G}_2$ (cf. [24]). Physically, S_e is just related to the entropy of the system with intensive energy e and an average coupling between next-nearest neighbors equal to $\mathcal{G}_2$. Thus the distribution of $\mathcal{G}_2$ is strongly peaked around the maximum of $S_e(\mathcal{G}_2)$ and has a width of the order $1/\sqrt{L}$, but its tails extend to nonthermal values of $\mathcal{G}_2$. Therefore, this is indeed a case where the width of the distribution of the matrix elements vanishes but the support does not due to the existence of rare states. Additionally, all the weights $|c_\alpha|^2$ can be computed exactly [24]. Their typical value is exponentially small in the size of the system. Thus they can bias significantly the microcanonical ensemble distribution

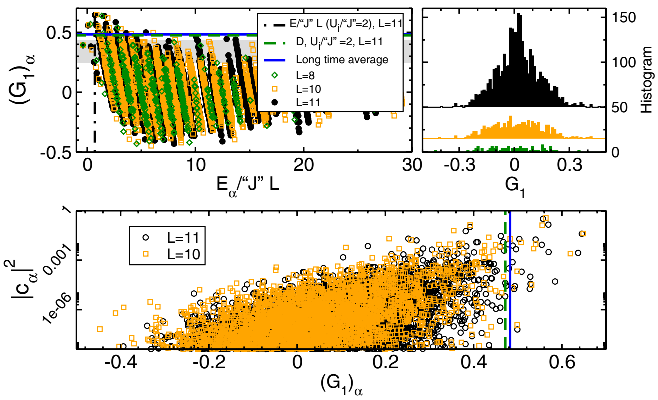

FIG. 1 (color online). Full diagonalization results of $(\mathcal{G}_1)_\alpha$ versus energy E_α in the even parity, $k = 0$ momentum sector for $U_f/J = 10$ (upper panels) and correlation of $|c_\alpha|$ versus $(\mathcal{G}_1)_\alpha$ for a quench from $U_i/J = 2$ (lower panel). Additionally, the average energy (dashed-dotted line) after the quench and the average value of $\mathcal{G}_1$ obtained from the time-dependent density matrix renormalization group method time evolution ($L = 100$; see [13]) (solid line) and the diagonal ensemble for $L = 11$ (dashed line) are shown. The shaded region corresponds to the microcanonical average [32]. Upper-right panel: Distribution of values $\mathcal{G}_1$ for the kinetic energy for the values $E_\alpha/LJ \in [4.5; 5.5]$. The average value is removed from the distribution, and the histograms are shifted vertically for visibility.

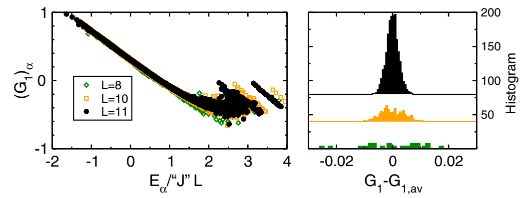

FIG. 2 (color online). Left panel: Full diagonalization results of $(\mathcal{G}_1)_\alpha$ versus energy E_α in the even parity, $k = 0$ momentum sector for $U_f/J = 1$. Right panel: Distribution of values $\mathcal{G}_1$ for $E_\alpha/LJ \in [-0.1, 0.1]$. The linear trend of the observable in the considered window is removed from the distribution, and the histograms are shifted vertically for visibility.

[27] by counterbalancing the difference in cardinality between rare and typical states. We find indeed that the distributions of $(\mathcal{G}_2)_\alpha$ in the microcanonical and diagonal ensembles become infinitely peaked but around two different values, in agreement with Ref. [12], thus explaining the absence of thermalization in this model [24].

The other example is the one-dimensional Bose-Hubbard model with one particle per site: $H = -\sum_j J(b_j^\dagger b_{j+1} + \text{H.c.}) + \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1)$, where $b_j^\dagger$ and b_j are the bosonic creation and annihilation operators, respectively, and $\hat{n}_j = b_j^\dagger b_j$ the number operators on site j. For most values of U and J, this model has been shown to be nonintegrable [28]. Only in special points, e.g., $(U = 0)$ and $(J = 0)$, is this model integrable. The first case we consider is a quench from the superfluid state $U_i/J = 2$ to $U_f/J = 10$. For this quench a nonthermal steady state has been found for long times [13,17]. The correlations $(\mathcal{G}_1)_\alpha = \sum_j \langle\alpha|b_j^\dagger b_{j+1}|\alpha\rangle/L$ in this nonthermal state (system sizes up to $L = 100$, solid horizontal line) do agree well with their diagonal ensemble average ($L = 11$, dashed horizontal line) but not with the microcanonical distribution (shaded region). In this nonintegrable situation it is more difficult to disentangle the role of rare states and finite size effects in the formation of a nonthermal state as we show in the following. First, let us start to consider the validity of Eq. (2). In Fig. 1 (upper-right panel), we show the correlations $(\mathcal{G}_1)_\alpha$ versus energy E_α/L. At low energies an (overlapping) band structure is seen. 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-right 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. In the upper-right panel the predicted narrowing of the half-width of the distribution with increasing system size is clearly visible. In contrast, the support does not seem to shrink which might point towards the existence of rare states. This is further supported in the lower panel of Fig. 1, where 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 the lower energy band edges [17] and are larger than the microcanonical average (shaded region in Fig. 1). A general decay of the weights towards lower values of the correlations is evident. This shows that the states which are important for the diagonal ensemble average do not have the microcanonical expectation value; i.e., rare states matter. Let us note that for the shown system sizes the average energy after the quench (marked by a vertical line) lies still within the lowest few energy bands. However, we estimated that, for the largest sizes considered by the time-dependent density matrix renormalization group method ($L = 100$), for which there is still no thermalization at accessible time scales, the eigenstates with considerable weight will be spread over tens of energy bands and the level statistics close to the Gaussian orthogonal ensemble [29]. We have also studied cases which should be easier from the point of view of thermalization since they are not close to an integrable point; in particular, we discuss $U_f/J = 1$ (Fig. 2). In this case the distribution of $(\mathcal{G}_1)_\alpha$ is much more peaked than for $U_f/J = 10$, and its width decreases when increasing system sizes. Additionally, the support of the distribution seems to decrease pointing towards thermalization. Certainly, larger system sizes are needed to make any firm statement.

As a conclusion, we find that the absence of thermalization for finite size systems can be attributed to two sources: (a) 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 for finite size systems and (b) states characterized by a value of $\mathcal{O}_\alpha$ different from the microcanonical value may have a considerable weight $|c_\alpha|^2$. All these phenomena clearly are at play for the finite size Bose-Hubbard model investigated above. Equation (2) and property (1) assure that the first origin of nonthermalization will be cured for large enough systems—the distributions will eventually become infinitely peaked—but not necessarily the second one. Indeed, we showed that in some integrable models the origin of nonthermalization stems from the existence of nonthermal eigenstates which are less numerous compared to the thermal ones but still exist and possibly bias a lot the diagonal expectation values. What happens for nonintegrable 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. Our results reveal two possible options to obtain thermalization: (i) The support of the distribution of $\mathcal{O}_\alpha$ around the thermal value shrinks to zero in the thermodynamic limit; i.e., rare nonthermal states disappear altogether (as at $U/J = 1$ seemingly), and (ii) rare states exist but the $|c_\alpha|^2$'s do not bias too much the microcanonical distribution toward them. Since the only *a priori* distinction between rare and typical states is that the latter are overwhelming more numerous, a plausible (but not necessary) assumption leading to thermalization is that the $|c_\alpha|^2$'s sample rather uniformly states with the same energy. Note that the existence of rare states for very large nonintegrable models is not completely unreasonable as suggested by mathematical physics results obtained in the semiclassical limit [5,30]. Both scenarios are testable in numerical experiments. One has to study how the support of the distribution of $\mathcal{O}_\alpha$ evolves with the size of the system to understand whether (i) is realized; see [24] for a first attempt. In order to study (ii), one can use the (von Neumann) Kullback-Leibler (KL) entropy S_{KL} [31] of the Gibbs distribution with respect to the diagonal ensemble. A "rather uniform sampling" would correspond to a zero intensive S_{KL} in the thermodynamic limit.

We conclude by stressing that thermalization after a quantum quench appears to be a property that emerges for large enough system sizes. Understanding the physics behind this "finite size thermalization length" and its dependence on the distance from integrability is a very interesting problem worth investigating in the future, especially because some cold atomic systems may well be below this thermalization threshold.

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[1] P. Castiglione, M. Falcioni, A. Lesne, and A. Vulpiani, *Chaos and Coarse Graining in Statistical Mechanics* (Cambridge University Press, Cambridge, England, 2008).

[2] P. Reimann, Phys. Rev. Lett. **101**, 190403 (2008).

[3] S. Goldstein *et al.*, arXiv:0907.0108.

[4] M. Srednicki, Phys. Rev. E **50**, 888 (1994).

[5] S. Nonnenmacher, Nonlinearity **21**, T113 (2008).

[6] U. Weiss, *Quantum Dissipative Systems*, Series in Modern Condensed Matter, Vol. 10 (World Scientific, Singapore, 2008).

[7] 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.

[8] J. von Neumann, Z. Phys. **57**, 30 (1929).

[9] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).

[10] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature (London) **440**, 900 (2006).

[11] 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.

[12] P. Calabrese and J. Cardy, J. Stat. Mech. (2007) P06008.

[13] C. Kollath, A. M. Läuchli, and E. Altman, Phys. Rev. Lett. **98**, 180601 (2007).

[14] S. R. Manmana, S. Wessel, R. M. Noack, and A. Muramatsu, Phys. Rev. Lett. **98**, 210405 (2007).

[15] M. Cramer *et al.*, Phys. Rev. Lett. **101**, 063001 (2008).

[16] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008).

[17] G. Roux, Phys. Rev. A **79**, 021608 (2009).

[18] M. Eckstein, M. Kollar, and P. Werner, Phys. Rev. Lett. **103**, 056403 (2009).

[19] M. Rigol, Phys. Rev. Lett. **103**, 100403 (2009).

[20] J. M. Deutsch, Phys. Rev. A **43**, 2046 (1991).

[21] M. Rigol, V. Dunjko, and M. Olshanii, Nature (London) **452**, 854 (2008).

[22] 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. [23].

[23] T. Barthel and U. Schollwöck, Phys. Rev. Lett. **100**, 100601 (2008).

[24] See supplementary material at http://link.aps.org/supplemental/10.1103/PhysRevLett.105.250401 for more details on the analytical and numerical analysis.

[25] But it is not equivalent to it, since the eigenstates α are, in general, not eigenstates of $\mathcal{O}$.

[26] Although $\mathcal{G}_2$ does not evolve with time, one can construct dynamical observables, by using two point correlation functions of ϕ_x, whose long-time limit is equal to $\mathcal{G}_2$. Thus, for simplicity, we just focus on $\mathcal{G}_2$.

[27] A correlation between large values of the weights to certain values of the observable have been noted for integrable systems in Ref. [21].

[28] A. R. Kolovsky and A. Buchleitner, Europhys. Lett. **68**, 632 (2004).

[29] C. Kollath *et al.*, J. Stat. Mech. (2010) P08011.

[30] F. Faure, S. Nonnenmacher, and S. D. Bièvre, Commun. Math. Phys. **239**, 449 (2003).

[31] T. Cover and J. Thomas, *Elements of Information Theory* (Wiley, New York, 2006), 2nd ed.

[32] The microcanonical average in these small systems depends 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 values obtained define the shaded region.