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## Weak and strong typicality in quantum systems

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We study the properties of mixed states obtained from eigenstates of many-body lattice Hamiltonians after tracing out part of the lattice. Two scenarios emerge for generic systems: (i) the diagonal entropy becomes equivalent to the thermodynamic entropy when a few sites are traced out (weak typicality); and (ii) the von Neumann (entanglement) entropy becomes equivalent to the thermodynamic entropy when a large fraction of the lattice is traced out (strong typicality). Remarkably, the results for few-body observables obtained with the reduced, diagonal, and canonical density matrices are very similar to each other, no matter which fraction of the lattice is traced out. Hence, for all physical quantities studied here, the results in the diagonal ensemble match the thermal predictions.

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Despite advances, the emergence of thermodynamics from quantum mechanics is still a subject under debate. How to derive, from first principles, proper ensembles leading to the basic thermodynamic relations is not yet entirely clear. According to the concept of canonical typicality [1], the reduced density matrix of a subsystem of most pure states of manyparticle systems is canonical. The proof of this statement requires a partition of the original system into a small "system" and a large "environment". However, for example, suppose that our universe is in a pure state and that we trace out only a finite number of degrees of freedom. Can we describe the rest of the universe using statistical mechanics? How much one needs to trace out, how well the notion of canonical typicality works in finite systems, and which quantities will be more or less affected by the fraction of the original system traced out are questions that have received little attention. They are the more pressing given the progress made in experiments with ultracold gases [2].

We can discuss these issues in the context of entropy. If one takes an eigenstate of a generic many-body Hamiltonian and traces out the "environment" ( $\mathcal{E}$ ), the grand canonical (GC) ensemble is the appropriate ensemble to describe the system ( $\mathcal{S}$ ) that is left, where the total energy and number of particles fluctuate. One immediately realizes that the GC-entropy,  $S_{\rm VR}$ , if only a small fraction of the original system is traced out. In this case,  $S_{\rm VN}$  is extensive in the size of the environment, instead of in the size of the system  $\mathcal{S} + \mathcal{E}$  in a pure state  $\hat{\rho} = |\Psi\rangle\langle\Psi|$ , the reduced von Neumann entropy is defined as

$$S_{\rm vN} \equiv -{\rm Tr}_{\mathcal{S}} \left[ \hat{\rho}_{\mathcal{S}} \ln \hat{\rho}_{\mathcal{S}} \right] \equiv -{\rm Tr}_{\mathcal{E}} \left[ \hat{\rho}_{\mathcal{E}} \ln \hat{\rho}_{\mathcal{E}} \right], \qquad (1)$$

where the Boltzmann constant is set to unity and the reduced density matrix  $\hat{\rho}_{S} = \text{Tr}_{\mathcal{E}}\hat{\rho}$  and similarly  $\hat{\rho}_{\mathcal{E}} = \text{Tr}_{S}\hat{\rho}$ .  $S_{vN}$ has been widely used to measure the entanglement in bipartite systems [3]. If the pure state is separable,  $\hat{\rho} = \hat{\rho}_{S} \otimes \hat{\rho}_{\mathcal{E}}$ , then  $S_{vN} = 0$ , while maximum entanglement leads to  $S_{vN} = \ln \mathcal{D}$ , where  $\mathcal{D}$  is the smallest dimension of the two subsystems. The source of the disparity between  $S_{vN}$  and  $S_{GC}$  is the information present in the off-diagonal elements of the reduced density matrix, which is not contained in the thermodynamic ensemble. When a large fraction of the original system is traced out, the equivalence between  $S_{\rm vN}$  and  $S_{\rm GC}$  is expected (canonical typicality). However, up to our knowledge, it has not been demonstrated for realistic systems.

Now suppose that instead of tracing out the environment, we physically cut it off and let the remaining system relax to equilibrium. We can then ask how much one needs to cut for the entropy of the reduced system to become equivalent to  $S_{GC}$ (if ever). After relaxation, this system is described by the diagonal ensemble [4, 5] obtained by writing the reduced density matrix ( $\hat{\rho}_S$ ) in the energy eigenbasis. The proper thermodynamic entropy in this case has been argued to be the diagonal entropy [6, 7], defined as

$$S_d \equiv -\sum_n \rho_{nn} \ln(\rho_{nn}),\tag{2}$$

where  $\rho_{nn}$  are the diagonal elements of the density matrix.  $S_d$  counts logarithmically the number of energy eigenstates which are occupied in S. Unlike  $S_{vN}$ ,  $S_d$  is extensive in the system size even if we trace a very small environment, e.g., a single degree of freedom. Cutting off the environment is equivalent to a sudden quench; it introduces to the system the (nonextensive) energy uncertainty  $\delta E_S$ . This uncertainty implies that if all the eigenstates of the subsystem Hamiltonian  $\hat{H}_S$  within the window  $\pm \delta E_S$  are occupied with roughly the same weights, then  $S_d \approx \log \Omega(E_S) \delta E_S$ , where  $\Omega(E_S)$  is the density of states in S. Up to subextensive corrections,  $S_d$ would then coincide with the thermodynamic entropy of S.

In this Letter, we study the properties of mixed states obtained from eigenstates of a many-body lattice Hamiltonian after tracing out or cutting off an increasingly large environment. One of our goals is to understand the structure of the remaining reduced density matrix and if it ever becomes thermal, which we monitor using  $S_{\rm vN}$ ,  $S_{\rm GC}$ , and  $S_d$ . We find that, for nonintegrable systems,  $S_d$  approaches  $S_{\rm GC}$  after cutting off a few (possibly one) sites, i.e., our hypothesis above is verified.  $S_{\rm vN}$ , on the other hand, remains different from  $S_d$  and  $S_{\rm GC}$  until a large fraction of the lattice is traced out [8]. This motivates us to distinguish between the conventional (or strong) typicality  $S_{\rm vN} \cong S_d \cong S_{\rm GC}$  and a weaker typicality in the sense that  $S_{\rm vN} \neq S_d \cong S_{\rm GC}$ . The latter implies that *only* the diagonal part of the density matrix of the reduced system in the energy eigenbasis exhibits a thermal structure.

Our results then show that the diagonal entropy satisfies the key thermodynamic relation:

$$\frac{\partial S_{\mathcal{S}}}{\partial E_{\mathcal{S}}} = \frac{\partial S_{\mathcal{E}}}{\partial E_{\mathcal{E}}} = \frac{1}{T},\tag{3}$$

where  $E_{\mathcal{S}}$  and  $E_{\mathcal{E}}$  are the energies of the subsystems. This follows from the fact that  $S_d$  coincides with the thermodynamic entropy for  $\mathcal{S}$  and  $\mathcal{E}$  simultaneously. In contrast,  $S_{vN}$  cannot satisfy this equality, as one can see by considering  $\mathcal{E} \gg \mathcal{S}$ . In this case,  $S_{vN} = S_{\mathcal{S}} = S_{\mathcal{E}}$  is proportional to the size of  $\mathcal{S}$ , while  $E_{\mathcal{E}}$  is proportional to the size of  $\mathcal{E}$ , so  $\partial S_{\mathcal{E}}/\partial E_{\mathcal{E}} \to 0$ .

Another of our main goals in this work is to understand the description of few-body observables in the mixed states obtained by the two procedures mentioned before. For that, we study their expectation values as given by the reduced density matrix, the diagonal ensemble, and the GC ensemble. The results for the first two are similar even if very few sites are traced out and the system sizes are small. This suggests that either tracing out part of the original system or removing the same number of sites and waiting for the reduced system to relax leads to the same results, up to non-extensive bound-ary terms. For all practical purposes both procedures are then equivalent. The agreement with the GC expectation values is also good and improves with increasing system size. This implies that, for few-body observables, only weak typicality is needed to observe thermal behavior in experiments.

*System.*– We study hard-core bosons in a one-dimensional lattice with open-boundary conditions described by

$$\hat{H} = \epsilon \left( \hat{n}_{1} - \frac{1}{2} \right)$$

$$+ \sum_{i=1}^{L-1} \left[ -t \left( \hat{b}_{i}^{\dagger} \hat{b}_{i+1} + \text{H.c.} \right) + V \left( \hat{n}_{i} - \frac{1}{2} \right) \left( \hat{n}_{i+1} - \frac{1}{2} \right) \right]$$

$$+ \sum_{i=1}^{L-2} \left[ -t' \left( \hat{b}_{i}^{\dagger} \hat{b}_{i+2} + \text{H.c.} \right) + V' \left( \hat{n}_{i} - \frac{1}{2} \right) \left( \hat{n}_{i+2} - \frac{1}{2} \right) \right],$$
(4)

where, t and t' [V and V'] are nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping [interaction], L is the chain size, and standard notation has been used [9]. Symmetries, and therefore degeneracies, are avoided by considering 1/3-filling and by placing an impurity ( $\epsilon \neq 0$ ) on the first site. In what follows, t = V = 1 sets the energy scale,  $\epsilon = 1/5$ , and t' = V'. When t' = V' = 0, the model is integrable [10]. As the ratio between NNN and NN couplings increases, the system transitions to the chaotic domain [9]. The results below depend on the regime (integrable vs nonintegrable), but not on specific values of the parameters.

For our calculations, we select an eigenstate  $|\Psi_j\rangle$  of  $\hat{H}$  (4), with energy  $E_j$  closest to  $E = \sum_j E_j e^{-E_j/T} / \sum_j e^{-E_j/T}$ 



FIG. 1: (Color online) (a),(b) Entropies per site vs temperature for R = L/3. (c),(d) Entropies per site vs R for a fixed temperature; T = 4. (a),(c) t' = V' = 0 (integrable); (b),(d) t' = V' = 0.32 (chaotic). All panels: L = 18.

corresponding to an effective temperature T. Since  $S_{\rm vN} = S_d = 0$ , this can be seen as the most distant choice for a state with a thermodynamic entropy. We then trace out a certain number of sites  $R \leq 2L/3$ , on the right side of the chain, and study the entropies and observables of the reduced system. The reduced density matrix  $\hat{\rho}_S$  describing the remaining system consists of different subspaces each with a number  $N \in [\max(L/3 - R, 0), L/3]$  of particles.

*Entropies.*– The von Neumann, diagonal, and GC entropies are given by Eq. (1), Eq. (2), and

$$S_{\rm GC} = \ln \Xi + \frac{E_{\mathcal{S}} - \mu N_{\mathcal{S}}}{T_{\rm GC}},\tag{5}$$

respectively. In Eq. (5),  $\Xi = \sum_{n} e^{(\mu N_n - E_n)/T_{GC}}$  is the grand partition function,  $T_{GC}$  is the GC temperature,  $\mu$  is the chemical potential, and  $E_S = \text{Tr}[\hat{H}_S \hat{\rho}_S]$  and  $N_S = \text{Tr}[\hat{N}_S \hat{\rho}_S]$  are, respectively, the average energy and number of particles in the remaining subsystem S.

*Results.*– In Fig. 1, we show results for  $S_{vN}$ ,  $S_d$ , and  $S_{GC}$  in the integrable [(a),(c)] and chaotic [(b),(d)] domains. Larger fluctuations are seen in Figs. 1(a) and 1(c) as characteristic of the integrable regime. Figs. 1(a) and 1(b) show the entropies vs different eigenstates, which are increasingly away from the ground state (*T* increases), when 1/3 of the sites are traced out. In the chaotic regime, and for all states selected, one can see that  $S_d$  is close to  $S_{GC}$ , while  $S_{vN}$  is quite far. This hints a thermal structure in the diagonal part of the reduced density matrix in the energy eigenbasis.

In Figs. 1(c) and 1(d) we show results for a fixed T as an increasingly larger fraction of the original system is traced out. One can see again that in the chaotic limit  $S_d$  is much closer to  $S_{GC}$  than to  $S_{vN}$ , even when very few sites are traced out. However, in both regimes, all entropies approach each other as the fraction of sites traced out increases. For the lattice sizes considered here, we need to trace out more than one half of the chain for the effects of the off-diagonal elements of the den-



FIG. 2: (Color online) (a)–(d) Entropies per site vs 1/L for T = 4 and a fixed ratio R/L (indicated). (e),(f) Full (empty) symbols:  $S_{GC} - S_d (S_{mc} - S_d)$  per site vs 1/L for R = 1, 2, and 3. (a),(c),(e) t' = V' = 0 (integrable); (b),(d),(f) t' = V' = 0.32 (chaotic).

sity matrix to become irrelevant in  $S_{\rm VN}$ , leading this entropy to finally approach  $S_d$  and  $S_{\rm GC}$ .

The results presented in Fig. 1 were obtained for L = 18, the largest system size that we can study with full exact diagonalization. Figure 2 depicts the scaling of the entropies in both domains, integrable [(a),(c)] and nonintegrable [(b),(d)], and for T = 4. In Figs. 2(a) and 2(b), when L/3 sites are cut off,  $S_d$  and  $S_{GC}$  approach each other as L increases, up to a possible non-extensive correction. This trend is seen for all systems we have studied in the chaotic regime [13], and opens up a new question: could cutting off an infinitesimal part of the original system lead  $S_d$  and  $S_{GC}$  to be equal in the thermodynamic limit? In Figs. 2(e) and 2(f), we show the difference between  $S_{GC}$  and  $S_d$  per site vs system size when tracing out one, two, or three sites. In the chaotic regime [Fig. 2(f)], the results are consistent with a vanishing difference in the thermodynamic limit (even when cutting one site [13]). This finding is reinforced with the empty symbols, which show the difference between the microcanonical entropy  $(S_{mc})$  and  $S_d$ . In this case, finite size effects are significantly reduced, leading to a much better agreement between the two entropies, which further improves with L [14]. Hence, one could argue that single eigenstates of many-body Hamiltonians have a thermodynamic entropy [8]. Close to the integrable point [Figs. 2(a), 2(c), and 2(e)], large fluctuations are observed for different values of T and t', V', which makes it difficult to draw general conclusions.

In Figs. 2(a) and 2(b), one can also see that for R = L/3, the von Neumann entropy (per site) saturates to a different value from  $S_d$  and  $S_{GC}$  (per site), as the lattice size increases. As shown in Figs. 2(c) and 2(d), it is only when R > L/2 that the three entropies become comparable. However, for our system sizes, this happens only in the chaotic regime. As one approaches the integrable point, we again find large fluctuations



FIG. 3: (Color online) (a),(b) Kinetic energy per site and (c),(d) n(k = 0) vs R; L = 18; T = 4. (a),(c) t' = V' = 0 (integrable); (b),(d) t' = V' = 0.32 (chaotic).

and the results depend on T and the values of t', V'. Fluctuations in the integrable regime are understandable. In the chaotic regime (and away from the edges of the spectrum) all eigenstates of the Hamiltonian that are close in energy have (i) a similar structure, as reflected by the inverse participation ratio and information entropy in different bases [9], and (ii) thermal expectation values of few-body observables [4, 5, 15, 16]. However, this is not the case close to integrability where most quantities fluctuate wildly between eigenstates close in energy [4, 5, 9, 16], and this is affecting our results here.

*Observables.*– An important question we are left to address is whether the extra information carried by the off-diagonal elements of the reduced density matrix is of relevance to quantities measured experimentally. We focus our analysis on fewbody observables. Their expectation values from the reduced, diagonal, and grand canonical density matrices are given by

$$O_{\rm vN} = {\rm Tr}[\hat{O}\hat{\rho}_{\mathcal{S}}], \quad O_d = \sum_n \rho_{nn} O_{nn}, \qquad (6)$$

$$O_{\rm GC} = \frac{1}{\Xi} \sum_{n} O_{nn} e^{(\mu N_n - E_n)/T},$$
(7)

respectively. Here,  $O_{nn} = \langle \psi_n | \hat{O} | \psi_n \rangle$  and  $| \psi_n \rangle$ 's are the eigenstates of the Hamiltonian in the reduced system.

Results.- Figure 3 shows results for the kinetic energy

$$\hat{K} = -t \sum_{i=1}^{L-R-1} \left( \hat{b}_i^{\dagger} \hat{b}_{i+1} + \text{H.c.} \right) - t' \sum_{i=1}^{L-R-2} \left( \hat{b}_i^{\dagger} \hat{b}_{i+2} + \text{H.c.} \right),$$
(8)

and the momentum distribution function,

$$\hat{n}(k) = \frac{1}{L-R} \sum_{j,l=1}^{L-R} e^{i\frac{2\pi k}{L-R}(j-l)} \hat{b}_j^{\dagger} \hat{b}_l,$$
(9)

for an increasingly large fraction of sites traced out. The results obtained with the three density matrices are comparable, independently of the regime, the number of sites traced out, and T (see [13]). In particular, the fact that  $O_{\rm vN}$  and  $O_d$  are so close demonstrates that both procedures, tracing sites out or cutting off part of the original system and then measuring the observables after relaxation, lead to similar outcome. The information contained in the off-diagonal elements of the reduced density matrix, which generates discrepancies between  $S_{\rm vN}$  and  $S_d \cong S_{\rm CG}$ , is therefore irrelevant to few-body observables. Our findings also open the interesting question: which experimentally measurable quantities (if any) could distinguish between tracing sites out or cutting them off?

We note that, in the chaotic regime, the GC results for both observables depart from those obtained with the reduced and diagonal density matrices as R increases. This is understandable because the GC results are obtained for a system with L - R sites and open boundary conditions, while the other two are obtained for a system with L sites from which R sites are either traced out or cut off. Hence, the more sites one cuts off (the larger the value of R), the smaller is the system remaining. Finite size effects are then expected to be stronger, in particular as the values of t', V' increase. It is also expected that they should vanish in the thermodynamic limit.

In Figs. 4(a)–4(d), we show the scaling behavior of the two observables from Fig. 3 for R = L/3. It is apparent that, in the chaotic regime [Figs. 4(b) and 4(d)], the observables calculated in the three ensembles approach each other with increasing system size. (Results for other temperatures and observables in the chaotic domain are presented in Ref. [13]). In the integrable limit [Figs. 4(a) and 4(c)], large fluctuations prevent us from reaching general conclusions. This is a regime that needs to be studied by other means, which may allow one to do a proper extrapolation to the thermodynamic limit.

A final important property of the mixed states studied here is that their effective thermodynamic temperature  $(T_{GC})$  is the same as the effective temperature T of the many-body eigenstate from which they are obtained. This is shown in Figs. 4(e) and 4(f), where we plot  $T_{GC}/T$  vs 1/L for R = L/3 [4(e)] and R = 2L/3 [4(f)], and for different values of t', V'. The two temperatures are close (except for the smallest systems sizes) and further approach each other as 1/L decreases, which is consistent with the idea of eigenstate thermalization where a single eigenstate exhibits thermal behavior [4, 15].

*Conclusions.*– We have found that, away from integrability, the diagonal and grand canonical entropies are very close to each other, even when a small portion (probably an infinitesimal fraction) of the lattice is cut off. They further approach each other with increasing system size. In contrast to  $S_d$ ,  $S_{vN}$  only approaches  $S_{GC}$  when a large part of the original system is traced out. This behavior reflects the non-diagonal structure of the reduced density matrix when only small fractions of the lattice are traced out. Led by these results, we identified two different regimes: weak typicality, where the diagonal ensemble develops a thermal structure, and strong (canonical) typicality, where the density matrix of the reduced system is thermal. Close to and at integrability further studies are necessary. Our results exhibit large fluctuations depending on the state selected and the values of t', V'.



FIG. 4: (Color online) (a)–(d) Observables vs 1/L for R = L/3. (e),(f) Ratio between the grand-canonical temperature and the temperature vs 1/L. (Black) Plus: t' = V' = 0.04; (red) cross: t' = V' = 0.08; (blue) star: t' = V' = 0.16; (green) diamond: t' = V' = 0.32; (purple) down-triangle: t' = V' = 0.64. In all panels: T = 4.

We also studied experimentally measurable few-body observables as determined from the reduced, diagonal, and grand-canonical density matrices. We find that they all lead to the same results as the system size increases, no matter how many sites are traced out. This demonstrates that the extra information contained in the off-diagonal elements of the reduced density matrix is irrelevant to those observables. Therefore, it is plausible to conjecture that the expectation values of *physical* observables in subsystems of any size obtained from generic many-body eigenstates can be entirely obtained from standard statistical ensembles. Our results show that even in relatively small systems, both procedures, tracing out the "bath" or cutting it off and letting the subsystem thermalize, lead to the same outcome.

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*Note added.*— After completion of this work, we have learned that the strong (canonical) typicality has been recently verified in translationally invariant systems [17].

- H. Tasaki, Phys. Rev. Lett. 80, 1373 (1998); S. Popescu, A. J. Short, and A. Winter, Nature Phys. 2, 754 (2006); S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, Phys. Rev. Lett. 96, 050403 (2006).
- [2] M. Greiner, O. Mandel, T. W. Hansch, and I. Bloch, Nature 419, 51 (2002); T. Kinoshita, T. Wenger, and D. S. Weiss, Nature 440, 900 (2006); S. Hofferberth *et al.*, Nature 449, 324 (2007); S. Trotzky *et al.*, Nature Phys. 8, 325 (2012).

- [3] C. Mejia-Monasterio, G. Benenti, G. Carlo, and G. Casati, Phys. Rev. A **71**, 062324 (2005); L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
- [4] M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008).
- [5] M. Rigol, Phys. Rev. Lett. 103, 100403 (2009); Phys. Rev. A 80, 053607 (2009).
- [6] A. Polkovnikov, Ann. Phys. (N.Y.) 326, 486 (2011).
- [7] L. F. Santos, A. Polkovnikov, and M. Rigol, Phys. Rev. Lett. 107, 040601 (2011).
- [8] J. M. Deutsch, New J. Phys. 12, 075021 (2010).
- [9] L. F. Santos and M. Rigol, Phys. Rev. E 81, 036206 (2010); Phys. Rev. E 82, 031130 (2010).
- [10] This system can be mapped onto a spin-1/2 chain [11]. In the presence of NN couplings only, the spin-1/2 model remains in-

tegrable even after the addition of a local impurity field on the edge of the chain [12].

- [11] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).
- [12] F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter, and G. R. W. Quispel, J. Phys. A 20, 6397 (1987).
- [13] See supplementary material.
- [14]  $S_{\rm mc}$  corresponds to an average of the microcanonical entropies of each subspace [13].
- [15] J. M. Deutsch, Phys. Rev. A 43, 2046 (1991); M. Srednicki, Phys. Rev. E 50, 888 (1994).
- [16] C. Neuenhahn and F. Marquardt, arXiv:1007.5306 (2010).
- [17] J. M. Deutsch, H. Li, and A. Sharma, arXiv:1202.2403.