Entropy of Isolated Quantum Systems after a Quench

Lea F. Santos,[1] Anatoli Polkovnikov,[2] and Marcos Rigol[3,4]
[1]Department of Physics, Yeshiva University, New York, New York 10016, USA
[2]Department of Physics, Boston University, Boston, Massachusetts 02215, USA
[3]Department of Physics, Georgetown University, Washington, D.C. 20057, USA
[4]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA
(Received 18 January 2011; revised manuscript received 7 March 2011; published 18 July 2011)

A diagonal entropy, which depends only on the diagonal elements of the system's density matrix in the energy representation, has been recently introduced as the proper definition of thermodynamic entropy in out-of-equilibrium quantum systems. We study this quantity after an interaction quench in lattice hard-core bosons and spinless fermions, and after a local chemical potential quench in a system of hard-core bosons in a superlattice potential. The former systems have a chaotic regime, where the diagonal entropy becomes equivalent to the equilibrium microcanonical entropy, coinciding with the onset of thermalization. The latter system is integrable. We show that its diagonal entropy is additive and different from the entropy of a generalized Gibbs ensemble, which has been introduced to account for the effects of conserved quantities at integrability.

DOI: 10.1103/PhysRevLett.107.040601 PACS numbers: 05.70.Ln, 02.30.Ik, 05.30.−d, 05.45.Mt

The notion of entropy was first used by Clausius in the mid-19th century and was soon put in the context of statistical mechanics by Boltzmann and Gibbs. Generalized to quantum mechanics by von Neumann in the 1930s and incorporated by probability theory by Shannon in the 1940s, entropy has manifested itself in different forms over the years. Despite the diversity, the consensus is that any physical definition of entropy must conform with the postulates of thermodynamics [1,2].

An appropriate definition of entropy, suitable also for isolated quantum systems out of equilibrium, is fundamental for advances in nonequilibrium statistical mechanics and for a better understanding of recent experiments with quasi-isolated quantum many-body systems, such as those realized with ultracold atoms [3]. von Neumann's entropy, defined as $S_N = -\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$, where $\hat{\rho}$ is the many-body density matrix (the Boltzmann constant here and throughout this Letter is set to unity), complies with the laws of thermodynamics when describing isolated quantum systems in equilibrium and quantum systems interacting with an environment, but it becomes problematic when dealing with closed systems out of equilibrium. Since in an isolated system S_N is conserved for any process, this entropy is not consistent with the second law of thermodynamics. This motivated the recent introduction of the diagonal (d) entropy [4], which is given by

$$S_d = -\sum_n \rho_{nn}\ln(\rho_{nn}), \tag{1}$$

where ρ_{nn} are the diagonal elements of the density matrix in the instantaneous energy basis. In equilibrium S_d coincides with the von Neumann's entropy. In addition, S_d was argued to satisfy the required properties of a thermodynamic entropy: it increases when a system in equilibrium is taken out of equilibrium, it is conserved for adiabatic processes, it is uniquely related to the energy distribution (and as such satisfies the fundamental thermodynamic relation), and it is additive.

More specifically, it was indicated in [4] that S_d should be equivalent to the equilibrium microcanonical entropy when the energy fluctuations are subextensive and the energy distribution is not sparse, assumptions expected to hold in nonintegrable systems. For integrable systems, the existence of a complete set of conserved quantities [5] invalidates those assumptions and precludes thermalization in the usual sense. However, it has been shown that few-body observables after relaxation can still be described by a generalized Gibbs ensemble (GGE) [6], which is a grand-canonical ensemble accounting for the conserved quantities [7].

Here, we study the d entropy in isolated quantum systems after a quench in both integrable and nonintegrable regimes. We consider two kinds of quenches in one dimension (1D): an interaction quench for hard-core bosons (HCBs) and spinless fermions, which have a nonintegrable regime [8], and a local chemical potential quench for HCBs (or spinless fermions) with a superlattice potential, which are integrable [6]. In the first case, as the system transitions to chaos, we show that the distribution function of energy becomes Gaussian-like and S_d approaches the thermodynamic entropy. This indicates that thermodynamically the system becomes indistinguishable from a thermal state. In the second case, S_d is shown to be additive and different from the entropy of the GGE. This difference scales linearly with the system size, suggesting the existence of additional correlations not captured by the GGE [9].

Quench and entropies.—We consider a particular initial state $|\psi_{\mathrm{ini}}\rangle$ which is an eigenstate of a certain initial

Hamiltonian. At time $\tau = 0$, the Hamiltonian is instantaneously changed (quenched) to a new one with eigenstates $|\Psi_n\rangle$ and eigenvalues E_n. The initial state then evolves as $|\psi(\tau)\rangle = \sum_n C_n e^{-iE_n\tau}|\Psi_n\rangle$, where $C_n = \langle\Psi_n|\psi_{\text{ini}}\rangle$ and $|C_n|^2$ correspond to the diagonal elements, ρ_{nn}, of the density matrix, $\hat{\rho}(\tau) = |\psi(\tau)\rangle\langle\psi(\tau)|$.

For generic systems, with nondegenerate and incommensurate spectra, the expectation values of few-body observables ($\hat{O}$) relax to the infinite time average $\overline{\langle\hat{O}(t)\rangle} = \sum_n \rho_{nn} O_{nn}$, which depends only on the diagonal elements ρ_{nn} and $O_{nn} = \langle\Psi_n|\hat{O}|\Psi_n\rangle$ [10,11]. Thus, the d entropy (1) is the entropy of the diagonal ensemble. It resembles the Shannon entropy, but with no arbitrariness in the basis. For sudden quenches, S_d is equivalent to S_N for the time averaged density matrix. The difference between S_d and thermodynamic entropies can help to quantify additional information contained in the diagonal part of the density matrix and not in the equilibrium ensemble.

One can write S_d as the sum of a smooth S_s and a fluctuating S_f part $S_d = S_s + S_f$ [4], where

$$S_s = \sum_n \rho_{nn} \ln[\eta(E_n)\delta E], \tag{2}$$

$$S_f = -\sum_n \rho_{nn} \ln[\rho_{nn}\eta(E_n)\delta E]. \tag{3}$$

Here $\eta(E_n)$ is the density of states at energy E_n: $\eta(E) = \sum_n \delta(E - E_n)$ and δE^2 is the energy variance: $\delta E^2 = \sum_n \rho_{nn}(E - E_{\text{ini}})^2$, where $E_{\text{ini}} = \langle\psi_{\text{ini}}|H|\psi_{\text{ini}}\rangle$ is the expectation value of the quenched Hamiltonian with respect to the initial state. In the continuum limit, $S_s = \int dEW(E)S_m(E)$ and $S_f = -\int dEW(E)\ln[W(E)\delta E]$, where $W(E) = \sum_n \rho_{nn}\delta(E - E_n)$ is the energy distribution. In S_s, the microcanonical entropy, $S_m(E) = \ln[\eta(E)\delta E]$, is the logarithm of the total number of accessible states in the range of energy $[E - \delta E/2, E + \delta E/2]$. If the system is large and finite-size effects become negligible, then up to nonextensive corrections, S_m becomes equal to the canonical entropy, $S_c = -\sum_n[Z^{-1}e^{-E_n/T}\ln(Z^{-1}e^{-E_n/T})]$, where T is the temperature related to the energy of the system and $Z = \sum_n e^{-E_n/T}$ is the partition function (see Ref. [12]).

When $W(E)$ is narrow, so that δE is subextensive, S_s becomes equivalent to the equilibrium microcanonical entropy. Moreover, if in addition $W(E)$ is a smooth function of energy, then S_f is also subextensive. These features are expected to be generic for the nonintegrable (chaotic) regime, where the eigenstates (away from the edges of the spectrum of systems with few-body interactions) become pseudorandom vectors [8,13].

In the integrable limit, on the other hand, conserved quantities reduce the number of eigenstates of the Hamiltonian that have a nonzero overlap with the initial state [11,14], so ρ_{nn} becomes sparse and S_f extensive. In this case, both terms S_s and S_f are expected to contribute to the d entropy. It then becomes appropriate to compare S_d with the entropy of the GGE introduced in Ref. [6], which accounts for the integrals of motion. The many-body density matrix of the GGE is given by $\hat{\rho}_{\text{GGE}} = Z_{\text{GGE}}^{-1}e^{-\sum\lambda_m\hat{I}_m}$, where $Z_{\text{GGE}} = \text{Tr}[e^{-\sum\lambda_m\hat{I}_m}]$, $\{\hat{I}_m\}$ is a complete set of conserved quantities, and λ_m are the Lagrange multipliers fixed by the initial conditions $\lambda_m = \ln[(1 - \langle\psi_{\text{ini}}|\hat{I}_m|\psi_{\text{ini}}\rangle)/\langle\psi_{\text{ini}}|\hat{I}_m|\psi_{\text{ini}}\rangle]$. Since the GGE is a grand-canonical ensemble, which can suffer from large finite-size effects for small systems, in addition to the entropy in the GGE, S_{GGE}, we also compute the entropy in its canonical version (GCE) as the trace $S_{\text{GCE}} = \text{Tr}[\hat{\rho}_{\text{GCE}}\ln(\hat{\rho}_{\text{GCE}})]_{\text{can}}$ where only eigenstates of the Hamiltonian with the same number of particles contribute to the trace.

Chaotic systems.—We consider periodic 1D chains with nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping and interaction, with the following Hamiltonian

$$H_B = \sum_{j=1}^{L}[-t(\hat{b}_j^\dagger\hat{b}_{j+1} + \text{H.c.}) - t'(\hat{b}_j^\dagger\hat{b}_{j+2} + \text{H.c.}) + V(\hat{n}_j^b - \tfrac{1}{2})(\hat{n}_{j+1}^b - \tfrac{1}{2}) + V'(\hat{n}_j^b - \tfrac{1}{2})(\hat{n}_{j+2}^b - \tfrac{1}{2})] \tag{4}$$

for hard-core bosons and similarly for spinless fermions (with $\hat{b}_j \to \hat{f}_j$, $\hat{b}_j^\dagger \to \hat{f}_j^\dagger$, and $\hat{n}_j^b \to \hat{n}_j^f$), where standard notation has been used [8]. L is the lattice size and we take the number of particles to be $N = L/3$. We use full exact diagonalization to compute all eigenstates of the Hamiltonian, taking advantage of conservation of total momentum k due to translational invariance. The initial states considered are eigenstates of Eq. (4) with parameters t_{ini}, V_{ini}, t', V' belonging to the $k = 0$ subspace. The final Hamiltonian (after the quench) has $t = V = 1$ and the same initial values of $t' = V'$. The initial states are selected such that their energies E_{ini} in the final quenched Hamiltonian are the closest to E at a chosen effective temperature T, computed as $E = Z^{-1}\sum_n E_n e^{-E_n/T}$. When $t' = V' = 0$ the system is integrable, while the addition of NNN terms eventually induces the onset of chaos [8].

Full exact diagonalization of the models above limits the system sizes that can be studied to a maximum of 8 particles in 24 sites and thus prevents proper scaling studies of the entropies with increasing system size. This is left to the integrable quenches where larger lattices can be explored. Here we compare S_d, S_s, S_f, S_m, and S_c for the two largest system sizes available and for various Hamiltonian parameters as one departs from the integrable point.

The main panels in Fig. 1 depict S_d and S_s for systems with $L = 24$ at different effective temperatures as t', V' increases. An agreement between S_d and S_s can be seen as one approaches the chaotic limit, improving with temperature and system size [cf. insets in Figs. 1(a) and 1(c)]. (By comparing the left and right panels, particle statistics does not seem to play much of a role.) Lower temperatures, for which S_d and S_s are seen to depart, imply initial states whose energies are closer to the edge of the energy spectrum. For finite systems, thermalization has been argued not to occur in those cases [8], and, from our results here, we expect that the idea of a thermodynamic description will break down if the temperature is sufficiently low. Increasing the system size is expected to increase the region of temperatures over which a thermodynamic description will be valid. Figure 1 also shows that different initial states give slightly different quantitative results (top vs bottom panels), although the overall qualitative behavior is the same.

The insets in Figs. 1(b) and 1(d), depict a comparison between S_d and the equilibrium entropies in thermodynamic ensembles whose energy has been chosen to be the same of the initial state after the quench. Explicit results for the microcanonical entropy with δE determined by the energy uncertainty are in surprisingly good agreement with those of S_d. Up to a nonextensive constant, the canonical entropy S_c can also be written in the same form as S_m (2) if we use the canonical width $\delta E_c^2 = -\partial_\beta E$. Results for S_c are shown for three different sets of eigenstates: (i) all the states in the N sector, (ii) only the states in the N sector with $k = 0$, (iii) only the states in the N sector with $k = 0$ and the same parity as the initial state. The latter, as expected, is the closest to S_m (also computed from eigenstates in the same symmetry sector as $|\psi_{\rm ini}\rangle$) and S_d. In the thermodynamic limit, all three sets of eigenstates should produce the same leading contribution to S_c, but for finite systems it is necessary to take into account discrete symmetries in order to get an accurate thermodynamic description of the equilibrium ensemble.

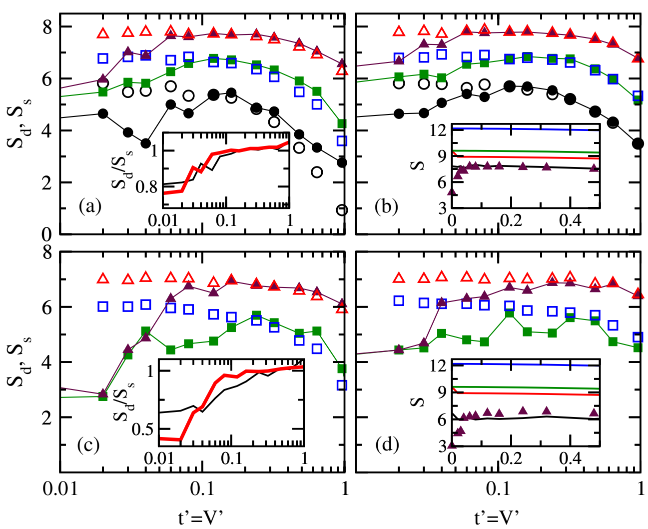

FIG. 1 (color online). Entropies vs $t' = V'$. Left: bosons; right: fermions; top: quench from $t_{\rm ini} = 0.5$, $V_{\rm ini} = 2.0$; bottom: quench from $t_{\rm ini} = 2.0$, $V_{\rm ini} = 0.5$. Filled symbols: d entropy (1); empty symbols: S_s (2); ○ $T = 1.5$; □ $T = 2.0$; △ $T = 3.0$. All panels: 1/3 filling and $L = 24$; insets of panels (a) and (c) show S_d/S_s for $L = 24$, thick (red) line, and $L = 21$, thin (black) line for $T = 3.0$. Solid lines in the insets of panels (b) and (d), from bottom to top: microcanonical entropy; canonical entropy S_c for eigenstates with $k = 0$ and the same parity as the initial state; S_c for eigenstates with $k = 0$ and both parities; and S_c for all eigenstates with $N = 8$.

The fact that $S_d/S_m \to 1$ in the chaotic limit and that the agreement improves with system size provide an important indication that S_f is small and subextensive. Information contained in the fluctuations of the density matrix becomes negligible in chaotic systems and only the smooth (measurable) part of the energy distribution contributes to the entropy of the system. Also, the close agreement between S_d and S_m in the insets of Figs. 1(b) and 1(d) suggests that S_d is indeed the proper entropy to characterize isolated quantum systems after relaxation. Results for the energy distribution $W(E)$ in Fig. 2 further support these findings.

Figure 2 shows $W(E)$ for HCBs for quenches in the integrable (left) and chaotic (right) domains. The sparsity of the density matrix in the integrable limit is reflected by large and well separated peaks, while for the nonintegrable case $W(E)$ approaches a Gaussian shape similar to $(\sqrt{2\pi}\delta E)^{-1} e^{-(E-E_{\rm ini})^2/(2\delta E^2)}$, as shown with the fits. The shape of $W(E)$ is determined by the product of the average weight of the components of the initial state and the density of states. The latter is Gaussian and the first depends on the strength of the interactions that lead to chaos, it becomes Gaussian for large interactions [15]. A plot of ρ_{nn} vs energy, on the other hand, does not capture so clearly the integrable-chaos transition [12].

Integrable systems.—We consider a 1D HCB model with NN hopping and an external potential described by

$$H_S = -t \sum_{j=1}^{L-1} (b_j^\dagger b_{j+1} + \text{H.c.}) + A \sum_{j=1}^{L} \cos\left(\frac{2\pi j}{P}\right) b_j^\dagger b_j. \quad (5)$$

This model is exactly solvable as it maps to spinless noninteracting fermions (see, e.g., Ref. [16]). The period P is taken to be $P = 5$, $t = 1$, and the amplitude A takes the values 4, 8, 12, and 16. We study systems with $L = 20, 25, \ldots, 55$ at 1/5 filling. For the quench, we start with the ground state of (5) with $A = 0$ and evolve the system with a superlattice ($A \neq 0$) and vice versa. Open boundary conditions are used in this case.

We first study how the deviation of S_d from S_s, as quantified by S_f/S_d, scales with increasing lattice size

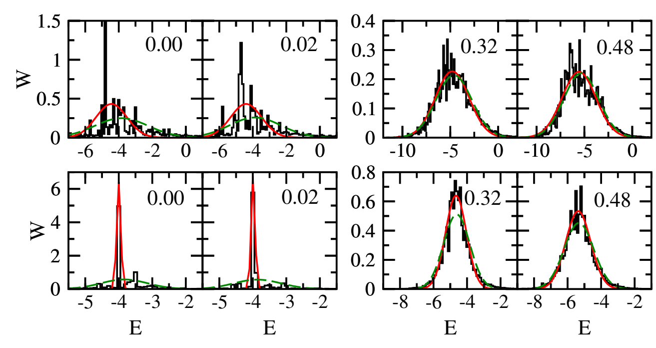

FIG. 2 (color online). Normalized distribution function of energy. Bosonic system, $L = 24$, $T = 3.0$ and the values of $t' = V'$ are indicated. Top panels: quench from $t_{\rm ini} = 0.5$, $V_{\rm ini} = 2.0$; bottom panels: quench from $t_{\rm ini} = 2.0$, $V_{\rm ini} = 0.5$. Solid smooth line: best Gaussian fit $(\sqrt{2\pi}a)^{-1} e^{-(E-b)^2/(2a^2)}$ for parameters a and b; dashed line: $(\sqrt{2\pi}\delta E)^{-1} e^{-(E-E_{\rm ini})^2/(2\delta E^2)}$.

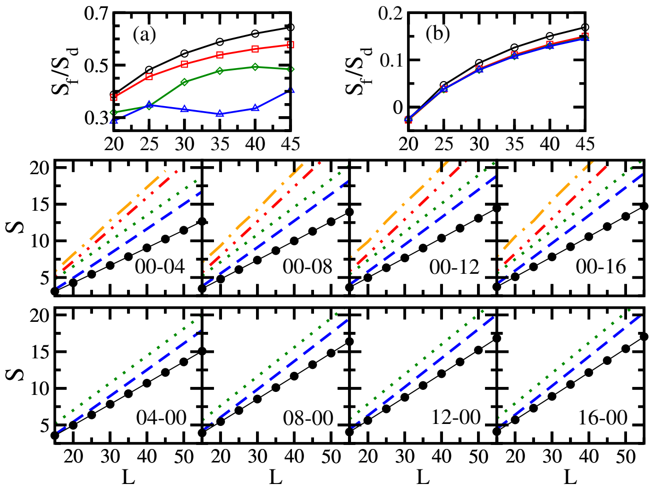

FIG. 3 (color online). Entropy vs system size. Panel (a): from top to bottom, quench to $A_{\rm fin} = 4$, 8, 12, 16; panel (b): quench from $A_{\rm ini} = 4$, 8, 12, 16, curves closely superpose. Lower panels: the quench type is indicated as (initial A)-(final A). Symbols: S_d; dashed lines: GCE entropy (the closest to the d entropy in all cases studied); dotted lines: GGE entropy; dashed double-dotted line: canonical entropy; and dash-dotted line: microcanonical entropy.

for different quenches. As shown in Figs. 3(a) and 3(b), S_f/S_d does not decrease as L increases, rather, we find indications that S_f/S_d saturates to a finite value in the thermodynamic limit. Hence, for these systems S_d is not expected to be equivalent to the microcanonical entropy.

In the lower panels of Fig. 3, we study the scaling of S_d with increasing system size for the same quenches. A clear linear behavior is seen, demonstrating that S_d is indeed additive. In these panels, we also show the microcanonical (with δE determined as for the interaction quenches [17]) and canonical ensembles. The latter two can be seen to increase linearly with L and with a similar slope. These two entropies are clearly greater than S_d indicating that the diagonal ensemble in this case is highly constrained. Finally, we show results for the GGE and GCE entropies. They also increase linearly with system size and with a similar slope, showing that in the thermodynamic limit their difference should be subextensive. Interestingly, the slopes of the GGE and GCE are greater than the slope of the diagonal entropy. This suggests the existence of additional correlations not fully captured by the generalized ensemble. The diagonal entropy in this case is a clear observable independent measure of such correlations. This finding opens an important question as to which ensemble should be appropriate to characterize the thermodynamic properties of isolated integrable quantum systems after relaxation following a quench and for which observables these additional correlations are relevant.

Summary.—We presented a study of the diagonal entropy following quenches in integrable and nonintegrable isolated quantum systems. In the nonintegrable regime, we showed that S_d has the properties expected from an equilibrium microcanonical entropy. In particular, the fact that S_d coincides with S_m up to subextensive corrections and is thus determined only by the energy of the system implies that basic thermodynamic relations can be applied to nonintegrable isolated systems (see also discussion in Ref. [4]). In the integrable limit, we demonstrated that S_d is additive and smaller than the entropy of generalized ensembles (recently shown to properly describe observables after relaxation following a quench). Our results open further questions as to how to characterize the thermodynamic properties of isolated integrable systems, and also motivate further studies for nonintegrable systems, in order to verify the scaling of S_d with system size and compare it to the one of the entropy in conventional statistical ensembles.

This work was supported by the Research Corporation (L. F. S.), by ONR and NSF under Grant No. PHY05-51164 (M. R.), by DMR-0907039, AFOSR under Grant No. FA9550-10-1-0110, and by the Sloan Foundation (A. P.). We thank the KITP at UCSB, where part of this work was done, for the hospitality.

[1] A. Wehrl, Rev. Mod. Phys. **50**, 221 (1978).
[2] O. Penrose, Rep. Prog. Phys. **42**, 1937 (1979).
[3] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature (London) **440**, 900 (2006); S. Hofferberth *et al.*, Nature (London) **449**, 324 (2007).
[4] A. Polkovnikov, Ann. Phys. (N.Y.) **326**, 486 (2011).
[5] B. Sutherland, *Beautiful Models* (World Scientific, Singapore, 2004).
[6] M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. **98**, 050405 (2007); M. Rigol, A. Muramatsu, and M. Olshanii, Phys. Rev. A **74**, 053616 (2006).
[7] M. A. Cazalilla, Phys. Rev. Lett. **97**, 156403 (2006); P. Calabrese and J. Cardy, J. Stat. Mech. (2007) P06008; M. Cramer *et al.*, Phys. Rev. Lett. **100**, 030602 (2008); T. Barthel and U. Schollwöck, Phys. Rev. Lett. **100**, 100601 (2008); M. Kollar and M. Eckstein, Phys. Rev. A **78**, 013626 (2008); D. Fioretto and G. Mussardo, New J. Phys. **12**, 055015 (2010).
[8] L. F. Santos and M. Rigol, Phys. Rev. E **81**, 036206 (2010); **82**, 031130 (2010).
[9] D. M. Gangardt and M. Pustilnik, Phys. Rev. A **77**, 041604 (R) (2008).
[10] M. Rigol, V. Dunjko, and M. Olshanii, Nature (London) **452**, 854 (2008).
[11] M. Rigol, Phys. Rev. Lett. **103**, 100403 (2009); Phys. Rev. A **80**, 053607 (2009).
[12] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.107.040601 for more information on diagonal entropy and energy distribution.
[13] M. V. Berry, J. Phys. A **10**, 2083 (1977).
[14] C. Neuenhahn and F. Marquardt, arXiv:1007.5306.
[15] V. V. Flambaum and F. M. Izrailev, Phys. Rev. E **56**, 5144 (1997).
[16] V. G. Rousseau *et al.*, Phys. Rev. B **73**, 174516 (2006).
[17] Note that S_m can be slightly larger than S_c because, here, the microcanonical ensemble is defined by taking the median (not the mean) energy to be $E_{\rm ini}$.