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The microscopic origin of thermodynamic entropy in isolated systems

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A microscopic understanding of the thermodynamic entropy in quantum systems has been a mystery ever since the invention of quantum mechanics. In classical physics, this entropy is believed to be the logarithm of the volume of phase space accessible to an isolated system [1]. There is no quantum mechanical analog to this. Instead, Von Neumann's hypothesis for the entropy [2] is most widely used. However this gives zero for systems with a known wave function, that is a pure state. This is because it measures the lack of information about the system rather than the flow of heat as obtained from thermodynamic experiments. Many arguments attempt to sidestep these issues by considering the system of interest coupled to a large external one, unlike the classical case where Boltzmann's approach for isolated systems is far more satisfactory. With new experimental techniques, probing the quantum nature of thermalization is now possible [3, 4]. Here, using recent advances in our understanding of quantum thermalization [5–10] we show how to obtain the entropy as is measured from thermodynamic experiments, solely from the self-entanglement of the wavefunction, and find strong numerical evidence that the two are in agreement for non-integrable systems. It is striking that this entropy, which is closely related to the concept of heat, and generally thought of as microscopic chaotic motion, can be determined for systems in energy eigenstates which are stationary in time and therefore not chaotic, but instead have a very complex spatial dependence.

The emergence of thermodynamics from underlying microscopic motion is still unclear. One of the hardest concepts to understand is that of entropy. Classically, the microscopic state of a system can be thought of as a single point in phase space and as it evolves, this point wanders in this space, filling up more of it as time progresses. Boltzmann's hypothesis relates the entropy to the volume that can be filled, and shows how microscopic motion determines large scale thermodynamic properties [1]. For a generic, that is a non-integrable, system, ergodicity implies that this volume will be the hypersurface of constant energy, but for integrable systems, the volume accessible depends on initial conditions so that such systems will not thermalize.

There are many different approaches and definitions for understanding entropy [11], but here we will be concerned with the experimental thermodynamic definition that is obtained, for example, by doing calorimetry measurements as related to the flow of heat. Classically, these thermodynamic measurements are not influenced by knowledge of the microscopic state of a system. For example, computer simulations are often used to predict thermodynamic quantities, such as entropy. However microscopic knowledge of the system allows one to extract work out of it by the well known example of Maxwell's demon. This would violate the second law of thermodynamics unless we correspondingly reduce the entropy to take into account this microscopic information [11]. Therefore classically there are two distinct uses of the word entropy: (*i*) obtained by performing macroscopic thermodynamic measurements, which we will call the thermodynamic entropy, and (*ii*) a measure of the lack of available information about a system's state.

The quantum mechanical situation is far less clear. Knowledge of the system through observation does alter the state of the system, so that it is not apparent if the thermodynamic

entropy is altered by this process. For a system with density matrix ρ , the Von Neumann entropy $S_{VN} = -\text{Tr}(\rho \ln \rho)$ which is identically zero for any system in a pure state, including an energy eigenstate. Because the state of the system is known completely, this reduces its entropy to zero as in case (*ii*). But what does this do to entropy (*i*)? If we do thermodynamic measurements on systems in pure states, that is, where the state is known completely to the experimenter, does this alter what is measured?

Furthermore, the quantum ensemble definition of entropy, case (*i*), is simply related to the density of states of the energy. But if the system is in a single energy eigenstate, it might appear to be impossible to get the density of states. This would argue that thermodynamic entropy measured for systems in pure states, would be different than for a system coupled to an external environment. Such questions until recently were purely theoretical but now with the emergence of experiments that study thermalization of isolated quantum systems or lack thereof [3, 4], a proper understanding of the microscopic origins of entropy has become increasingly important.

Here we find convincing evidence that for pure states, there is a way of defining an entropy as in case (*i*) for a non-integrable quantum mechanical system with a large number of degrees of freedoms which is identical to the thermodynamic definition and give an explicit prescription for its construction from a knowledge of the eigenstate alone, thus successfully linking the thermodynamic entropy with its underlying microscopic origins. Throughout this work we will be concerned with the thermodynamic limit of a large number of degrees of freedom, N , and will not consider non-extensive corrections to the entropy for finite systems. Furthermore in this limit, the microcanonical and canonical ensembles give identical results [1]. Therefore we can freely choose which ensemble to consider.

Statistical mechanics is concerned mainly with computing the time average of observables that depend on only a few variables, and relates this time average to an average over an ensemble. Thus for a system with average energy $\langle E \rangle$, statistical mechanics posits the relation between the time average of some observable \hat{O} and its average over the microcanonical ensemble of states, the latter being far easier to compute:

$$\overline{\langle \hat{O} \rangle} = \text{Tr}(\rho_{\text{micro}, \langle E \rangle} \hat{O}) \quad (1)$$

where the bar on the left hand side denotes a time average and the microcanonical density matrix at energy E_0 is

$$\rho_{\text{micro}, E_0} \equiv \frac{1}{\mathcal{N}_{\text{states}}} \sum_{E_0 < E < E_0 + \Delta E} |E\rangle\langle E| \quad (2)$$

and ΔE is much greater than the average distance between neighboring energy levels but much less than the macroscopic energy scale E_0 , and $\mathcal{N}_{\text{states}}$ is the number of terms in the sum. In quantum mechanics, the fluctuation in the energy can be large [5] but in practice is taken to be small so that $\langle E \rangle$ is a good measure of the energy. The way to see the connection between the underlying quantum evolution needed on the left hand side of Eq. 1 of a generic system and the ensemble methods of statistical mechanics has recently become much better understood. The idea is the ‘‘Eigenstate Thermalization Hypothesis’’ (ETH) [5–7]: for large N , the expectation value of an observable in an energy eigenstate becomes equal to the microcanonical average at the same energy, that is

$$\text{Tr}(\rho_E \hat{O}) = \text{Tr}(\rho_{\text{micro}, E} \hat{O}) \quad (3)$$

where ρ is the density matrix for the wavefunction $|E\rangle$ at energy E , $\rho_E = |E\rangle\langle E|$. Put more simply, the expectation value of \hat{O} will vary very little between neighboring energy levels for large N , implying that the expectation value of \hat{O} in any energy eigenstate is the microcanonical average (at that energy). There is strong numerical evidence and analytic arguments to support this for a variety of systems [5–10]. Not all systems obey this hypothesis [12, 13]. In particular, integrable systems, do not do so. Note that $\rho_E \neq \rho_{\text{micro}, E}$, as there a large number of constants of motion, even for generic Hamiltonians, such as projection operators[14] that violate Eq. 3. This is why the choice of observables satisfying this equation is restricted.

Below we shall extend these ideas to understanding entropy. In the thermodynamic limit statistical mechanics posits the formula for the thermodynamic entropy $S_{\text{thermo}} = -\text{Tr}(\rho_{\text{micro}} \ln \rho_{\text{micro}})$ where ρ_{micro} could be equivalently replaced with the thermal density matrix in the canonical ensemble in the limit that we are considering. We want to see if this can be calculated from the properties of the wavefunction itself without any recourse to ensembles.

We consider homogeneous systems for simplicity with short range interactions and start by following the standard textbook scenario: the system is divided into two parts, the larger part, B , can act as a bath in contact with the smaller

one, A , that is our system of interest. If the complete system starts out in a pure state, then by doing a partial trace over B , the reduced density matrix for A , $\rho_A = \text{Tr}_B \rho$ becomes mixed because it is entangled with B . This is part of a common but non-rigorous argument for how a canonical distribution of energies emerge for the smaller system A , where the temperature T is given by the statistical mechanical relation between T and the average energy. If the complete system was actually integrable this argument fails and thermalization does not occur.

The *entanglement entropy* is defined as

$$S_{\text{Ent}}(A, B) = -\text{Tr}(\rho_A \ln \rho_A). \quad (4)$$

which has been studied in detail for a wide variety of systems and is very important in the study of quantum information theory[15], black holes [16] and quantum phase transitions [17]. This will also be important in what follows.

If instead we considered the complete system to already be described by the microcanonical density matrix, then $\rho_{A, \text{micro}} \equiv \text{Tr}_B \rho_{\text{micro}}$ must behave with canonical statistics even for integrable systems, and the entanglement entropy in that case is $S_{\text{Ent}, \text{micro}}(A, B) \equiv -\text{Tr}(\rho_{A, \text{micro}} \ln \rho_{A, \text{micro}})$ which is the statistical mechanical expression for the entropy. This entropy is what one measures experimentally in thermodynamic experiments. Thus

$$S_{\text{thermo}}(A) = S_{\text{Ent}, \text{micro}}(A, B) = -\text{Tr}(\rho_{A, \text{micro}} \ln \rho_{A, \text{micro}}) \quad (5)$$

This argument is very similar to most treatments of entropy in textbooks[18] however there is more evidence than that this to support it. Rigorous analysis [19] gives an canonical entanglement entropy for one dimensional models in agreement with the thermodynamic results [20].

This *does not* connect thermodynamic entropy with the wavefunction of a system because the right hand side of Eq. 5 involves the microcanonical average and is similar to the right hand side of the ETH as written in Eq. 3, but differs because of the nonlinear logarithmic factor which is not an observable operator. Thus we ask whether we can extend the ETH to quantities of this form; that is, for a generic quantum system in an energy eigenstate can we replace $\rho_{A, \text{micro}}$ with ρ_A ? In other words is

$$S_{\text{thermo}}(A) = -\text{Tr}(\rho_A \ln \rho_A)? \quad (6)$$

This form was recently hypothesized using other less direct analytical arguments [21]. Although this is the thermodynamic entropy for a subsystem of $A + B$, the entropy is extensive so we can obtain the entropy for the full system by adding the entropies for individual subsystems together. In the particular case of a homogeneous system, the above equation can easily give us the thermodynamic entropy per unit volume. Thus entropy defined this way is a measure of *self-entanglement*.

Now we employ exact diagonalization on a number of systems to determine if Eq. 6 is satisfied, and how it scales with

system size. Because system sizes are still far from the thermodynamic limit we minimize finite size effects by asking equivalently using Eq. 5, does

$$-\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_{A,micro} \ln \rho_{A,micro})? \quad (7)$$

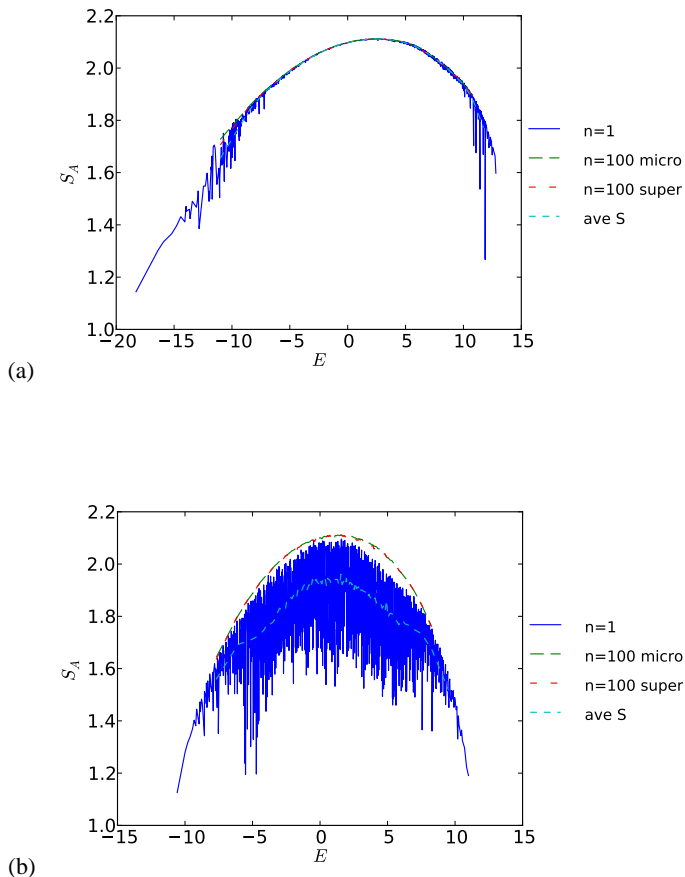


FIG. 1. (a) The entanglement entropy $S_{Em}(A,B)$ (Eq. 4), for a non-integrable system of 6 hard core bosons on 27 sites where A has 4 sites and B has 23. The blue curve $n = 1$ is obtained from the entanglement entropy of individual energy eigenvectors. The dashed green curve is the microcanonical entropy obtained by averaging the density matrix over $n = 100$ neighboring eigenvectors. The dashed red curve is obtained from the entanglement entropy of a wave function that is a random superposition of 100 neighboring levels. The light blue dashed curve is the curve $n = 1$ smoothed over 100 neighboring energy levels. (b) The same as in (a) but for an integrable system $t' = V' = 0$.

We study systems that have been previously shown to give rise to energy eigenstate thermalization. Following some of these previous studies [8–10] we consider spinless fermions and hard core bosons on a one dimensional lattice with nearest neighbor (NN) and next nearest neighbor (NNN) hopping, and interaction. The hopping strengths for NN and NNN are t

and t' , likewise we denote the interaction strengths V and V' . We study these systems for parameters where they are known to obey ETH and for integrable parameters where they do not. Following previous work, we use periodic boundary conditions in the subspace with wavevector $k = 1$, rather than $k = 0$ to avoid a parity symmetry. Throughout this work we set the energy scale to have $t = V = \hbar = 1$.

For both the fermions and hard core boson cases, $t' = V' = 0.96$ which is non-integrable and should obey the ETH. We calculate the entanglement entropy for each energy eigenstate for a range of different bath and system sizes. Our largest size was $N = 27$ lattice sites with $N_p = 6$ particles. We trace over the bath sites and calculate the entanglement entropy Eq. 4, and do this as a function of the number of lattice sites of A , denoted m . For these cases, we plotted the entanglement entropy as a function of m . As is well known [22] $S_{ent}(m) = S_{ent}(N - m)$ so for $m > N/2$ the entanglement entropy must go back down to zero. As we display in the supplementary information in the case of hard core bosons, it is very close to linear behavior over a substantial range of m , for the non-integrable case, as is expected due to the extensive nature of entropy.

However the behavior for integrable systems, $t' = V' = 0$, is more erratic and the linearity depends much more strongly on the eigenvector. Similar results were also obtained for the fermion model as well as is shown in the supplementary material.

We directly checked to see if Eq. 7 is supported numerically. We calculated the left hand side of this equation for different values of m and because of the linearity of the entanglement entropy with m , the results are insensitive to this value. In Fig. 1 it is shown for $m = 4$. We also calculate the microcanonical reduced density matrix by taking the partial trace of Eq. 2. We average the reduced density matrix over 100 neighboring eigenvectors, and use that to calculate the entanglement entropy as done on the right hand side of Eq. 7. The result for 6 hard core bosons on 27 sites is shown in Fig. 1(a). The blue line is no microcanonical averaging ($n = 1$) and the green dashed curve is the microcanonical average over $n = 100$ neighbors. The two curves are very close to each other in most of the range where the density of states is high and one has eigenstate thermalization. The light blue dashed curve takes the entanglement entropy with no microcanonical averaging and averages it over 100 neighboring energy levels. The dashed red line will be discussed below.

In contrast, Fig. 1(b), for the integrable case $t' = V' = 0$, one sees that the fluctuations are much larger and that the microcanonical average is much further from the entanglement entropy for individual eigenstates. Similar results are seen in the one dimensional spinless fermion system. To quantify this difference further, we examine the standard deviation of fluctuation of the entanglement entropy for both the integrable and non-integrable cases.

We calculated the standard deviation $\sigma(S)$ of the entanglement entropy $S_{ent}(A,B)$ around the maximum of the curves in Fig. 1 for different lattice sizes, 16, 18, 20, 25, and 27, all

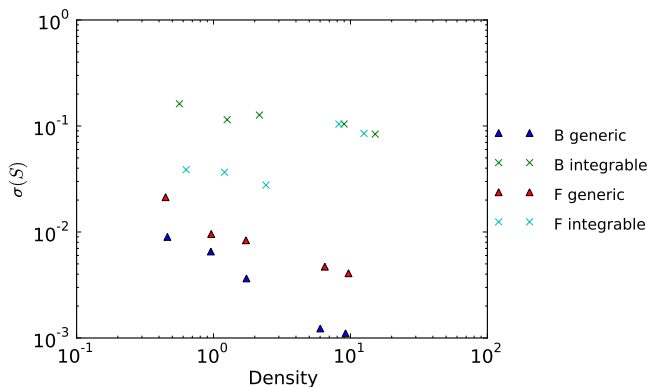


FIG. 2. The fluctuations in the entanglement entropy for both non-integrable (generic) and integrable systems of 6 hard core bosons (B) but with a different number of lattice sites, and the same quantity for the spinless fermion model (F). The standard deviation of the entanglement entropy $S_{ent}(A, B)$ is plotted against the density of states. This is done around the point of maximum entanglement entropy.

with 6 particles in Fig. 2. $\sigma(S)$ is computed over 100 neighboring energy levels, and this is shown as a function of the density of states on a log-log plot for both the hard core boson models (B) and spinless fermions (F), and for both the non-integrable and integrable cases. As is apparent, the integrable fluctuations are substantially higher. This is also the case for observables as has been shown previously [7]. The behavior as a function of the density of states and system size is qualitatively different. The fluctuations are diminishing much more rapidly in the non-integrable case. This is similar to slower diminution of fluctuations of observables predicted for integrable versus non-integrable systems, where in the former case we expect a power law decrease as a function of the number of degrees of freedom and in the latter case it is predicted to be an exponential [5].

The above studies provide excellent numerical evidence for the equivalence of the thermodynamic entropy of non-integrable systems with the entanglement entropy when the wavefunction is in an energy eigenstate. We also studied two dimensional hard core bosons and fermions and reached the same conclusion (see supplementary materials). Now we ask what happens with more general initial states. If one starts the system off in a state with fluctuations in energy in a window, then we can ask how this evolves for long times. We expect thermalization of observables, and that the entropy should also be the thermodynamic entropy. We can test to see if this is the case numerically.

Over long times, the energy eigenvector components of non-integrable wave functions will have random phases [23]. Therefore we test this case to see if the entanglement entropy still looks like the microcanonical entanglement entropy. In Fig. 1(a) the dashed red line computes the entanglement entropy at each energy by using wavefunctions that are the superposition of 100 neighboring energy eigenvectors with Gaussian amplitudes and random phases. As can be seen, this

matches the predictions of the microcanonical entanglement entropy very well, and the same conclusion is also reached in the fermion case. The closeness of the reduced density matrix to the canonical result is expected for general initial conditions where many energy eigenstates are present [24]. Our above analysis shows that for generic systems, when the system is put in an energy eigenstate, we still obtain the microcanonical entropy, which is crucial, as otherwise thermodynamics would fail in this important case.

Therefore the equivalence of thermodynamic and the entanglement entropy for long times should be correct, starting from a wide range of initial states.

We can now answer the questions that we originally posed. Although the statistical mechanical entropy is most simply understood from the density of states, for a generic Hamiltonian, the self-entanglement of a single energy eigenstate can be used to obtain the same result as well. Knowledge of neighboring levels is not necessary as this entropy as we have seen, is a property of a single energy eigenvector. Going back to our earlier comparison with classical physics, we can now answer our original question. A complete knowledge of the system's quantum state, does not affect its behavior with respect to macroscopic measurements of the entropy. An experimenter who measured a system's state precisely, will in subsequent measurements obtain the same answers as someone who is not made privy to this information, despite the latter describing the system in a mixed state. For long times, a system in a pure state and one in an statistical ensemble have identical thermodynamic entropies in the limit of large systems. This is because the entropy in such experiments measures the system's self-entanglement, not the lack of knowledge of it.

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Supplementary materials to: The microscopic origin of thermodynamic entropy in isolated systems

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We start by considering two kinds of one dimensional lattice systems, hard core bosons (HCB) and spinless fermions (SF). We choose periodic boundary conditions and add both nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping and interactions. Following the notation of Santos and Rigol [2], the Hamiltonian for bosons H_B and for fermions H_F are

$$H_B = \sum_{i=1}^L \left[-t \left(b_i^\dagger b_{i+1} + h.c. \right) + V n_i^b n_{i+1}^b - t' \left(b_i^\dagger b_{i+2} + h.c. \right) + V' n_i^b n_{i+2}^b \right], \quad (1)$$

and

$$H_F = \sum_{i=1}^L \left[-t \left(f_i^\dagger f_{i+1} + h.c. \right) + V n_i^f n_{i+1}^f - t' \left(f_i^\dagger f_{i+2} + h.c. \right) + V' n_i^f n_{i+2}^f \right]. \quad (2)$$

Here, L is the length of the chain, b_i and b_i^\dagger are bosonic and f_i and f_i^\dagger are the fermionic annihilation and creation operators for site i . $n_i^b = b_i^\dagger b_i$ is the boson and $n_i^f = f_i^\dagger f_i$ is the fermion local density operator. Hardcore bosons cannot occupy the same site, and the operators commute on different sites. The NN and NNN hopping strengths are respectively t and t' . The interaction strengths are V and V' respectively. We take $\hbar = t = V = 1$.

Because of translational invariance and particle number conservation, the Hamiltonian divides into independent blocks each with fixed total momentum k . As previously pointed out [2], to avoid degeneracy associated with parity symmetry at $k = 0$, we take $k = 1$ and checked that the energy levels obey Wigner-Dyson statistics.

Using exact diagonalization, we computed the eigenvalues and eigenvectors of the Hamiltonian in the $k = 1$ sector. We studied the cases $V' = t' = .96$, and $V' = t' = 0$. The HCB results for the entanglement entropy $S_{ent}(m)$ are shown in Fig. 1(a) for the non-integrable case $V' = t' = .96$ and the in integrable case Fig. 1(b) $V' = t' = 0$. Here the number of lattice sites $N = 27$, and the number of particles $N_p = 6$. The five plots sample different eigenvectors and are evenly spaced as a function of the eigenvector index. The plots start at $m = 3$ because for m smaller than a correlation length, we do not expect to obtain the correct entropy. The corrections to linearity are well fitted with a small exponential term. For the integrable case (b), the behavior is much more erratic and less straight than in the non-integrable case(a). Fig. 2 we display the analagous results for spinless fermions with the same parameters.

We show the same quantities as shown in Fig. 2 of the letter for spinless fermions in Fig. 3, with the same parameters as used for the hard core bosons.

Because of the strong linearity in the entanglement entropy as a function of m , we can take the difference $\Delta S \equiv S_{ent}(4) - S_{ent}(3)$ to be an estimate for the entropy of the system per lattice site. The results are very similar to those obtained using $\Delta S \equiv S_{ent}(5) - S_{ent}(4)$ instead. The results for hard core bosons are displayed in Fig. 4. This difference displays the same features as the full entanglement entropy and still shows very

good agreement with the microcanonical results in the case of a non-integrable system, but does not agree well for the integrable case.

We next consider the same quantities for a two dimensional square lattice of hard core bosons with periodic boundary condition. We chose the total momentum sector to be zero. Hard core bosons in two dimensions have also been shown to satisfy energy eigenstate thermalization [1]. We consider 6 hard core bosons on a 5 by 5 lattice. We choose repulsive nearest neighbor interactions $V = 0.1$ and a nearest neighbor hopping strength $t = 1$. As above we chose $\Delta S \equiv S_{ent}(4) - S_{ent}(3)$

Fig. 5 shows the results from exact diagonalization of this model. As we found in one dimensional non-integrable systems, the microcanonical entanglement entropy is in very good agreement with the entanglement entropy.

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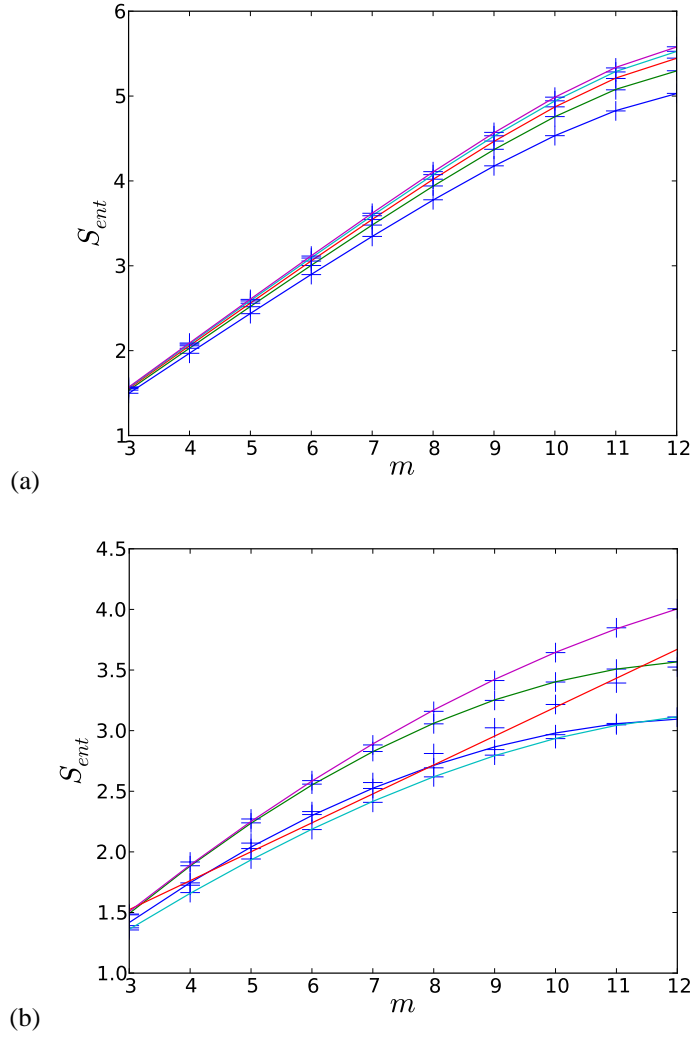


FIG. 1. The entanglement entropy for single energy eigenstates of hard core bosons shown for a number of different levels in the non-integrable case. The levels were chosen to be evenly spaced and are 548 (lowest), 1096, 1644, 2192, 2740 (highest) out of a total of 10966 states in the $k = 1$ sector (a) The non-integrable case, for $t' = V' = 0.96$. The fit was to a straight line plus an exponential correction and the standard deviation of the error for each curve is less than 3.4×10^{-3} for all of these levels. (b) The integrable case $t' = V' = 0$.

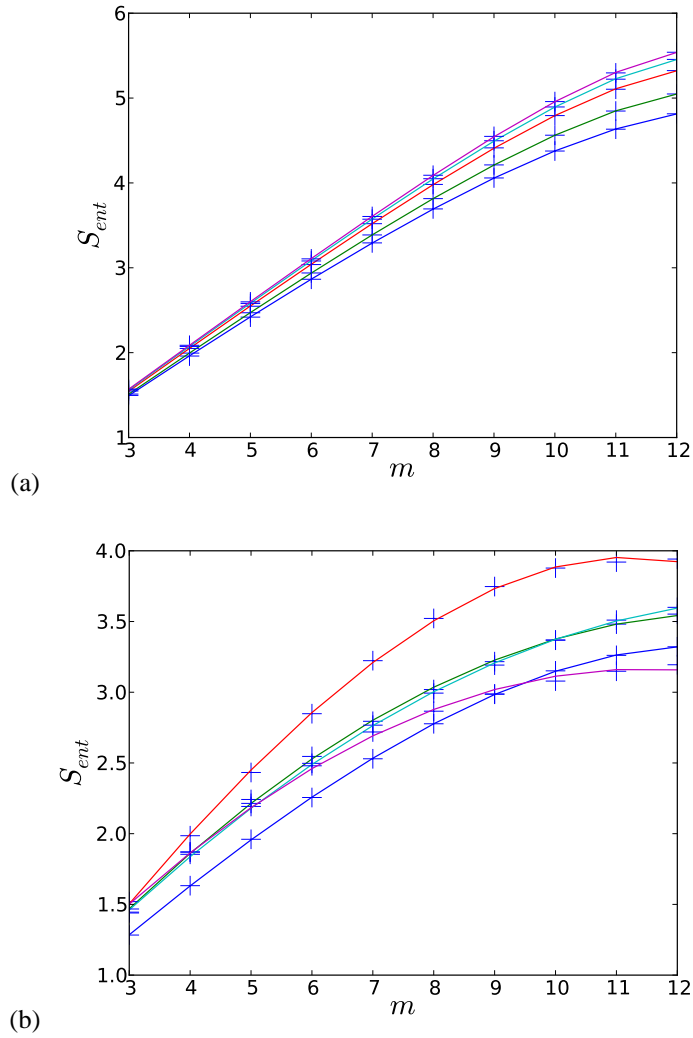


FIG. 2. The entanglement entropy for single energy eigenstates of spinless fermions shown for a number of different levels in the non-integrable case. The levels were chosen to be evenly spaced and are 548 (lowest), 1096, 1644, 2192, 2740 (highest) out of a total of 10966 states in the $k = 1$ sector (a) The non-integrable case, for $t' = V' = 0.96$. The fit was to a straight line plus an exponential correction and the standard deviation of the error for each curve is less than 3.1×10^{-3} for all of these levels. (b) The integrable case $t' = V' = 0$.

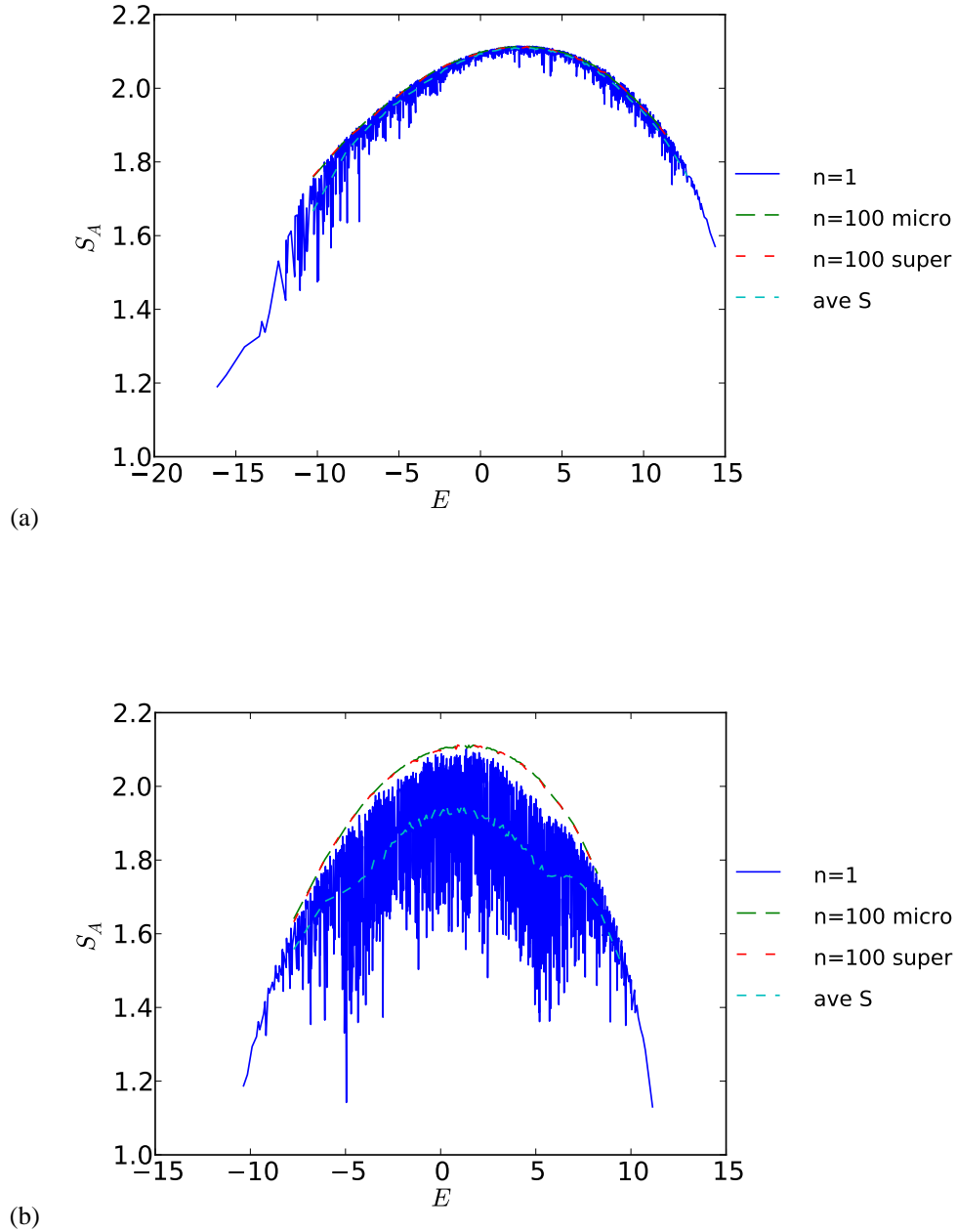


FIG. 3. (a) The entanglement entropy $S_{Ent}(A, B)$, for a non-integrable system of 6 spinless fermions on 27 sites where A has 4 sites and B has 23. The blue curve $n = 1$ is obtained from the entanglement entropy of individual energy eigenvectors. The dashed green curve is the microcanonical entropy obtained by averaging the density matrix over $n = 100$ neighboring eigenvectors. The dashed red curve is obtained from the entanglement entropy of a wave function that is a random superposition of 100 neighboring levels. The light blue dashed curve is the curve $n = 1$ smoothed over 100 neighboring energy levels. (b) The same as in (a) but for an integrable system $t' = V' = 0$.

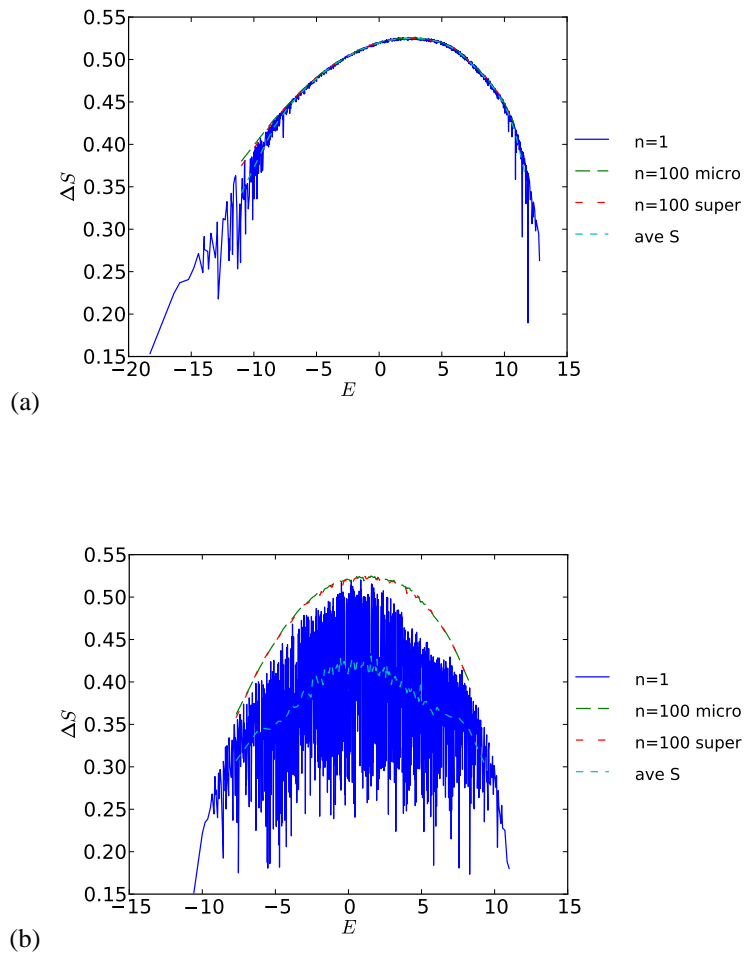


FIG. 4. (a) The entanglement entropy difference for a non-integrable system of 6 bosons on 27 sites for the same system as Fig. 1 of the accompanying letter. Here $\Delta S \equiv S_{ent}(4) - S_{ent}(3)$. The blue curve $n = 1$ is obtained from the entanglement entropy of individual energy eigenvectors. The dashed green curve is the microcanonical entropy obtained by averaging the density matrix over $n = 100$ neighboring eigenvectors. The dashed red curve is obtained from the entanglement entropy of a wave function that is a random superposition of 100 neighboring levels. The light blue dashed curve is the curve $n = 1$ smoothed over 100 neighboring energy levels. (b) The same as in (a) but for an integrable system $t' = V' = 0$.

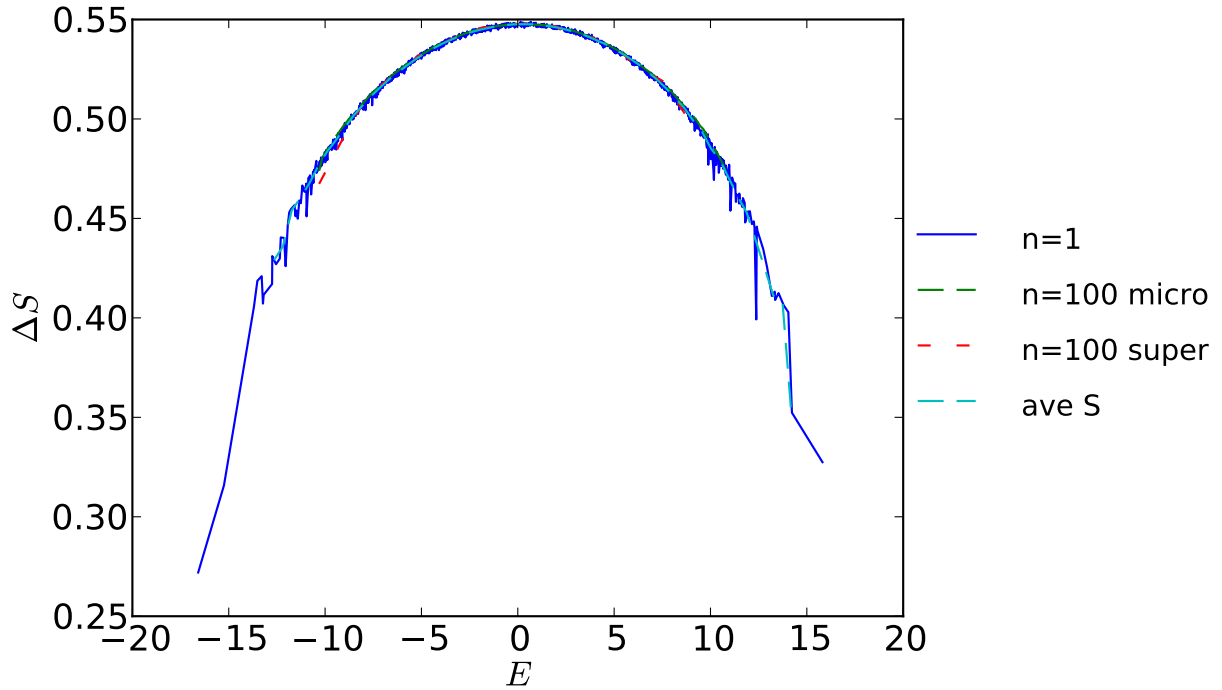


FIG. 5. The entanglement entropy difference for a non-integrable system of 6 hard core bosons on a two dimensional 5×5 lattice. Here $\Delta S \equiv S_{ent}(4) - S_{ent}(3)$. The blue curve $n = 1$ is obtained from the entanglement entropy of individual energy eigenvectors. The dashed green curve is the microcanonical entropy obtained by averaging the density matrix over $n = 100$ neighboring eigenvectors. The dashed red curve is obtained from the entanglement entropy of a wave function that is a random superposition of 100 neighboring levels. The light blue dashed curve is the curve $n = 1$ smoothed over 100 neighboring energy levels.