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Locality, entanglement, and thermalization of isolated quantum systems

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A way to understand thermalization in an isolated system is to interpret it as an increase in entanglement between subsystems. Here we test this idea through a combination of analytical and Krylov-subspace based numerical methods applied to a quantum gas of bosons. We find that the entanglement entropy of a subsystem is rapidly generated at the initial state of the evolution, to quickly approach the thermal value. Our results also provide an accurate numerical test of the Eigenstate Thermalization Hypothesis (ETH), according to which a single energy eigenstate of an isolated system behaves in certain respects as a thermal state. In the context of quantum black holes, we propose that the ETH is a quantum version of the classical no-hair theorem.

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A basic tenet of thermodynamics is that macroscopic isolated systems evolve towards a final state of maximum entropy. (Applied to the entire universe this is sometimes called the "heat death of the universe.") On the other hand, quantum mechanics predicts that an initial pure state evolves into another pure state; since pure states have zero entropy, no entropy can ever be generated. The problem of how to reconcile these apparently conflicting views has been greatly sharpened recently by the degree to which it is now possible to isolate and manipulate quantum systems in cold-atom experiments [1, 2].

To understand the problem more concretely, consider a quantum system with Hamiltonian H, Hilbert space of dimension N and energy eigenstates $|E_\nu\rangle$. Take an initial state $|\psi_0\rangle = \sum_{\nu=1}^{N} c_\nu |E_\nu\rangle$ with a narrow spread in energy ΔE around a mean value E. At later times the state is given by

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle = \sum_{\nu=1}^{N} c_\nu e^{-iE_\nu t}|E_\nu\rangle. \qquad (1)$$

Consider an observable $\hat{A}$ associated with a subsystem—a small part of the full isolated system. According to thermodynamics, the time-dependent expectation value

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \sum_{\nu,\nu'=1}^{N} c^*_{\nu'} c_\nu e^{-i(E_\nu - E_{\nu'})t} \langle E_{\nu'}|\hat{A}|E_\nu\rangle, \quad (2)$$

should reach, after an appropriate thermalization time t_{th}, a constant value independent of the initial state and given by the thermal expectation value, as computed in the subsystem. The basic idea is that this happens because the phases $e^{-i(E_\nu - E_{\nu'})t}$ that are initially ($t = 0$) all equal, at later times ($t \gg t_{th}$) become incoherent leading to a cancellation of the time dependent terms. More precisely, the Eigenstate Thermalization Hypothesis (ETH) put forward by Deutsch and Srednicki [3–7] states that the off-diagonal matrix elements, $\langle E_{\nu'}|\hat{A}|E_\nu\rangle$ for $\nu \neq \nu'$, are small (of order $1/\sqrt{N}$) and the diagonal matrix elements are (to order $1/\sqrt{N}$) smooth functions of the energy, meaning that $\langle E_\nu|\hat{A}|E_\nu\rangle = A(E_\nu)$ are approximately equal for all eigenstates $|E_\nu\rangle$ within the narrow spread of energy ΔE. Under these conditions,

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle\Big|_{t\gg t_{th}} \simeq \sum_{\nu=1}^{N} |c_\nu|^2 A(E_\nu) \simeq A(E)\,, \qquad (3)$$

independently of the initial state $|\psi_0\rangle$.

Given the importance of the ETH, it is essential to test it numerically. However, since the corrections of order $1/\sqrt{N}$ have to be negligible, a direct test requires diagonalization of a large $(N \times N)$ Hamiltonian matrix. This is a difficult task, although recently important progress in this direction has been reported [8–11]. In addition to systems representing cold atoms (for a review, see [12]), motivation for this line of work comes from models of quantum computation, where individual qubits can thermalize due to interactions even if the whole system is perfectly isolated [13]. Other, perhaps less expected, area that has been a focus of recent attention [14–16], where understanding the precise mechanism of thermalization is required, is the physics of black holes, in particular, the properties of the Hawking radiation. In fact, the AdS/CFT correspondence [17–19] relates thermalization of a quantum isolated system to the formation of black holes in quantum gravity, a process for which there is no clear theoretical description. In particular in [20] it has been argued that an arrow of time appears in the field theory side of the correspondence by using arguments similar to ETH.

While the ETH readily explains the independence of averages for local observables of time (at large times), as well as their independence of the initial state, it still remains to connect it to more conventional measures of thermalization, such as the growth of entropy. Here we establish this connection for a model system, a two-dimensional lattice gas of bosons with hard-core repulsion and an additional nearest-neighbor repulsive interaction.

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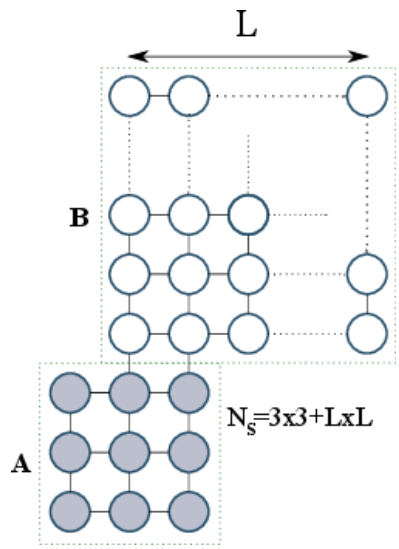


FIG. 1: The type of lattice used in our numerical computations. A gas of bosons is initially contained in region A and expands into regions $A+B$.

L	N_s	N_b	N
5	34	3	5,984
4	25	5	53,130
6	45	5	1,221,759
8	73	5	15,020,334

TABLE I: Various values of the parameters considered: size L, number of sites N_s, number of bosons N_b, and total size of the Hilbert space N.

The Hamiltonian is

$$H = J_1 \sum_{\langle i,j \rangle} (a_i a_j^\dagger + a_i^\dagger a_j) + 2J_0 \sum_{\langle i,j \rangle} n_i n_j \,, \qquad (4)$$

where the sum is over pairs of near neighbors and, for concreteness, we take $J_1 = -1$, $J_0 = \frac{1}{4}$. The shape of the lattice is shown in Fig. 1, and the parameters are listed in Table I.

We start our study by showing that various local observables satisfy a somewhat weakened version of the ETH, namely, the ETH in the Krylov subspace, the latter obtained by applying powers of the Hamiltonian to the initial state $|\psi_0\rangle$. A Krylov subspace of a relatively modest size allows us to follow the evolution well beyond the thermalization time, for systems that are much larger than those accessible to complete diagonalization. If the ETH is true in the full Hilbert space, it must also be true in the Krylov subspace (although, of course, not the other way around). So, our method provides an accurate test of the original ETH, pertaining to systems much larger than those previously considered.

For the system under consideration, the energy is bounded both from below and from above. Therefore, the series

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle = \sum_{p=0}^{\infty} \frac{(-i)^p}{p!} H^p \, |\psi_0\rangle \qquad (5)$$

is absolutely convergent and, to any desired finite precision, can be truncated at a finite number n of terms. This shows that only the Krylov subspace

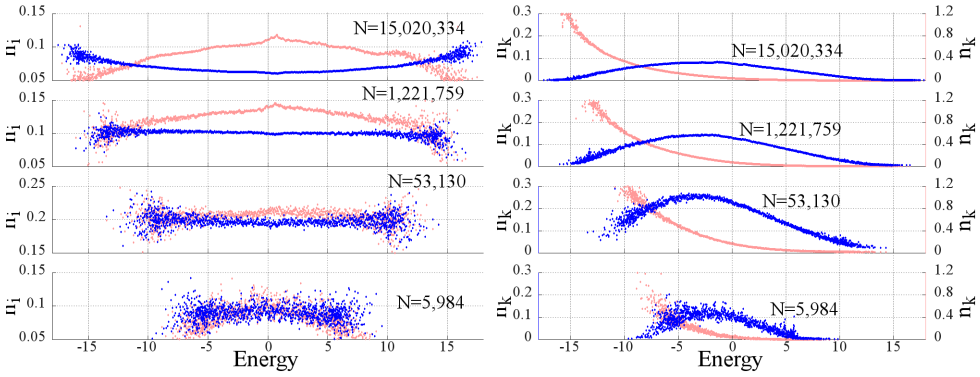
$$\mathcal{K}_n = \{H^p|\psi_0\rangle, p = 0 \ldots n-1\} \qquad (6)$$

is required to follow the evolution [21]. For fixed precision, the larger the time we wish to access, the larger the dimension n of the Krylov subspace that needs to be considered. Since t_{th} depends only weakly on the linear size L, to reach $t = t_{th}$ it is typically enough to consider n that is vastly smaller that the total size N of the Hilbert space. Defining $\mathbb{P}_n$ as the projector onto $\mathcal{K}_n$ we can approximate $|\psi(t)\rangle \simeq \mathbb{P}_n|\psi(t)\rangle$ and

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle \simeq \sum_{\ell,\ell'=1}^{n} \tilde{c}^*_{\ell'} \tilde{c}_\ell \; e^{-i(\tilde{E}_\ell - \tilde{E}_{\ell'})t} \, \langle \tilde{E}_{\ell'}|\hat{A}|\tilde{E}_\ell\rangle \qquad (7)$$

where the so-called Ritz vectors $|\tilde{E}_\ell\rangle$ are the eigenstates of the projected Hamiltonian $\tilde{H} = \mathbb{P}_n H \mathbb{P}_n$. Applying to eq. (7) the same reasoning as we did above to eq. (2), we conclude that the ETH should also apply to the matrix elements $\langle \tilde{E}_{\ell'}|\hat{A}|\tilde{E}_\ell\rangle$ (of the observable $\hat{A}$ in the Ritz basis), at least as long as the difference $|\tilde{E}_\ell - \tilde{E}_{\ell'}|$ is much larger than $1/t_{\max}$, where $t_{\max}$ is the largest time that the Krylov subspace with a given n allows us to access.

Numerically we considered a Krylov subspace of dimension $n = 1241$. For operators $\hat{A}$, we took the occupation numbers n_i of various lattice sites and also the occupation numbers $\tilde{n}_k$ of single particle eigenstates. The single particle eigenstates are the eigenstates $|\epsilon_k\rangle$ of the Hamiltonian (4) when only one particle is present. In that way, the Hamiltonian (4) can be equally written as $H = \sum_k \epsilon_k \tilde{n}_k + 2J_0 \sum_{\langle i,j \rangle} n_i n_j$. The $\tilde{n}_k$ are not local observables but should also thermalize in weakly interacting or sufficiently dilute systems. In Fig. 2 we display the mean values of such operators as functions of the Ritz energy, for systems with dimensions of the total Hilbert spaces varying from $N \sim 6,000$ to $N \sim 1.5 \times 10^7$ (see Table 1). It is clear that the functions become smoother as N becomes larger, in agreement with the ETH. Perhaps it is useful to clarify that these are mean values in the quantum sense. A single measurement should, of course, result in an integer value of n_i or $\tilde{n}_k$. Although they are not plotted here, the off-diagonal matrix elements can be computed and are found to become smaller as N increases. Finally, we checked, for a selection of Ritz states, that the single particle occupation numbers $\tilde{n}_k$ followed an approximate Bose-Einstein distribution, namely they are thermal. All this put together provides *strong numerical evidence* for the validity of the ETH in the present system.



(a) $n_i(\tilde{E}_\ell)$ (b) $\tilde{n}_k(\tilde{E}_\ell)$

FIG. 2: (Color online) Left: Mean values $\langle \tilde{E}_\ell | n_i | \tilde{E}_\ell \rangle$ for two different sites as functions of the energy eigenvalue $\tilde{E}_\ell$ in a fixed dimension $n = 1241$ Krylov subspace. The lighter colored dots correspond to a site in region A and the darker (blue) dots to a site in region B. The values of n_i are larger for region A since the initial state has all the bosons there. Right: the same for two different single particle state occupation numbers, the lighter colored curve for the lowest energy state and the darker (blue) curve for an excited state, which is occupied only when the total energy is large enough. The dimension of the full Hilbert space N increases from bottom to top, the plots clearly showing that the functions become smoother as a result.

Diagonalization of the reduced Hamiltonian was done using the Lanczos method in which the Hamiltonian becomes tridiagonal. The resulting matrix is equivalent to the one of a tight-binding Hamiltonian for a particle hopping on a one-dimensional chain with site and bond disorder. This analogy allows us to apply results pertaining to Anderson localization phenomena to understand some properties of the Ritz states. In particular, the states at the edges of the spectrum, for which Lanczos iterations have already converged, correspond to localized states in the Anderson problem, and the states in the middle of the band, for which $\langle \tilde{E}_\ell | \hat{A} | \tilde{E}_\ell \rangle$ varies smoothly, to the extended states.

Following the time evolution via (7) shows that the occupation numbers n_i thermalize, that is, become to a good accuracy time-independent at sufficiently large times. We now show how thermalization can be understood as a consequence of generation of a large entanglement entropy between subsystems. Dividing the system in fig.1 into subsystem A, the 3×3 block, and subsystem B (the large block), we consider the entanglement entropy given by $S_{AB}(t) = -\mathrm{tr}(\rho_A \ln \rho_A)$, where ρ_A is the density matrix associated with subsystem A. Numerically, we consider an initial state with all bosons in region A and compute $S_{AB}(t)$; the result is plotted in Fig. 3b. The overall shape of the curve with the entropy rising and then decreasing is similar to that discussed by Page [22] in relation to the entropy generation in black hole formation and evaporation. That the entanglement entropy thermalizes suggests that it should also obey the ETH, a fact that is made evident in Fig. 3a.

The behavior of $S_{AB}(t)$ at $t \to 0$ can be understood analytically. The density matrix can be Taylor expanded as

$$\rho_A(t) = \rho_A(0) + t^p \rho_A^{(p)} + \dots \tag{8}$$

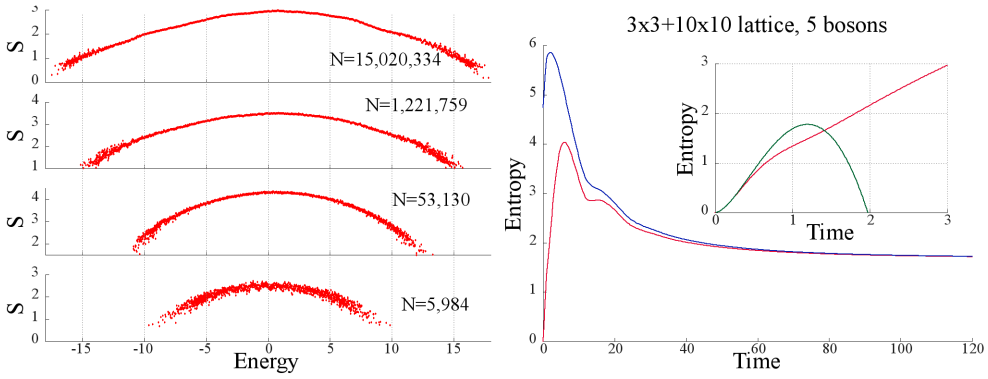
where p is an integer and $\rho_A^{(p)}$ is traceless. From the definition of the entropy, combined with perturbation theory to compute the eigenvalues of $\rho_A(t)$, it follows that

$$S_{AB}(t) = \langle \psi_A(0) | \rho_A^{(p)} | \psi_A(0) \rangle t^p \ln t^p + \dots \tag{9}$$

where $|\psi_A(0)\rangle$ is the initial state of subsystem A. This is a quite generic result. For the system and initial state we considered, a simple calculation shows that $p = 2$, in good agreement with the numerical result. At later times, the growth of entropy stops since the entanglement entropy is bounded by the thermal entropy; the latter is defined as the entropy of the canonical ensemble at the temperature and chemical potential corresponding to the average energy and particle number of the subsystem. Further, as more and more bosons leave the small box, the available thermal entropy decreases and so does the entanglement entropy as can be seen in the plot.

The asymptotic value $S_{AB}(t \gg t_{th})$ is close to the thermodynamics entropy, as expected [23, 24]. A surprising result from the numerics, however, is that the entanglement entropy becomes quite close to the thermal entropy much earlier than the thermalization time t_{th} of the entire system (t_{th} corresponding roughly to the largest times in the plot). Thus, by streaming particles into vacuum, subsystem A quickly reaches a mixed state close to thermodynamic equilibrium. This explains why local observables behave thermally and thus provides the sought after connection between thermalization of local observables, as envisioned by the ETH, and the growth of entropy.

We conclude with a comment on an application of the ETH to quantum gravity. As previously mentioned, black hole formation can be seen as a thermalization process. In classical gravity, the metric settles, independently of the initial state, to a time-independent value



(a) $S(\tilde{E}_\ell)$ (b) $S(t)$

FIG. 3: Left: Entanglement entropy $S_{AB}(\tilde{E}_\ell)$ as a function of the (Ritz) energy eigenvalue $\tilde{E}_\ell$ in a fixed dimension $n = 1241$ Krylov subspace. Right: Entanglement entropy (lower curve) and thermal entropy (upper curve) as functions of time. Inset: Initial growth of the entanglement entropy. At short times, the numerical result (monotonically increasing curve) matches the result of the series expansion.

characterized by a few conserved numbers (total energy, angular momentum, charge). This is known as the no-hair theorem [25]. If we accept the ETH as the general reason for thermalization in quantum systems, we are led to the conclusion that the quantum counterpart of the no-hair theorem is the statement that the metric is an operator obeying the ETH. Thus, we propose a **no-hair=ETH** equivalence, which asserts that the metric has the same average and the same few-point correlations functions in all energy eigenstates with close-by values of energy (charge and angular momentum). This point of view is consistent with the idea that quantizing the metric is not the right way to identify the microscopic degrees of freedom that describe a black hole, any more than quantizing sound waves is sufficient for discovery of the molecular nature of matter [26].

In summary, by using Krylov subspace techniques, we have extended numerical tests of the ETH to systems much larger than those amenable to direct diagonalization. We have also provided evidence that thermalization of isolated systems, even those in individual pure states, can be understood at the level of subsystems in terms of a rapid growth of the entanglement entropy. The close parallel between the ETH and the no-hair theorem of classical gravity suggests an application of these ideas to quantum physics of black holes.

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