Project report: Numerical study of the many body localization transition

David J. Luitz*
Institute for Condensed Matter Theory,
University of Illinois at Urbana-Champaign and
Department of Physics T42, Technische Universität München, Germany
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This project addressed important fundamental questions concerning thermalization and information transport in strongly interacting generic quantum matter. It provided important details for a better understanding of the mechanism of thermalization in isolated quantum systems and the nature of the many-body localization transition. We were able to perform exact simulations of very large systems up to $L = 31$ spins $1/2$, which is a particularly challenging task due to the exponential growth of the Hilbert space which was as large as $3 \cdot 10^8$.

Our results led to the discovery of subdominant corrections to the eigenstate thermalization hypothesis in subdiffusive systems and surprising features of the probability distributions of matrix elements of local operators in the eigenbasis of the Hamiltonian. They pointed to a coexistence of thermal and localized states at the many-body localization transition and they identified slow information transport prior to the transition, which is reflected in a power law light cone structure of the out of time ordered correlation function.

I. PROJECT INFORMATION

Title: "Numerical study of the many body localization transition".
Type: Illinois exploratory allocation.
Period: November 20, 2015 until December 31, 2016.
PI: **Dr. David J. Luitz**.
Institution: Technische Universität München, Germany.
Usage of Computational resources: 50000 node hours.

II. DESCRIPTION OF RESEARCH ACTIVITIES AND RESULTS

A. Key Challenges

We focus on one dimensional isolated quantum systems which are relevant for our fundamental understanding of statistical mechanics and thermodynamics as well as in their experimental realization in cold atomic systems. Generically, such systems are expected to thermalize via the so called *Eigenstate thermalization hypothesis* (ETH)[1–4], which assumes that matrix elements of local operators in the eigenbasis of the Hamiltonian become a smooth function of energy in the thermodynamic limit. For finite systems, ETH predicts noise on top of this smooth function of energy, which has a Gaussian probability distribution whose variance decreases exponentially with system size. ETH ensures that a finite system relaxes to thermodynamic equilibrium in the limit of very long times, if prepared initially to a nonequilibrium state and in the absence of a heat bath or any other contact to the environment.

While such a behavior is expected for generic interacting quantum systems without conservation laws that might prevent thermalization, surprisingly it turns out that there are strongly disordered systems which do not thermalize even though they are strongly correlated. The mechanism for this absence of thermalization is similar to what happens in disordered noninteracting models that exhibit Anderson localization[5]: The systems develops robust integrability at strong enough disorder through the formation of local conserved quantities, which are called l-bits[6–9] and becomes *many-body localized*[10,11] (MBL).

Many numerical studies[12–15] on small systems have observed so far the phenomenology in one dimensional spin models that at weak disorder ETH is valid, while at strong disorder it is broken and the system is in the MBL phase, however a detailed theory of the MBL transition is still lacking. Therefore, it is important to obtain accurate results for very large systems in order to understand the influence of finite size effects and to approach the sizes relevant for experiments (several hundred particles[16]). In this project, we studied the random field Heisenberg chain given by the Hamiltonian

$$\mathbf{H} = J \sum_i \mathbf{S}_i \mathbf{S}_{i+1} + h_i S_i^z, \tag{1}$$

where the disordered magnetic fields h_i on site i are randomly drawn from a box distribution between $-W$ and W, with the disorder strength W in units of the interaction strength $J = 1$. Previous studies[12,14] established that this model exhibits an MBL transition at a critical disorder strength $W_c \approx 3.7$. At intermediate disorder, in the ergodic phase, it was suggested that the dynamics in the system is slower than diffusive[13,17,18].

The key challenges we focussed on in this project, were

1. to provide *high precision* numerical evidence for slow dynamics in the ergodic phase and the consequences for ETH.

2. to study the nature of transport of quantum information in the ergodic phase, where particle transport is subdiffusive.

3. to address the nature of the MBL transition.

B. Why it Matters

The impact of this project is both fundamental and technical. Clearly, a theoretical understanding of thermalization and the conditions for its failure is an important contribution to fundamental research. By providing exact numerical results in realistic model systems, it is possible to consider in great detail various aspects of thermalization and numerical observations will drive future theoretical work, for which we already made first steps in this project.

The technological aspect is to push the feasible problem dimensions on an extremely powerful machine, exploring limitations of current numerical methods. Here, we have used a method for the calculation of eigenpairs in the middle of the spectrum of very large sparse matrices using a shift and invert technique. The inversion step is based on a massively parallel implementation of the Gauss elimination algorithm provided by the `MUMPS` library[19,20], allowing us to push the problem dimension to more than 700000. The second method that we use is exact time evolution of quantum wave functions. It is based on the product of the matrix exponential $\exp(-i\mathsf{H}t)$ and the wave function vector $|\psi\rangle$, where t is the time variable and H is the (sparse) Hamiltonian operator. The action of the matrix exponential on the wave function vector can be efficiently calculated[21] by projecting the matrix exponential onto the Krylov space spanned by the wave function at time t=0, which can be carried out in a massively parallel way. Using this methods, we were able to simulate problems with dimensions up to $3 \cdot 10^8$ using 64 Blue Waters XE nodes with 2048 highly optimized MPI processes. Our code is based on the `PETSC`[22,23] and `SLEPC`[24] libraries.

Our experience from these calculations is very useful for future projects.

C. Why Blue Waters

Blue Waters is a uniquely powerful computational resource which permits scientific achievements which are otherwise not possible. The research questions on thermalization in interacting isolated quantum systems which we addressed in this project can be formulated as challenging linear algebra problems, which are ideally suited for Blue Waters since the can be carried out in a massively parallel way. However, these problems are not embarrassingly parallel, since communication between the MPI processes involved in one simulation is paramount. In particular, the largest problems we were able to simulate do not fit in the memory of a single XE node and can therefore only be solved by distributing the memory over a large number of nodes.

In order to efficiently exploit a massively parallel machine like Blue Waters, it is important to base all codes on vendor optimized libraries for fast inter node communication like `MPI` and for Linear Algebra like Cray's `libsci`. The Blue Waters staff was extremely helpful in helping to compile the relevant codes and to link them against optimal implementations of MPI. The quick responsiveness and competence of the staff allowed for an efficient execution of the project, such that the all research goals were met and could be extended far beyond the scope of the initial proposal.

A crucial ingredient for the success of this project was the flexible extension of the initial timeframe which permitted the study of information propagation in a very large scale calculation[25], which required much more time to prepare than anticipated and could be completed successfully at the end of the extended allocation period.

D. Accomplishments

The allocation of resources on Blue Waters and in particular the generous availability of more than twice the amount of CPU cycles initially granted by using the "low" queue allowed us to address a large number of research questions which led to 5 well appreciated publications. The following accomplishments could be achieved.

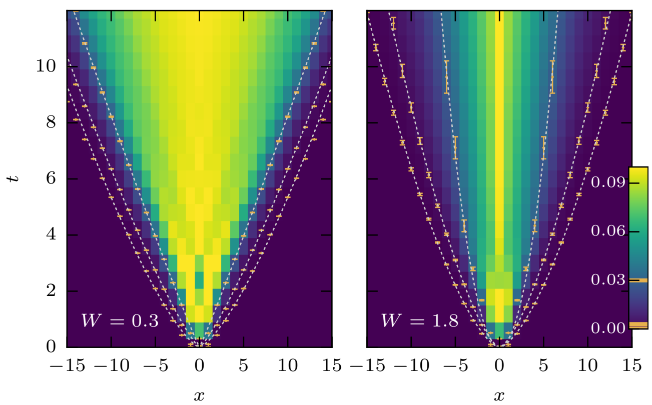

FIG. 1. Power law light cone structure in the operator norm of the commutator $[S_i^z, S_j^z]$ as a function of time t and separation $x = i - j$. i is fixed to 0 and two disorder strengths W are displayed for the $L = 31$ Heisenberg chain. These results are averaged over 50 to 100 disorder realizations.

- Better understanding of the MBL transition. In this subproject, we considered the scaling of the entanglement entropy in high energy eigenstates with subsystem size very close to the MBL transition. We were able to demonstrate that the probability distribution of the slope of the entanglement entropy (as a function of subsystem size) becomes bimodal at the MBL transition *even in single realizations of disorder.* This is an important observation and points to a highly nontrivial nature of the transition. This research was published in Ref.[26].

- Generalized Thermalization Hypothesis. Using a very large scale simulation of the random field Heisenberg chain, partly relying on data from a previous project carried out on EOS (CALMIP, France), we studied matrix elements of local operators in the eigenbasis of the Hamiltonian to test ETH. In the subdiffusive regime, we discovered *strongly non-Gaussian* probability distributions using a tremendous amount of matrix elements to obtain very high precision statistics and to resolve the tails of the distribution. In a subsequent work, we could connect the offdiagonal matrix elements of the local magnetization to spin transport after a quench, which we simulated on Blue Waters using exact time evolution techniques. This led to the discovery of a generalized thermalization ansatz, which exhibits a slower scaling of the variance of the noise distribution with system size in systems which have subdiffusive transport. We have published these findings in Ref.[27] and[28].

- Review article on the ergodic side of the MBL transition. The current knowledge of the nature of the slow transport prior to the MBL transition at intermediate disorder is based on numerics of small to intermediate system sizes and full of puzzles. We have classified and thoroughly discussed the state of the literature and provided a detailed comparison of numerical results for transport exponents, adding new results obtained on Blue Waters to test important relations between these exponents. The review article is available as a preprint in Ref.[29].

- Information propagation in isolated quantum systems. We have studied the information transport in the random Heisenberg chain in terms of the time evolution of the commutator of two local operators $[S_i^z, S_j^z]$, which vanishes at time t=0 for $i \neq j$. Due to information propagation, the commutator acquires a finite value after a time which depends on the separation $i - j$ of the two operators. We have developed a method based on Lévy's lemma that allows for the calculation of the operator norm of the commutator by exact propagation of typical wave functions in time. This allowed us to obtain exact results for unprecedented system sizes, up to $L = 31$ spins, corresponding to a Hilbert space dimension of about $3 \cdot 10^8$ and more than doubling the system size of previous calculations. These large system sizes allowed us to study the shape of the "light-cone" within which information propagates and to establish that slow information transport leads to a power law shape of the light cone in contrast to a linear light cone which we find in the case of clean diffusion. An illustration of the main result obtained from the largest simulation using 64 Blue Waters XE nodes for a single disorder realization is shown in Fig. 1. We also tested important predictions on the growth of the commutator with time and the decay with separation and found that surprisingly there is no exponential regime. This research is potentially of very high impact and available as a preprint in Ref.[25].

III. LIST OF PUBLICATIONS

Research in this Blue Waters project led to 5 publications[25–29], one of which is published in Physical Review Letters, two in Physical Review B and two preprints, one submitted to Annalen der Physik[29] and one to Nature Physics[25].

- **D. J. Luitz** and Y. Bar Lev, *"Information propagation in isolated quantum systems"*, arXiv:1702.03929, Ref. 25
- **D. J. Luitz** and Y. Bar Lev, *"The Ergodic Side of the Many-Body Localization Transition"*, arXiv:1610.08993, Ref. 29
- **D. J. Luitz** and Y. Bar Lev, *"Anomalous thermalization in ergodic systems"*, Phys. Rev. Lett. **117**, 170404 (2016), arXiv:1607.01012, Ref. 28
- X. Yu, **D. J. Luitz** and B. K Clark, *"Bimodal entanglement entropy distribution in the many-body localization transition"*, Phys. Rev. B **94**, 184202 (2016), arXiv:1606.01260, 26
- **D. J. Luitz**, *"Long tail distributions near the many body localization transition"*, Phys. Rev. B **93**, 134201 (2016), arXiv:1601.04058, 27

* david.luitz@tum.de

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