Accessing Many-Body Localized States through the Generalized Gibbs Ensemble

Stephen Inglis and Lode Pollet

Phys. Rev. Lett. **117**, 120402 — Published 13 September 2016

DOI: 10.1103/PhysRevLett.117.120402

Accessing many-body localized states through the Generalized Gibbs Ensemble

Stephen Inglis[1] and Lode Pollet[1]

[1]*Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 Munich, Germany*

We show how the thermodynamic properties of large many-body localized systems can be studied using quantum Monte Carlo simulations. We devise a heuristic way of constructing local integrals of motion of high quality, which are added to the Hamiltonian in conjunction with Lagrange multipliers. The ground state simulation of the shifted Hamiltonian corresponds to a high-energy state of the original Hamiltonian in case of exactly known local integrals of motion. The inevitable mixing between eigenstates as a consequence of non-perfect integrals of motion is weak enough such that the characteristics of many-body localized systems are not averaged out, unlike the standard ensembles of statistical mechanics. Our method paves the way to study higher dimensions and indicates that a fully many-body localized phase in 2d, where (nearly) all eigenstates are localized, is likely to exist.

Introduction – Many-body localization (MBL) addresses the fundamental question under which conditions quantum systems can avoid ergodicity and thermalization, thereby generalizing Anderson localization to interacting systems [1–7]. The widely accepted mechanism for thermalization in quantum systems is the eigenstate thermalization hypothesis [8–10]: Under very mild assumptions, (almost) every eigenstate of the system is thermal. This implies that the reduced density matrix of a small subsystem, obtained by tracing out the degrees of freedom of the considered (eigen)state outside the subsystem, is indistinguishable from the thermal density matrix with an effective temperature that depends on the energy density of the chosen eigenstate. MBL states, on the contrary, retain knowledge of their initial local conditions in local operators for asymptotically large times. The picture of local integrals of motion (LIOM) [11–16] can explain most of the unusual phenomenology of MBL states: its area law [17] leads to a logarithmic growth of the entanglement entropy, and the dc conductivity is identically zero. The LIOMs are the conserved quantities that prevent a MBL system from thermalizing – if one tried to construct them in the ergodic case, one would find that each operator is delocalized over the entire system. Dynamics is a decisive characteristic to distinguish between thermal and MBL states: experiments on trapped ions [18] and 1d cold atoms [19] demonstrated memory of the initial conditions over long periods of time for sufficiently strong disorder.

The thermodynamic predictions of a single-eigenstate ensemble differ fundamentally from the ones of the standard (micro-/grand-)canonical ensembles of statistical mechanics in the MBL phase. Obtaining a single, or even a certain class of eigenstates in the middle of the spectrum in order to prevent the averaging over all states with the same energy, which inevitably occurs in the standard ensembles, is a daunting task from a computational point of view because the mean level spacing decreases exponentially with system size. If one wants to study sufficiently large MBL systems, say of size at least 100 in 1d, the mean level spacing is far below the machine precision, meaning typical computational codes would be unable to differentiate them at all. So far exact diagonalization (ED) for disordered spin-1/2 systems could be performed for 22 sites using a shift-invert method [20]. With Density Matrix Renormalization group (DMRG) methods one could go to larger system sizes by using energy projection [21–23] according to $(\hat{H}-\sigma)^2$, with σ the target energy, or by using the successful shift invert $(\hat{H}-\sigma)^{-1}$ method [21], or performing the matrix product selection on the basis of explicit LIOMs [24].

In this Letter we show how quantum Monte Carlo methods can be used to study the equilibrium properties of MBL states provided the picture of LIOMs holds, which is the case in the fMBL (full-MBL) phase, where nearly all many-body eigenstates are localized [25–28]. The key idea is that, if by some technique a finite density of LIOMs can be constructed, they can be added to the action in conjunction with Lagrange multipliers. This creates a generalized Gibbs ensemble (GGE), which allows one to map MBL excited states to ground states, amenable to quantum Monte Carlo simulations for models without the sign problem. We provide a heuristic way of constructing LIOMs, whose quality can be tested a posteriori. Our method allows us to put a lower bound on the size of LIOMs, which can be used to positively identify the MBL phase when the localization length is below this bound. The present method can identify an ergodic phase whenever the LIOM construction fails entirely but only in the MBL phase can the properties of high-energy states be studied; we focus in particular on the eigenvalues and eigenvectors of the reduced one-body density matrix [29], which we apply here to hard-core bosonic instead of fermionic systems. The benefit of using quantum Monte Carlo is that it scales in a way that even 3d systems are attainable for a given set of LIOMs. Nevertheless, the quantum Monte Carlo part can be replaced by any other ground state method such as DMRG, and extended to arbitrary fermionic and spin models (as long as the sign problem is absent or remains tolerable).

Method – Our first objective is to generate a set of LIOMs (which are not unique) of sufficiently good quality such that the eigenstates are (nearly) unaffected when adding them to the action in conjunction with Lagrange multipliers. A number of procedures have been suggested in the literature, including infinite time evolution [15], self-similar transformations [30], renormalization methods [31] and perturbative approaches [14]. Although these approaches could be applied here, we need the LIOMs in a form compatible with existing quantum Monte-Carlo worm-type algorithms [32] in the implementation of Ref. [33], *i.e.*, we look for LIOMs in the form of L-bit operators $\mathbf{L}$ [6], defined over a finite support S, which contain operators that are only of nearest-neighbor hopping, local density or nearest-neighbor density-density type. Specifically, in 1d they take the form

$$\mathbf{L}^{(p)} = \sum_{i\in S} \mu_i^{(p)} n_i + \sum_{i,i+1\in S} t_i^{(p)} (b_{i+1}^\dagger b_i + h.c.) + V_i^{(p)} n_i n_{i+1}, \tag{1}$$

The coefficients $\mu_i^{(p)}, t_i^{(p)}$, and $V_i^{(p)}$ are optimization parameters for the L-bit defined on patch p. The support S is a strict subset of the sites p, $S \subset p$. We take the patches to be non-overlapping spatial sections of the full Hamiltonian. We seek to find the single best-possible L-bit of the above form over the patch p in the sense that the norm of the matrix of terms connecting different eigenstates (similar to the commutator) is as small as possible. In a fMBL system the proximity of the atomic limit suggests that Eq. (1) is a good parametrization. L-bits defined over different patches have an exponentially small overlap. Note that our design consists of finding some approximate L-bits (not all possible ones) which in general have a spectrum of more than 2 states (hence the notion L-bit also acquires the meaning of *enlarged* bits). Other design criteria are possible but left for future work.

To find the L-bits we use full diagonalization [16]. We enforce that the width of the L-bit spectrum be equal to 1 in order to meaningfully compare the quality of the proposed L-bits. We rotate the L-bit to the eigenbasis of the patch Hamiltonian, $\tilde{\mathbf{L}} = \mathbf{U}^\dagger \mathbf{L} \mathbf{U}$ with U the matrix of eigenvectors of the patch Hamiltonian. In case that $[\mathbf{L}^{(p)}, H^{(p)}] = 0$, $\tilde{\mathbf{L}}^{(p)}$ is a diagonal matrix. We define the cost function as the Frobenius norm of the off-diagonal elements of matrix $\tilde{\mathbf{L}}^{(p)}$. A non-linear minimization solver is used to find the optimal parameters $\mu_i^{(p)}, t_i^{(p)}$, and $V_i^{(p)}$. Other ways to construct the L-bits can certainly be thought of (and avoid full diagonalization), and may perhaps be better suited to combine with tensor network state methods or yield a smaller value for the commutator; our goal is merely to show that using the GGE is realistic and robust.

To check whether the operators thus found are L-bits of good enough quality, we shift the original Hamiltonian with the optimal L-bits found over the N_p patches and examine the ground state of the GGE Hamiltonian

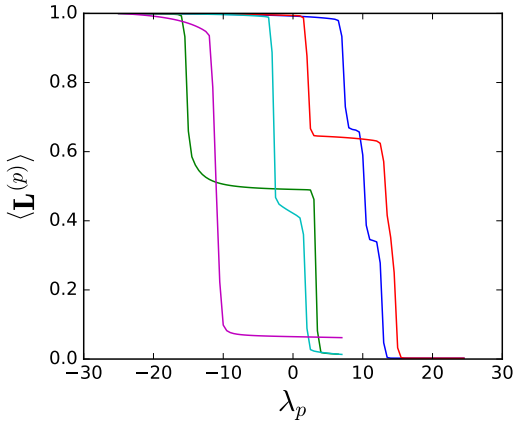

FIG. 1: (Color online). Expectation value of 5 different L-bits with 5 independent λ for $\Delta = 6$ on a support of 3 sites in a patch of 11 sites for the 1d Heisenberg model in a random magnetic field. Distinct plateaus are seen for each $\langle \mathbf{L}^{(p)} \rangle$ showing that the L-bits represent well-defined quantities.

$$\mathbf{H}_G(\lambda_1, \ldots \lambda_{N_p}) = \mathbf{H} + \sum_{p=1}^{N_p} \lambda_p \mathbf{L}^{(p)}. \tag{2}$$

We investigate each of the $\langle \mathbf{L}^{(p)} \rangle$ as a function of λ_p in a quantum Monte Carlo simulation. Our tests show that the value of the $\langle \mathbf{L}^{(p)} \rangle$'s can, to a very good accuracy, be set by the respective λ_p independently of the L-bits on the other patches. If successful, $\langle \mathbf{L}^{(p)} \rangle$ shows large plateaus separated by sharp jumps, *i.e.*, the L-bit selects the ground state based on the expectation of the L-bit for that state without mixing the states. When no plateaus can be found, the L-bit must be discarded. If no L-bits at all can be found, then the procedure failed and the system is very likely ergodic or has a very large localization length. Deviations from a flat plateau are an indication of how much hybridization took place as a consequence of non-ideal L-bits and the truncation of their exponential tails. This averaging is however tolerable because it averages low energy states within the GGE (which are all within a given L-bit sector), in contrast to the (micro)-canonical averaging which averages over all orientations of the L-operators within a narrow energy window. In the MBL phase one can move states around in the spectrum by choosing the λ_p according to different plateau values. The difference in energy between the plateaus is proportional to the energy gain in the many-body spectrum. Note that, in contrast to textbook Legendre transformations, our L-bits are intensive operators and we need a finite density of them in order to reach high-energy states.

Results in 1d – We now apply this construction to the 1d spin-1/2 Heisenberg chain with disorder in the magnetic field. For convenience, we write the Hamiltonian

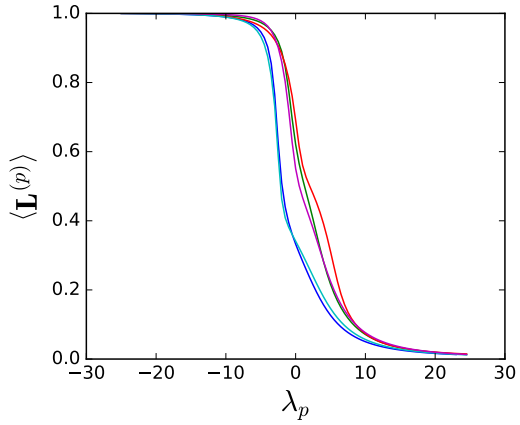

FIG. 2: (Color online). Expectation value of 5 distinct L-bits for $\Delta = 1$ on a support of 3 sites in a patch of 11 sites for the 1d Heisenberg model in a random magnetic field. No plateaus are seen in the range $\lambda \in]-10, 10[$; all attempted L-bits are hence discarded.

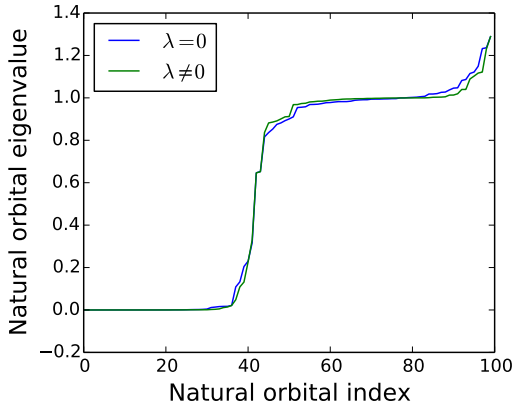

FIG. 3: (Color online). Comparison between the sorted eigenvalues corresponding to the natural orbitals in the ground state and a MBL state for the 1d Heisenberg model for $\Delta = 6$. We constructed 12 L-bits on a system of size 100. The ground state energy is $E/J = -180.67(1)$ and the energy of the excited state is $E/J = -135.98(1)$.

in the hard-core boson language as $H = -t\sum_i b_i^\dagger b_{i+1} + 2t\sum_i n_{i+1}n_i + \sum_i \mu_i n_i$, where μ_i is drawn uniformly from $[-\Delta, \Delta]$ and the hopping amplitude is set to one, $t = 1$. The system is fMBL for $\Delta > 3.5$ according to the full diagonalization results of Ref. [20] (However, Ref. [34] shows that truly zero dc conductivity may require much larger disorder strength).

First, we compare the quality of the plateaus as a function of the value of the corresponding Lagrange multiplier in the fMBL phase (Fig. 1) and in the ergodic phase (Fig. 2). In the fMBL phase, sharp plateaus are observed indicating that the respective L-bits (nearly) commute with the Hamiltonian. For $\lambda_p = 0$ we always see a well-defined plateau, corresponding to the localized ground state of the original Hamiltonian. By contrast, in the ergodic phase no clear plateaus can be discerned, which is also obvious from the strong hybridization at $\lambda_p = 0$.

To judge the quality of the L-bits, we define a measure

$$Q = \sum_k^n \left(\langle \mathbf{L}(\lambda^k) \rangle - \langle \mathbf{L}(\lambda^{k+1}) \rangle \right)^2 \qquad (3)$$

where λ^k are a mesh of points and $\mathbf{L}(\lambda^k)$ is the value the L-bit takes in $H_G(...)$. The number of λ^k points is fixed for every L-bit, and the spacing is determined by the energy density of the original ground state because, typically, the magnitude of λ needed to change $\langle \mathbf{L} \rangle$ scales with this quantity. This measure is inspired by the inverse participation ratio, and has a maximal value of 1 in the case of a single large jump of size 1 (the width of the L-bit spectrum) separating two perfectly flat plateaus.

Second, when good plateaus are found, we invoke transitions by selecting values of the Lagrange multipliers corresponding to plateaus found for $\lambda_p \neq 0$. The quantum Monte Carlo simulation projects on the ground state of the shifted Hamiltonian and gives us access to its thermodynamic properties, including the single particle density matrix, from which we can extract the localization length and which we diagonalize in order to obtain the natural orbitals (effective single particle picture) and their corresponding eigenvalues. According to Ref. [29], the sorted eigenvalues show a sharp jump in the MBL phase for a fermionic system. This is also seen in Fig. 3: the jump seen for the ground state of the GGE Hamiltonian is very similar to the one of the original Hamiltonian. We were able to reach excited states that correspond to 25% above the ground state towards the anti-groundstate of the original bounded Hamiltonian. Furthermore, our results for local quantities remain invariant when increasing the system size and we saw no signs of superfluidity which would imply delocalization. Given the current state-of-the art of quantum Monte Carlo simulations with worm-type updates, fMBL properties of systems of several thousands of sites are feasible.

When we apply the same procedure to intermediate disorder strengths $\Delta \sim 3$, where the exact diagonalization results of Ref. [20] found a mobility edge (which is however contentious [35]), we can still find good L-bits but considerably fewer than in the fMBL phase. In Fig. 4 we see that the L-bits are always of poor quality in the ergodic phase (and must hence be discarded), almost always of good quality in the fMBL phase, whereas in the intermediate regime we get a broad distribution. Discarding the poor L-bits but making use of the high-quality ones, we could go up about 15% in energy for 9 L-bits over a system of size 100 for $\Delta = 3$. The properties of the natural orbitals indicate insulating behavior and we obtained a zero superfluid response, suggesting

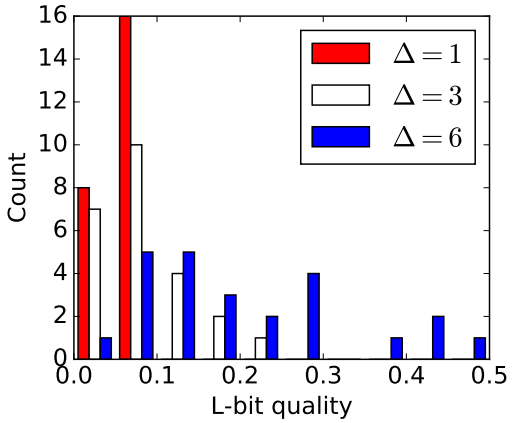

FIG. 4: (Color online). Histogram of the quality of the L-bit for different disorder strength using Eq. (3), where an ideal L-bit has a quality of one.

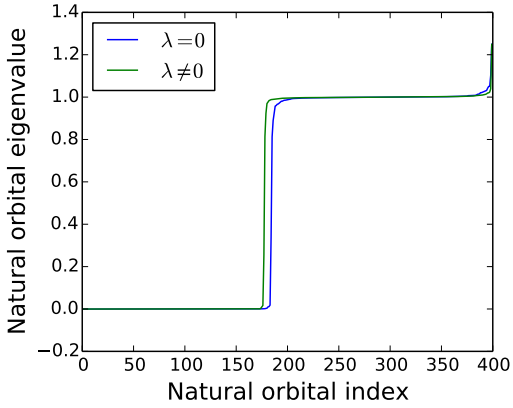

FIG. 5: (Color online). Sorted eigenvalues of the natural orbitals for the 2d Heisenberg model in the ground state and for a system with 40 L-bits obtained by quantum Monte Carlo simulation of size 20×20. The L-bits may change the particle number compared to the ground state, causing the shift in the location of the jump.

that at least some states in the spectrum are localized.

Results in 2d – The most appealing feature of a quantum Monte Carlo approach is the possibility to go to higher dimensions, which we demonstrate here by studying the 2d generalization of the disordered 1d Heisenberg model introduced before. Deep in the fMBL phase (assuming it exists) we take for the support a 2×2 cluster which is diagonalized over a 12 site patch (a 4×4 square excluding the 4 corners), and allow the same site- and bond-operators as in the 1d case. To test the quality of the L-bits, we embed them in a 20×20 lattice and measure the plateaus using quantum Monte Carlo simulations. For $\Delta/J = 40$ we are able to find L-bits with good plateaus, as shown in Fig. 6. Also the sorted eigenvalues of the natural orbitals of the system with an energy about 25% (40 L-bits were constructed) above the ground state

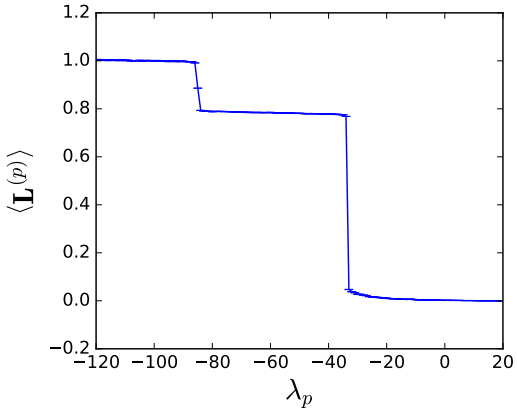

FIG. 6: (Color online). Illustration of the plateaus found for a single $\mathbf{L}$ as a function of λ for a 4-site L-bit embedded in a two dimensional 20×20 lattice with $\Delta = 40$. With large Δ effective L-bits can be optimized even when the embedding Hamiltonian is small.

show a pronounced jump similar as in the ground state. Fig. 5 demonstrates how the addition of the L-bits in 2d does not affect the natural orbital structure suggesting that fMBL can also be realized in 2d [36].

Conclusions – We have demonstrated the ability to find and implement L-bits, effectively allowing us to access excited states of a model as the ground states of a modified Hamiltonian which is related by a Legendre transform to the original model. When the L-bits do not exactly commute with the Hamiltonian, mixing occurs in the original Hamiltonian, but this does not destroy the MBL properties because local observables can distinguish between nearby eigenstates in the MBL phase. The system sizes that could be reached are substantially larger than with other methods, and the approach opens the way to study fMBL in dimensions higher than one. Our approach can also be combined with DMRG where more complicated operators in the L-bit construction can be taken into account, as long as the localization length remains sufficiently small. With a basic framework in place, there are a few natural extensions that can be explored in future work. It would be interesting to use a cost function which does not involve exact diagonalization over the patch, such as for instance DMRG or a stochastic optimization based on the quality of the plateaus as a function of the Lagrange multiplier, which could all be highly parallelized. Our approach relies crucially on the existence of the LIOMs and as such it is not clear whether it can be used to study the transition (or perhaps crossover [34]). Studying roperties such as the entanglement entropy (in higher dimensions) and observing resonances would be interesting.

Note – During the final stages of this work, a cold-atom experiment claimed the existence of a MBL phase in two dimensions [37] where the ground state is superfluid.

Acknowledgments – The authors would like to acknowledge inspiring discussions with E. Altman, B. Bauer, E. Demler, F. Heidrich-Meisner, D. Huse, D. Luitz, D. Pekker, N. Prokof'ev, F. Pollmann, and U. Schneider. This work was supported by FP7/ERC starting grant No. 306897 and FP7/Marie-Curie CIG Grant No. 321918. Part of the work of LP was performed at the Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1066293

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