Fixed Points of Wegner-Wilson Flows and Many-Body Localization

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Fixed points of Wegner-Wilson flows and many-body localization

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Many-body localization (MBL) is a phase of matter that is characterized by the absence of thermalization. Dynamical generation of a large number of local quantum numbers has been identified as one key characteristic of this phase, quite possibly the microscopic mechanism of breakdown of thermalization and the phase transition itself. We formulate a robust algorithm, based on Wegner-Wilson flow (WWF) renormalization, for computing these conserved quantities and their interactions. We present evidence for the existence of distinct fixed point distributions of the latter: a Gaussian, white noise-like, distribution in the ergodic phase, a $1/f$ law inside the MBL phase, and scale-free distributions in the transition regime.

Recent progress on the theory of many-body localization (MBL) demonstrates clearly that the conventional quantum statistical description of interacting many-body problems is incomplete. Concrete analytic [1], numerical [2–5] and mathematical [6, 7] results establish the existence and robustness of many-body localized phases in sufficiently strongly disordered and/or low dimensional interacting models at finite extensive entropy. While the understanding of the transition between thermal and MBL phases is only beginning to emerge [8–12] several distinct new directions of inquiry related to MBL and the fundamental issue of ergodicity in quantum many-body systems have taken shape. These include the interplay of MBL with spontaneous symmetry breaking and topological order [13–16], self-localization (glassiness) in translationally invariant quantum systems [17–20] and MBL in driven systems [21–23]. MBL has also stimulated considerable progress in developing tools for describing excited eigenstates of many-body systems [12, 24–28]. MBL has been realized in recent experiments [29, 30] and may also have important implications for quantum engineering problems, e.g. quantum computing [31–35].

One natural route to the breakdown of thermalization is via proliferation of a large number of conserved quasilocal quantities. The extreme version of such a proposal has gained considerable traction as a model phenomenology [36] of the so-called fully-MBL regime, where the entire many-body spectrum is localized. Consider a generic system, e.g. the n-site spin 1/2 random field Heisenberg chain (see Eq. 7), which is diagonalized by a (non-unique) unitary matrix U. This diagonal Hamiltonian may *always* be expressed in terms of n two-level systems (ℓ-bits) $\tau_j = U\sigma_j U^+$, such that the entire spectrum is correctly captured by a simple (classical) energy functional on τ_j^z's only (σ's are Pauli matrices representing microscopic spins). Importantly, we expect that for sufficiently strong disorder τ's can be made quasi-local [37], i.e. with finite overlap with the microscopic spin operators $\mathrm{Tr}[\sigma_j \cdot \tau_j] \neq 0$ in the thermodynamic limit and rapidly (exponentially) decaying tails. This overlap is analogous to the quasiparticle residue in Fermi liquids which allows for direct access to elementary excitations (τ's in our case) using external probes coupling to microscopic degrees of freedom (σ's). Although there is no universally accepted method for constructing ℓ-bits [38–42] as of yet, one may take finite overlap [40] as one design criterion (see Fig. 1 for a specific example of well behaved ℓ-bits obtained in this work, as explained below). In this letter we take a constructive definition of ℓ-bits as being generated by the unitary U obtained using the Wegner-Wilson flow (described below). Having constructed the finite residue ℓ-bits (τ's) we may ask about the structure of the effective Hamiltonian of the system, $H_{\mathrm{eff}}[\{\tau_j^z\}] \equiv UHU^+$ – this is referred to as the ℓ-bit Hamiltonian and its structure is the main focus of this work.

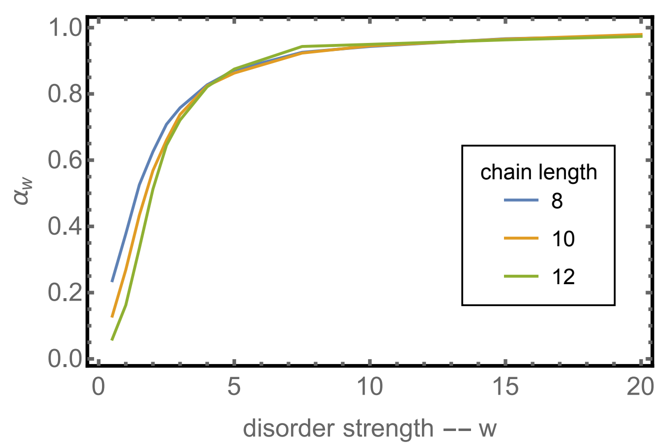

FIG. 1. Mean overlap α_w between physical- and ℓ-bit operators σ_1^x and τ_1^x as a function of disorder strength. The disorder averaging of the overlap was computed as $\alpha_w = \exp\left[\mathrm{mean}_{\mathrm{disorder}}(\log|\mathrm{Tr}\,\sigma_1^x\tau_1^x|)\right]$.

Results: We find that ℓ-bit Hamiltonians in the MBL phase are special because of a universal feature of their coupling constants: as we coarse-grain our view of the system to consider only coupling constants at large range, these coupling constants approach a broad power-law distribution similar to the broad distributions that are commonly associated with so-called infinite randomness critical points. This behavior contradicts mean-field-like form of spin-spin interactions characterized by a single decay length. In spite of the ℓ-bit phenomenology being the primary description of MBL, this is a heretofore unknown qualitative feature of these Hamiltonians and hence, of the MBL phase. Extension of this construction into the critical and ergodic regimes finds scale-invariant and narrowing distributions, respectively. This is suggestive of three kinds of fixed points - stable, MBL, and ergodic phases (with concomitant flows to 1/f and narrow distributions) and unstable critical point (scale invariant distributions). This structure addresses a key question about the universality of the transition and puts the MBL transition on the same footing as more general critical phenomena. Finite overlap with microscopic spin operators should enable observation of these distributions experimentally in finite chains and especially inside the MBL phase, using dynamical protocols such as DEER [43].

Methods: Here we describe how we construct the unitary using WWF. While all unitaries have the same values in them, they may differ from each other by the permutations of the columns and by a sign on each column. Wegner-Wilson flow is a robust algorithm for generating a unitary which constructs (numerical) functional renormalization flow from a given many-body Hamiltonian to its diagonalized form. In perturbative cases it correctly reproduces results obtained using Feynman diagrams [44], however, its true value lies in its nonpertubative nature, rooted in convergence properties for finite systems akin to those of the Jacobi rotation method for exact diagonalization [44, 45]. Unlike the typical renormalization group schemes, where one integrates out short distance/high energy degrees of freedom to obtain an effective action for the remaining low energy degrees of freedom, WWF works by decoupling degrees of freedom that are separated by large energies without removing any degrees of freedom. The flow generator, η, is computed [44, 46–48] by separating the Hamiltonian into diagonal (H_0) and off-diagonal (V) pieces with respect to a physically motivated basis (which we pick once at the beginning of the flow)

$$H(\beta) = H_0(\beta) + V(\beta), \tag{1}$$
$$\eta(\beta) = [H_0(\beta), V(\beta)], \tag{2}$$
$$\frac{dU(\beta)}{d\beta} = \eta(\beta), \tag{3}$$
$$\frac{dH(\beta)}{d\beta} = [H(\beta), \eta(\beta)] \ . \tag{4}$$

where β is the flow parameter ranging from 0 to ∞. Note that we are generally interested not only in $H(\beta)$ but also in $U(\beta)$, the transformation between $H(\beta)$ and $H(0)$ Note that $U(\beta = \infty)$ is the transformation which diagonalizes $H(0)$ and from which all other transformed operators may be obtained, e.g. τ's. WWF is a non-linear flow, with the off-diagonal part of $H(\beta)$ flowing to zero and therefore simultaneously reducing the size of η. Such flows only slow down when the problem is nearly diagonal, blithely integrating past would-be resonances that complicate ordinary perturbative treatments. The initial conditions for the flow are

$$U(\beta = 0) = \mathbb{1}, \tag{5}$$
$$H(\beta = 0) = H, \tag{6}$$

where H is the Hamiltonian we are diagonalizing in the original basis, and $U(\infty)$ and $H(\infty)$ are the quantities of interest.

A few comments are in order before we discuss the results. First, the WWF method is entirely deterministic, with an outcome which only depends on the initial basis choice. The method does bear some resemblance to other iterative diagonalization methods, such as Jacobi rotations or consecutive displacement transformations[42], and flow equation method with alternate generators [49], but it is not equivalent to them. For example, while Jacobi pivots away the largest off-diagonal matrix elements, WWF targets matrix elements connecting the largest energy splittings; alternately, the consecutive displacement transformations appear to be organized in the order of number of spin flips they induce. Also, while other methods are often comprised of discrete steps, WWF is a continuous flow, which may be an important advantage – in our side-by-side comparison studies (to be published in a separate longer paper) the outcomes of WWF consistently produces more local unitaries, as measured by entanglement of the unitaries, the locality of the ℓ-bits, and the locality of the diagonal ℓ-bit Hamiltonian, compared to those from methods such as bipartite matching [41] and Jacobi iterations (see supplement). In fact, we suspect that this may be true generally. This strong locality suggests that the $\ell-$bits constructed from WWF are reasonable ones.

For the purposes of this Letter, we only compress the structure of $H(\beta)$ and $U(\beta)$ by using sparse representation of these matrices; we show, however, (see Supplement) that $H(\beta)$ and $U(\beta)$ can be efficiently described by a low bond-dimension matrix-product-operator in the MBL phase and, so, using matrix-product technology could be a fruitful direction to pursue [12, 26, 41, 50–52]. In this work, we focus on obtaining and analyzing the ensemble of fixed points $H(\infty)$ and $U(\infty)$ using numerical integration of the flow equations Eqs.(1)-(4).

To improve performance, we used several tricks. Particular technical details include (1) Numerical integration was performed using Dormand-Prince method [i.e. Runge-Kutta(4,5)]. (2) WWF flow involves a very wide range of RG time scales, spanning from roughly the inverse many-body band-width to the inverse many-body level spacing. To accommodate this wide range of timescales, without resorting to an implicit integration scheme, in the course of integration the very small matrix elements in $H(\beta)$, associated with the short RG timescales, were dropped thus allowing the RG time step to grow as the WWF flow progressed. (3) WWF is only needed to decide on the permutation of columns and signs. Therefore we run WWF with a time-step that is too large to get values of the unitary to machine precision but small enough to faithfully capture the discrete permutation of columns/signs. We then execute a standard exact diagonalization routine (LAPACK) to generate exact eigenvectors which are used to replace the approximate WWF eigenvectors (keeping the WWF order and signs).

Model and analysis: We consider the random field Heisenberg model

$$H = \frac{1}{4}\sum_i \sigma_i \cdot \sigma_{i+1} + \frac{1}{2}\sum_i h_i \sigma_i^z, \quad (7)$$

on open chains where the h_i's are chosen from a uniform distribution $[-w, w]$. We focus on the analysis of $H(\infty)$ for (1) a range of chain lengths $L = \{8, 10, 12\}$, (2) disorder strength spanning the range from $w = 0.5$ to $w = 20$, and (3) a large number of disorder realization (500-1000 disorder realizations were generated for each L and w).

Before we begin the analysis of $H(\infty)$, we examine the possibility of *probing* it using external excitations, e.g. transverse field coupling to σ_j^x. To that end we compute and present overlaps between microscopic spin-flip operators σ_i^x and ℓ-bit spin-flip operators τ_i^x associated with the same site of the chain (see Fig. 1). In the MBL phase, these overlaps appear to be large and chain length independent. It is likely that these large overlaps persist in the $L \to \infty$ limit. On the other hand, in the ergodic phase, the overlaps are strongly chain length dependent, quickly shrinking as the chain length increases. The fact that the ℓ-bit spin-flip operators show a healthy overlap with corresponding microscopic spin-flip operators on the same site implies, among other things, that external time-dependent but local-in-space manipulations can be used to target ℓ-bit configurations.

We now focus on the analysis of $H(\infty)$

$$H(\infty) = E_0 + \sum_i J_i \tau_i^z + \sum_{i,j} J_{ij} \tau_i^z \tau_j^z + \sum_{i,j,k} J_{ijk} \tau_i^z \tau_j^z \tau_k^z + \dots. \quad (8)$$

Since WWF preserve all of the information about the many-body problem and because we only have results for few system sizes we need to introduce an additional parameter to elucidate scaling properties of the $\beta \to \infty$ problem. As with ordinary criticality, we expect real-space resolution of observables to be a natural direct way to proceed. Hence, we introduce the range r which is used to group the coupling constants $J_{i,j,\dots,k}$ that appear in Eq. (8) by the size of their footprint, i.e. the range for the terms $J_{2,5}$, $J_{2,4,5}$, and $J_{4,5,7}$ is $r = 4$. For a given r and w, we define $\mathcal{F}_{r,w}(J)$ as the distribution function of $|J_{i,j,\dots,k}|$'s sampled over all disorder realizations.

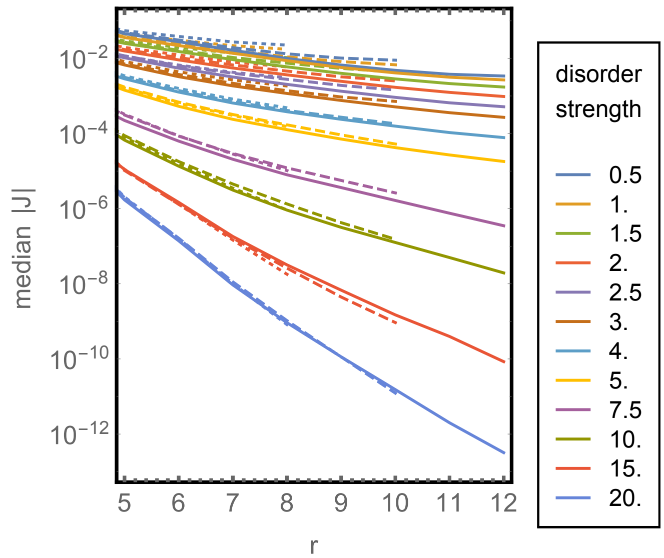

FIG. 2. Median $|J|$ as a function of range and disorder strength, for three different chain length ($L = 8$ dotted lines; $L = 10$ dashed lines, $L = 12$ solid lines.

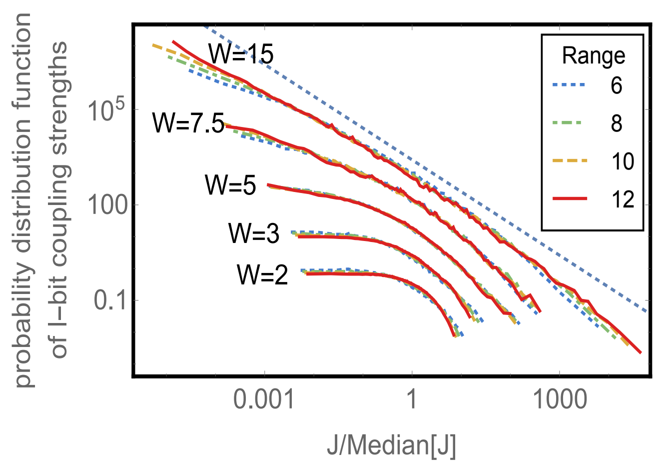

FIG. 3. Evolution of normalized ℓ-bit couplings with disorder (vertical offset: $W = 2, 3, 5, 7.5, 15$) and range (colors, see legend and explanation in text). The straight dotted line corresponds to slope -1, i.e. $\sim 1/|J|$ distribution.

We begin by focusing on the gross feature – the dependence of the typical value of $|J_{i,j,\dots,k}|$ on the range shown in Fig. 2. As expected, there is a strong, approximately exponential decay of median coupling with r in the MBL phase. As the exponential fit is not terribly good, and we do not know an improved functional ansatz (beyond simple exponential) inside the MBL phase, we do not extract an explicit value of the localization length. Also, perhaps surprisingly, there is an approximately exponential decay of couplings in the ergodic regime. While, at first sight,

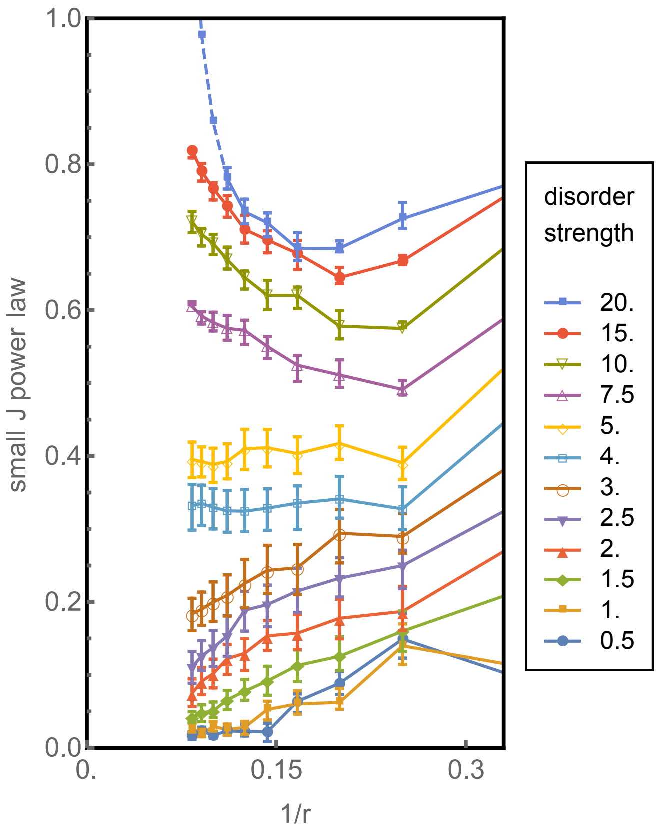

FIG. 4. Flows of the end-point Hamiltonian as a function of coarse graining and disorder strength. Specifically, we extract the small J power law from the distributions $\mathcal{F}_{w,r}(J)$ and plot these as a function of $1/r$ for various w's. Observe that flows at weak disorder tend to flat distributions (J^0), while flows at strong disorder tend to the ($1/J$) distribution. In between these two regimes (for $3 \lesssim w \lesssim 7.5$) the power law appears to be independent of the range indicating that the distributions $\mathcal{F}_{w,r}(J)$ are scale-free. The error bars indicate the uncertainty in fitting the small J data to a power law. The dashed line segments for $w = 20$ indicate that $\mathcal{F}_{w,r}(J)$ include J's that are below machine precision, and hence an accurate measurement of the power law was not possible.

the behavior in the weak disorder case is surprising, it is indeed consistent with Gaussian orthogonal ensemble (GOE) level statistics and hence ergodicity. Specifically, in order to observe GOE statistics for a given range r the typical value of $|J_{i,j,\ldots,k}|$ must exceed the level spacing $r2^{-r}$. This condition is indeed satisfied for our data in the weak disorder regime $w \lesssim 4$.

We now turn to the full counting statistics of J's which appears to show a much clearer flow with r than the median J itself, see Fig. 3. There are three clearly distinguishable regimes: (i) the couplings flow to the $1/|J|$ law everywhere in the MBL phase; (ii) the couplings flow to the approximately constant distributions (possibly gaussian?) in the ergodic phase; (iii) the couplings do not flow in the intermediate, critical, regime. The full distribution functions $\mathcal{F}_{r,w}(\mathcal{J})$ appear to form a one-parameter family $\mathcal{F}_{f(r,w)}(\mathcal{J})$, where $\mathcal{J} = |J|/\text{Median}[|J|]$ and the median is over all J's at given r and w (see Supplement). Due to the system size we are able to access, it is difficult to establish if there is a single scale-free intermediate fixed point or a critical phase between the ergodic and MBL phases.

Focusing on the small $|J|$'s we can recast these qualitative observations into a quantitative fit to power-law behavior $\mathcal{F}_{r,w}(\mathcal{J}) \propto \mathcal{J}^{-\alpha_{r,w}}$ for the small $\mathcal{J}$ part of the curve. We plot $\alpha_{r,w}$ as a function of $1/r$ in Fig. 4. As already foretold visually in Fig. 3 there is a flow (as $r \to \infty$) in α towards respectively white noise and $1/f$ laws below and above the critical regime residing near $3 \lesssim w \lesssim 7.5$.

Summary and outlook: We have applied a numerical implementation of the Wegner-Wilson flow renormalization group to random field Heisenberg chains. The properties of the fixed point (diagonal) Hamiltonians and corresponding unitaries are consistent with the phenomenology of fully MBL matter [36] when disorder is sufficiently strong. We have investigated the range-dependence of the end-point diagonal Hamiltonians produced by Wegner-Wilson flow. We found robust flow towards broad $1/f$-type distributions in the MBL phase and narrow white-noise-like distributions in the ergodic phase. At intermediate disorder, we found what appears to be a scale-free critical point or critical phase that demarcates the boundary between the ergodic and the MBL phases. To quantify these trends, we analyzed power laws in the small-J tails of the distribution. The dependence of the extracted power laws on range revealed bifurcating flows that seem to be an essentially universal feature of the MBL transition.

The $1/f$ type distributions we find bear some resemblance to the power-law distributions previously found in random $SU(2)_k$ and Heisenberg models using RSRG-X [16, 53]. We also note that the perturbative framework, e.g. as set up in Ref. 37, may provide a fruitful approach for obtaining such distributions deep inside MBL phases of generic models. We further speculate that our finding of scale-free distribution in the transition region may stimulate analytic work towards understanding localization-delocalization in interacting disordered models.

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