Letter

Local integrals of motion and the quasiperiodic many-body localization transition

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We study the many-body localization (MBL) transition for interacting fermions subject to quasiperiodic potentials by constructing the local integrals of motion (LIOMs) in the MBL phase as time-averaged local operators. We study numerically how these time-averaged operators evolve across the MBL transition. We find that the norm of such time-averaged operators drops discontinuously to zero across the transition; as we discuss, this implies that LIOMs abruptly become unstable at some critical localization length of order unity. We analyze the LIOMs using hydrodynamic projections and isolating the part of the operator that is associated with interactions. Equipped with these data we perform a finite-size scaling analysis of the quasiperiodic MBL transition. Our results suggest that the quasiperiodic MBL transition occurs at considerably stronger quasiperiodic modulations and has a larger correlation-length critical exponent than previous studies had found.

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Intuition suggests that isolated many-body systems initialized out of equilibrium should "thermalize" under their intrinsic unitary dynamics, in the sense of approaching a state in which *local* observables and correlation functions exhibit equilibrium behavior [1–4]. Since Anderson's work [5], it has been understood that thermalization is not fully generic: Systems subject to strong quenched randomness can instead exhibit a many-body localized (MBL) phase, in which thermalization fails, and the system instead retains a local memory of its initial conditions to arbitrarily late times [4,6–11]. This memory is due to the existence in the MBL phase of (quasi-)local operators that are *exact* integrals of motion, called local integrals of motion (LIOMs) or l-bits [11–19]. The existence of the MBL phase and of LIOMs has been established under minimal assumptions in one-dimensional random spin chains [11]; experimental evidence for the MBL phase exists in many different settings [20–33] (but see Refs. [34–41]). Rare regions—i.e., regions of a sample in which the disorder is anomalously weak or strong—play a central part in our understanding of MBL, determining the nature of the MBL transition [42–51], response on both sides of the transition [52–63], and even the stability of the MBL phase in higher dimensions [56,64]. However, many experiments on the MBL phase treat systems subject to *quasiperiodic* (QP) rather than random potentials [20,24,65–72]. Noninteracting 1d QP systems have a localized phase [73], which appears to be perturbatively stable in the presence of interactions [65]. However, rare regions are absent in QP systems, so it seems that the MBL transition—and the response near it—must differ qualitatively from the random transition [66]. The numerical evidence on the QP-MBL transition is mixed, with some studies casting doubt on whether a transition exists at all [74], while others find a breakdown of diffusion [67,75], potentially even in a regime where single-particle states are delocalized [76,77].

Most work on QP-MBL systems has worked in the Schrödinger picture, considering the properties of typical individual eigenstates across the transition. The response of typical eigenstates in the MBL phase to a probe will involve both the external QP potential and the self-generated *configurational* randomness from the random pattern of occupation of localized orbitals (which exert random Hartree shifts on one another). Thus from the eigenstate perspective there is no clear distinction between random and QP MBL systems; since the transition is really an instability of the MBL phase, one might be led to conclude that the transition should also be the same. In the present work, we instead take the *Heisenberg* perspective and focus on the properties of the LIOMs as operators [78]. In the QP-MBL phase, the pattern of LIOMs is QP, with LIOMs approximately repeating at regular distances that are rational approximants to the QP pattern; there are no rare regions with anomalous LIOMs. Thus from this operator perspective the QP and random MBL phases differ, and one would also expect the transition at which LIOMs cease to exist to differ, if rare regions are indeed important. (Whether this transition coincides with the transition into the thermal phase is an issue we revisit below).

In the present work we explicitly construct LIOMs in QP systems by time-averaging local operators, as first proposed in Ref. [15]. We perform the infinite-time average explicitly via full diagonalization {we also explore tensor-network methods [79] (see, also, references [80–84] therein)}. We analyze these LIOMs by computing the fraction of the operator norm that comes from n-fermion terms in the expansion $O = A_{ij}c_i^\dagger c_j + B_{ijkl}c_i^\dagger c_j^\dagger c_k c_l + \ldots$ using tensor-network methods to efficiently extract these quantities [79]. These n-fermion weights give us a handle on the specifically *many-body* effects that occur at the transition: Unlike transport and entanglement, it is not contaminated by the single-particle critical point, which lies somewhat near the apparent many-body transition.

We find that the n-fermion weights and the norm of the LIOMs give us new ways of analyzing the transition, pointing to a transition that occurs at larger values of the QP potential, with different critical exponents, than previously expected. This transition has notable similarities to the random case; in particular, the LIOMs slightly on the MBL side of the transition are tightly localized. Thus, as in the random case, it seems that the QP-MBL transition is an instability of the localized phase, which sets in at some critical value of the localization length. The microscopic origin of this instability remains unclear.

Model.– We consider the following model,

$$H = \sum_{i=1}^{L-1}(X_iX_{i+1} + Y_iY_{i+1} + VZ_iZ_{i+1}) + \sum_{i=1}^{L} h_iZ_i, \quad (1)$$

where X, Y, Z denote the Pauli matrices and $h_i = h\cos(2\pi/\varphi(i - L/2) + \phi)$, where $\varphi = \frac{1+\sqrt{5}}{2}$ and ϕ is a phase offset that we tune to translate our window. When $V = 0$, this is the noninteracting Aubry-André model which has localized eigenstates for $h > 2$ and extended eigenstates for $h < 2$. At nonzero V, finite-size exact-diagonalization studies [65–67] of the average eigenstate entanglement and level statistics ratio have found an MBL transition at $h_c \approx 3$ with a critical exponent $\nu \sim 1$. (However, studies on longer spin-chains using the time-dependent variational principle have seen a larger critical point, consistent with ours [70]). In this letter we set $V = 1/2$.

Following [15], we construct LIOMs for this model by time averaging a local operator O, which we choose to be $Z_{L/2}$. The time average of O is given by

$$\bar{O} \equiv \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\ O(t) = \sum_E \langle E|O|E\rangle |E\rangle\langle E|, \quad (2)$$

where $|E\rangle$ are eigenstates of H. In the MBL phase, we expect $\bar{O}$ to be an approximately local operator with exponential tails, i.e., we expect there is some operator O_n with support on n sites such that $\|O - O_n\|_F \leqslant e^{-n/\xi}$ where ξ is a characteristic localization length and $\|\cdot\|_F$ denotes the Frobenius norm. In the ergodic phase, the time average instead produces a non-local integral of motion, predominately the projection of O onto conserved charges. We construct $\bar{O}$ by full exact diagonalization, using Eq. (2). We explore finite-time averages, performed using exact diagonalization as well as matrix-product methods, in [79].

Fermion weights.— We analyze the LIOMs by expanding them in a basis of n-fermion operators. These are related to the Pauli operators by a Jordan-Wigner transformation, and evidently form a complete basis:

$$\bar{O} = \sum_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} w_1^{\alpha_1} w_2^{\alpha_2} \cdots w_{2L}^{\alpha_{2L}}, \quad (3)$$

where $\{w_i, w_j\} = 2\delta_{ij}$ are Majorana fermions. In what follows we will focus on two quantities: the Frobenius norm of the operator, $\mathcal{N} \equiv \mathrm{Tr}(\bar{O}^2)$, and its two-body weight f_2, defined by

$$f_2 = \frac{1}{\mathcal{N}}\sum_{|\boldsymbol{\alpha}|=2} |c_{\boldsymbol{\alpha}}|^2, \qquad \mathcal{N} = \sum_{\boldsymbol{\alpha}} |c_\alpha|^2. \quad (4)$$

We can also define four- and six-body weights accordingly. As f_2 is 1 for quadratic fermion operators, $1 - f_2 = f_4 + f_6 + \ldots$ measures the many-body content of the operator. (These weights can be efficiently computed using matrix-product operator methods; we outline these methods and present results on the weights f_n with $n > 2$ in [79]). Note that $\mathcal{N}$ and f_2 probe complementary aspects of the time evolution: $\mathcal{N}$ addresses how much of the initial-state information survives in the time average, while f_2 addresses what fraction of this information is encoded in "simple" (i.e., few-body) operators.

Hydrodynamic modes.— Fig. 1(a) shows the average and distribution of f_2. As we might expect, f_2 approaches 1 and we also find that $\mathcal{N}$ is of order unity in the MBL phase, since in this phase the LIOMs are approximately single-site occupation numbers. Less obviously, f_2 also approaches 1 deep in the thermal phase (although $\mathcal{N}$, not shown, goes to zero with system size). One can understand this as follows. The operator $O = Z_i$ has some overlap with the total conserved charge, $I_1 \equiv \sum_i Z_i$, which is conserved (and is a two-fermion operator), and also with the Hamiltonian $I_2 = H$ (which contains two- and four-point operators). More generally, in a system of size L, there are 2^L nonlocal conserved operators, i.e., projectors onto eigenstates, while the operator Hilbert space is 4^L-dimensional. Since the operator O at late times under chaotic dynamics is essentially random, its projection onto the conserved eigenstates would be exponentially small in L if it were not for local conservation laws. Neglecting these exponentially small components, one can write $\bar{O}$ in the thermal phase as its projection onto hydrodynamic modes using the (super) projector

$$\mathcal{P} = \sum_{l,k=1,2} |I_k\rangle\rangle C_{kl}^{-1} \langle\langle I_l|, \quad (5)$$

where $I_1 = \sum_i Z_i$ and $I_2 = H$ the conserved charges, acting on a Hilbert space $\mathcal{H}$, are now viewed as states on the doubled Hilbert space $\mathcal{H}\otimes\mathcal{H}$, and $C_{kl} = \langle\langle I_k|I_l\rangle\rangle$ the susceptibility matrix with $\langle\langle A|B\rangle\rangle \equiv 2^{-L}\mathrm{tr}(A^\dagger B)$. Since H and Q are both composed of two- and four-body operators, f_2 remains of order unity throughout the thermal phase.

Since the hydrodynamic modes exist on both sides of the transition and the projection of an operator onto these modes is a property of the $t = 0$ operator that is insensitive to critical properties, we subtract the projection onto this hydrodynamic subspace and define the "subtracted operator"

$$\bar{O}_{\mathrm{sub}} \equiv \frac{\bar{O} - \mathcal{P}(O)}{\|O - \mathcal{P}(O)\|}. \quad (6)$$

The denominator in Eq. (6) corrects for the fact that the hydrodynamic projection of O smoothly increases with increasing disorder, since the Hamiltonian is dominated by single-site potential terms. (Empirically, we find that not fixing the normalization of $\bar{O}_{\mathrm{sub}}$ leads to spurious finite-size drifts in small-system numerics). The norm $\mathcal{N}_{\mathrm{sub}}$ is defined as for the full operator. We also introduce the subtracted two body component, $\tilde{f}_{2\mathrm{sub}}$, defined as

$$\tilde{f}_{2,\mathrm{sub}} \equiv \frac{\sum_{i<j} |\mathrm{tr}(\bar{O}_{\mathrm{sub}} w_i w_j)|^2}{\sum_{i<j} |\mathrm{tr}(O_{\mathrm{sub}}(0) w_i w_j)|^2}. \quad (7)$$

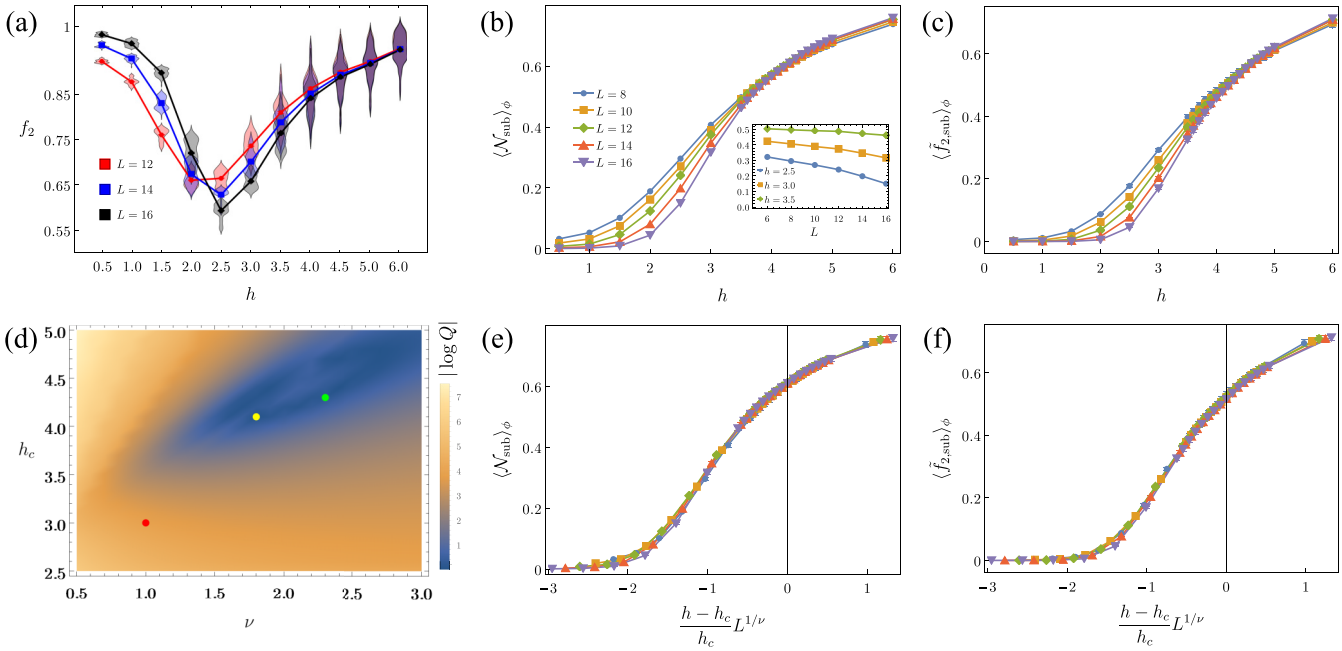

FIG. 1. (a) Evolution of the fraction f_2 of the weight of the time-averaged operator $\bar{O}$ that comes from fermion bilinears vs QP potential h. The solid lines are the average over the phase offset ϕ and the "violin" shapes indicate the distribution over ϕ (to see the behavior of the distributions one only needs to look at the "left" or "right" half of the violin). (b) Subtracted norm $\mathcal{N}_{\rm sub}$ of $\bar{O}$ vs h, where the subtracted operator is defined by projecting out hydrodynamic modes, Eq. (6). Note the crossing at $h \approx 4$. Inset shows the evolution of $\mathcal{N}_{\rm sub}$ with system size, indicating an instability that sets in as the system size is increased, even for $h = 3.5$ where previous studies have seen an MBL phase. (c) Two-body component of the subtracted operator, defined in Eq. (7); once again, this shows a crossing that is consistent with a discontinuous jump at the MBL transition. (d) The quality factor, Q, of the finite-size scaling collapse of the curves in (b, c) as a function of the chosen collapse parameters h_c, ν. Q is optimal when it is equal to 1 and in general $Q \geqslant 1$. The yellow dot marks the minimum of the cost function; by eye, the best collapse is for slightly different parameters (green dot) [these collapses are shown in (e) and (f)]. The transition seen in level statistics is marked by the red dot; our data are clearly inconsistent with these values. For all figures, averaging was performed over 200 phases equally spaced in the interval $(0, 2\pi)$. The color scheme for different system sizes is shared for (b), (c), (e), and (f).

The rationale behind this normalization is, once again, to correct for the changes in the four-fermion weight of the subtracted operator as a function of h.

Results.—Our results are summarized in Fig. 1. Figure 1(a) shows the two-body weight f_2 of the full time-averaged operator (which, as noted above, is always $Z_{L/2}$); as we expect, this is non-monotonic because it is dominated by hydrodynamic modes on the thermal side of the transition and by single-site operators deep on the MBL side of the transition. The sample-to-sample (or, equivalently, site-to-site) fluctuations of this quantity are large and size-independent deep in the MBL phase, negligible deep in the thermal phase, and intermediate in magnitude near the transition. Note that there is clear finite-size drift of f_2 for fields as large as $h = 4$, which previous literature [65–67] has assumed to be deep in the MBL phase.

We now turn to the properties of the subtracted operator (6). Fig. 1(b) shows its norm, which decreases with system size in the thermal phase but saturates in the MBL phase. The decrease in the thermal phase is consistent with an exponential [79], which is what we would expect since we projected out hydrodynamic contributions. Similarly, the subtracted two-body component $\tilde{f}_{2,\rm sub}$ decreases continuously in the thermal phase and saturates in the MBL phase: This is, again, expected since the residual finite-size contributions to $\bar{O}_{\rm sub}$ in the thermal phase are highly nonlocal and have negligible two-body components.

While both quantities vanish identically in the thermodynamic limit throughout the thermal phase, it is not *a priori* obvious whether they should rise continuously from zero or jump discontinuously at the MBL transition. Our numerical results strongly suggest the latter: The curves for both $\mathcal{N}_{\rm sub}$ and $f_{2,\rm sub}$ vs system size cross in the interval $h \in (4, 4.5)$; moreover, the crossing shifts weakly to larger h with increasing system size, suggesting that there are relatively "simple" LIOMs (with large two-body component) all the way up to the transition. This is consistent with a picture where the QP-MBL phase becomes unstable to thermalization at some critical value of the QP potential, but remains deeply localized all the way up to the transition. In the random case, "avalanche"-based theories of the MBL transition generally predict this behavior, and it is also consistent with the available numerical evidence [57,59,85–87]. However, since avalanches do not obviously occur in QP systems, this behavior is unexpected (and had not previously been numerically observed to our knowledge).

Another unexpected feature of these results is that the transition point and its critical properties differ quite strongly from those seen in previous numerical studies [Figs. 1(d)–1(f)]. Collapsing our finite-size data to the single-parameter scaling form $\phi(L, h - h_c) = \phi(L^{1/\nu}|h - h_c|/h_c)$, where ν is the correlation-length exponent, we find that the data collapses well in the parameter range $h_c \in (4, 4.5)$, with values of $\nu \in$

(2, 3). These results are very different from the expectation (gleaned, e.g., from studying the level statistics) that $h_c \approx 3$ and $\nu \approx 1$. In Fig. 1(d) we have plotted the figure of merit (specifically, the log quality factor $|\log Q|$ extracted from the Python package pyfssa [88]) for attempted data collapses with various possible combinations of h_c and ν: Our numerical data for the transition in the LIOMs are evidently inconsistent with previous predictions for the critical point. If anything, our scaling collapses show weak drift to larger values of h_c, suggesting that the transition might occur even deeper in the apparent MBL phase than our estimates above.

A clue as to why our results look so different from previous studies can be gleaned from the inset to Fig. 1(b). For $h = 3, 3.5$ (which would conventionally be regarded as critical and localized respectively), $\mathcal{N}_{\text{sub}}$ remains large for all the system sizes we study. However, it decreases with system size in a way that is *accelerating* at larger L. This pattern is not consistent with the expected finite-size effects in the MBL phase, which should scale as $e^{-L/\xi}$, where ξ is the correlation length, and should therefore flatten out at larger sizes. Rather, these results support a scenario in which the system seems localized on short scales, but then (beyond some critical scale ξ) realizes it is unstable. The scale ξ diverges as h is increased toward h_c and can be regarded as a correlation length.

Discussion.— In this work we studied the properties of LIOMs across the QP MBL transition, constructing them as time-averaged local operators. In the thermal phase, these time-averaged operators are just projectors onto global conserved quantities like the total energy and charge; once these hydrodynamic parts are subtracted out, the remainder of the operator vanishes rapidly. In the MBL phase, instead, a time-averaged local operator retains a finite norm, since it has nonhydrodynamic projections onto the LIOMs. There is a transition at which these LIOMs cease to exist and the norm of the subtracted time-averaged operator vanishes. This apparent transition has a critical point and critical exponents that are inconsistent with the apparent transition in observables such as eigenstate entanglement and nearest-neighbor-level statistics. Notably, the apparent correlation-length exponent $\nu \in (2, 2.5)$ that we extract from the finite-size scaling of the LIOMs is much larger than the Luck bound $\nu \geqslant 1$ (whereas previous results had $\nu = 1$, saturating the Luck bound). Indeed, we should emphasize that the results we have presented do not constitute strong evidence for the existence of an MBL phase at all and are in principle consistent with a transition that occurs at $h_c = \infty$; however, the MBL phase is perturbatively stable for sufficiently large h, and no nonperturbative instabilities have yet been identified, so we take the point of view that there is a transition in the window where we see one. A counterintuitive implication of our results is that if $\nu \geqslant 2$, the QP-MBL critical point is *perturbatively stable* against weak randomness by the Harris criterion [89]. (We note that a similar result was found using a real-space RG scheme in Ref. [68]). This could suggest either that there is a critical value of randomness required to change the universality class of the QP-MBL transition or that both the QP-MBL critical point and some part of the QP-MBL phase undergo a nonperturbative instability for infinitesimal randomness.

How can we reconcile our observations with the results on level statistics and entanglement? One possibility is that there are two separate transitions with distinct critical properties, one at which the level statistics changes its character and another at which LIOMs cease to exist. This could happen, for example, if there were an intermediate phase with a many-body mobility edge [90,91]. However, it is unclear whether such many-body mobility edges can exist [91] and, even if they do, the transition in entanglement should occur once the entire spectrum is localized. Thus it is not clear how this scenario could apply to our case. A second possibility is that the LIOMs we study here have weaker finite-size effects than the level statistics because they are less affected by state-to-state fluctuations that are large in finite systems [66]. (All known finite-size effects favor the MBL phase, so a higher h_c value is more plausible, assuming there is a single transition).

Our results shed light on the nature of this transition at which LIOMs cease to exist, which we tentatively identify with the MBL transition. In particular, we find that LIOMs even slightly on the MBL side are mostly fermion bilinears with large norm; thus, they overlap strongly with microscopic spins. The QP transition, like the random one, appears to be an *instability* of the MBL phase that sets in at some critical localization length as one increases the system size. In random systems, such an instability is thought to be seeded by rare regions that are locally thermal. Although rare regions do not exist, strictly speaking, in QP systems, one might still expect the instability to occur first in some parts of the sample. One might expect LIOMs to be unusually delocalized in samples that contain these parts. However, we do not see much evidence of enhanced heterogeneity at the transition (Fig. 1). It therefore seems that the instability we are seeing is due to the proliferation of many-body resonances in *typical* regions of the sample. The origin of these resonances remains to be identified.

Our work, like all ED studies, is inherently limited to small system sizes. An important question for future work is whether one can construct LIOMs for much larger systems. We attempted to do so by time-evolving local operators via time-evolving block decimation (TEBD) applied to matrix-product operators [79] and averaging over finite time windows. Unfortunately, to get a good approximation to the LIOMs away from the deeply localized limit, one must average over such long time windows (comparable to the Heisenberg time) that TEBD is impractical [79], because the bond dimension needed to describe the operator grows intractably large. Whether other forms of explicit time-averaging, e.g., based on Krylov-space methods [61,92], can provide access to larger systems and sufficiently long times is an interesting question for future work.

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