One-particle-density-matrix occupation spectrum of many-body localized states after a global quench

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The emergent integrability of the many-body localized phase is naturally understood in terms of localized quasiparticles. As a result, the occupations of the one-particle density matrix in eigenstates show a Fermi-liquid like discontinuity. Here we show that in the steady state reached at long times after a global quench from a perfect density-wave state, this occupation discontinuity is absent, which is reminiscent of a Fermi liquid at a finite temperature, while the full occupation function remains strongly nonthermal. We discuss how one can understand this as a consequence of the local structure of the density-wave state and the resulting partial occupation of quasiparticles.

Introduction.—One of the basic notions of condensed matter physics is adiabatic continuity [1]. The Fermi liquid, a major example, is adiabatically connected to the Fermi gas by slowly turning on interactions: the ground state of the Fermi gas evolves into that of the Fermi liquid and low-energy excited states evolve into excited quasiparticle states with identical quantum numbers [2, 3]. The quasiparticle density operators commute with the effective low-energy Fermi-liquid Hamiltonian and represent conserved quantities. The Fermi-liquid Hamiltonian is diagonal in the quasiparticle basis but is not quadratic as it contains quasiparticle density-density interaction terms that represent the back action of all the other particles on excitations. The Fermi liquid fundamentally relies on reduced scattering of quasiparticles due to limited phase space, provided by the Fermi-sphere structure of the ground state, and is therefore only a valid description at low temperatures compared with the Fermi temperature [2, 3].

Closed interacting disordered quantum systems can exhibit many-body localization (MBL) [4, 5], resulting in an ideal insulator with vanishing charge and thermal conductivities at finite, or even infinite [6, 7], temperatures. This MBL insulator is adiabatically connected to the Anderson insulator and therefore shares many features with the Fermi liquid [8, 9]. In contrast to the Fermi liquid, where only the ground state and the lowly excited states are adiabatically connected, in an MBL insulator *every* eigenstate is adiabatically connected to some eigenstate of the Anderson insulator—for example in fully many-body-localized systems [10] (with exceptions [11]) where the relation can be provided by a finite-depth quantum circuit [12]. The MBL phase is thus an emergent integrable phase [10, 13, 14] characterized by conserved quasiparticle densities, which are the density operators of Anderson orbitals locally dressed by particle-hole excitations [15–18]. The eigenstates are product states of these quasiparticles and therefore satisfy an area law of entanglement [12, 19, 20], necessarily violating the eigenstate thermalization hypothesis [21–23]. The construction of the conserved quantities (which in spin systems are commonly referred to as l-bits) is extensively studied [15–18, 24–31]. As in the Fermi liquid, the MBL Hamiltonian is diagonal in the quasiparticle basis, but contains quasiparticle density-density interaction terms, which are absent in the Anderson insulator [10, 13]. These interaction terms give rise to dephasing in dynamics that results in a logarithmic growth of entanglement entropy [32–34] (for examples of other quantum information measures, see [35–42]), and a slow relaxation of observables towards nonergodic stationary states at long times [43]. The adiabatic connectivity of the MBL phase to the Anderson insulator relies on the stability of Anderson localization against interactions and not directly on phase space arguments [4, 5, 15–17].

This formal analogy between MBL and Fermi liquids was further developed in Refs. 8 and 9, which evinced a Fermi-liquid-like discontinuity in the occupations of the one-particle density matrix (OPDM) in many-body eigenstates, analogous to a finite quasiparticle weight (see also Ref. 44). The discontinuity signals Fock-space localization and produces phase diagrams consistent with those obtained from other observables [20, 45]. The eigenvectors of the OPDM give localized orbitals, the natural orbitals, that can be used to construct an optimized single-particle approximation to the quasiparticles [9].

In a Fermi liquid the occupation spectrum is strictly discontinuous only at zero temperature; any nonzero temperature leads to a smooth and continuous occupation spectrum. With the MBL eigenstates providing an analog to a zero-temperature Fermi liquid, it is natural to ask if there is also a finite-temperature analog. We limit our consideration to temperature effects on quasiparticle occupations and assume that quasiparticle lifetimes are not affected. In this phenomenological analogy, in which each MBL eigenstate is a zero-temperature reference state, this requires partial occupations of quasiparticles compared with the reference occupations in a

given eigenstate. A generic combination of eigenstates, described by a mixed density matrix, does not work as this corresponds to summing over different random occupations of quasiparticles, or to mixing reference states. Instead, we propose that a global quench from a product state of local densities provides the physics we are after. Intuitively, a local density has a large overlap with some quasiparticle density. An expansion of such a local density in the quasiparticles will therefore mainly contain the quasiparticles localized close-by, as if they were excited by a relatively small effective temperature. In the remainder, we focus on a perfect density-wave state as the initial state. Such a product state still has systematic phase differences between different quasiparticles unlike in thermal states. During time evolution, however, this quasiparticle superposition dephases such that the initial phase relationship is scrambled in the infinite-time steady state. The main result of our work is a characterization of this steady state with one-particle density matrix occupations that indeed mimic occupation effects of temperature in a Fermi liquid. We further discuss the important difference between instantaneous and time-averaged density matrices in the many-body localized phase.

An initial density-wave state is also used in the ultracold atoms experiments [46–48] that observed a finite imbalance between the density on even and odd sites as a signature of the absence of thermalization [46] (see [49–52] for further experiments). As a corollary result we therefore obtain a relation between the OPDM occupations and experiments. In particular, we introduce an OPDM occupation imbalance, the difference in occupations between mainly occupied and mainly unoccupied natural orbitals, which behaves similar to the density imbalance, but with a slower relaxation towards the steady state, thereby capturing dephasing.

Model and methods.—We use a standard model of many-body localization, namely a system of spinless fermions hopping and repulsively interacting with their nearest neighbours in a disordered 1D lattice. Such a system is described by the Hamiltonian

$$H = J\sum_{i=1}^{L}\Big[-\frac{1}{2}(c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) + \epsilon_i\Big(n_i - \frac{1}{2}\Big) + V\Big(n_i - \frac{1}{2}\Big)\Big(n_{i+1} - \frac{1}{2}\Big)\Big], \tag{1}$$

where $c_i^\dagger$ creates a fermion on site i (among L sites) and $n_i = c_i^\dagger c_i$ is the number operator. Energies are expressed in terms of the hopping constant J, whereas disorder and interaction strengths are denoted by the dimensionless quantities W and V, respectively. The disorder is diagonal and taken from a box distribution $\epsilon_i \in [-W, W]$. We set $J = V = 1$ throughout this work, in which case the localization-delocalization transition is found to be at $W_c = 3.5 \pm 1$ for energies in the middle of the spectrum [7, 8, 20, 45, 53].

Using exact diagonalization, we study the system described in (1) for different system sizes L and average over 10^4 ($L = 8, 10, 12$), 5×10^3 ($L = 14$) and 4×10^3 ($L = 16, 18$) disorder realizations. We use periodic boundary conditions and fix the number of particles to half filling $N = L/2$. The symbol $\langle\cdot\rangle$ denotes the disorder average.

The initial state is a perfect density-wave state,

$$|\Psi_0\rangle = \prod_{i=1}^{L/2} c_{2i}^\dagger |0\rangle, \tag{2}$$

which then evolves under the Hamiltonian (1) according to (we set $\hbar = 1$) $|\Psi(t)\rangle = \exp(-iHt)|\Psi_0\rangle$. To characterize the state $|\Psi(t)\rangle$, we calculate the instantaneous one-particle density matrix

$$\rho_{ij}(t) = \langle\Psi(t)|c_i^\dagger c_j|\Psi(t)\rangle \tag{3}$$

and diagonalize it. The eigenvalues $\{n_\alpha(t)\}$, with $\alpha = 1, 2, \ldots, L$, are the occupations and the eigenfunctions $\{|\phi_\alpha\rangle\}$ are the natural orbitals. For each time, we order the OPDM occupation spectrum in descending order $n_1(t) \geq n_2(t) \geq \cdots \geq n_L(t)$, noting that the total particle number is conserved $\sum_{\alpha=1}^{L} n_\alpha(t) = \mathrm{tr}\,\rho(t) = N$ at all times.

Evolution of occupations.—We first address the nature of the temporal relaxation dynamics of the occupations $\{n_\alpha(t)\}$. In the initial state $|\Psi_0\rangle$, half of the occupations are equal to one and the other half equal to zero, i.e., $n_\alpha(0) = 1$ for $\alpha \leq N$ and $n_\alpha(0) = 0$ for $\alpha \geq N + 1$. It is worth noting that in the absence of interactions, for any finite W, the system is an Anderson insulator and both halves of the OPDM spectrum continue to be equal to one and zero at all times.

The time evolution of the occupation spectrum in the MBL phase is plotted in Fig. 1(a). Initially, the spectrum captures a fast expansion up to the localization length, followed by a slow relaxation in which the occupations approach their saturation values as a power law $\nu\, t^{-\gamma} + \delta$, starting at times of the order of $t \sim 10^2$ (see the inset). The power-law parameters δ, ν, and γ depend non-universally on α with the exponent γ ranging between 0.3 and 0.6. In Fig. 1(b), the time evolution of the single occupation $\langle n_N(t)\rangle$ is shown for both phases and at the transition ($W \approx W_c$). In the MBL phase ($W > W_c$), it undergoes a slow relaxation towards a non-thermal stationary state at long times ($t \sim 10^8$). This slow relaxation is due to dephasing and is characteristic of the MBL phase [43]. The instantaneous natural orbitals evolve from the initial onsite densities towards localized orbitals at long times, and the instantaneous occupations $\{n_\alpha(t)\}$ can therefore be seen as expectation values of local observables. In this sense, their approach to their stationary values is consistent with general arguments for power-law relaxation of local observables [43]. In the ergodic phase ($W < W_c$), in contrast, we observe a fast relaxation towards a thermal stationary state.

Steady-state properties.—On the basis of the above, it is natural to ask about the behavior of the occupation spectrum in the steady-state limit. To this end, we

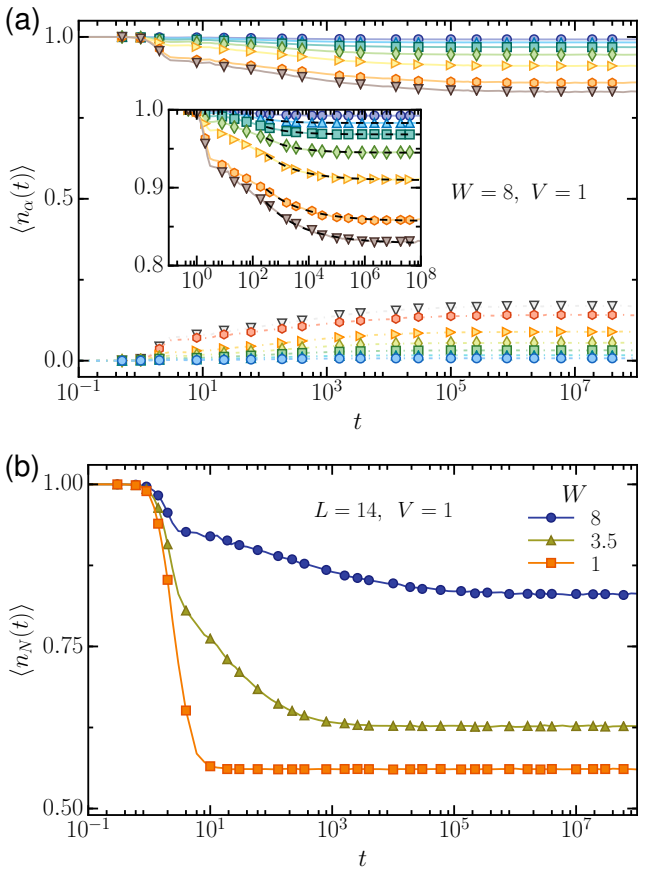

FIG. 1. (a) Evolution of the disorder-averaged occupation spectrum $\langle n_\alpha(t)\rangle$ deep in the MBL phase ($W = 8$). In the inset, the power-law relaxation (dashed lines, fits to the data) for the upper half of the spectrum is shown. (b) Evolution of a single occupation number, namely $\langle n_N(t)\rangle$, for both phases ($W = 1, 8$) and at the transition (W=3.5). $L = 14$ in both panels.

explore the asymptotic behavior ($t \to \infty$) of the time-averaged density matrix, which we can compare to density matrices that capture the separate effects of dephasing and thermalization. As we will see, the steady-state density matrix at long times is described by the diagonal ensemble in both the MBL and the ergodic phase; only the latter is additionally reproduced by a thermal ensemble. Specifically, expanding $|\Psi_0\rangle = \sum_n a_n|n\rangle$ in terms of the many-body eigenstates $H|n\rangle = E_n|n\rangle$, the time-evolved state takes the form $|\Psi(t)\rangle = \sum_n e^{-iE_n t}a_n|n\rangle$, and the density matrix is

$$\rho_{ij}(t) = \sum_{n,m} e^{-i(E_n-E_m)t}a_m^* a_n \langle m|c_i^\dagger c_j|n\rangle. \tag{4}$$

Taking the time average (denoted by $\bar{\cdot}$) yields

$$\bar{\rho} = \lim_{T\to\infty}\frac{1}{T-t_0}\int_{t_0}^{T}\rho(t)\,dt, \tag{5}$$

$$\bar{\rho}_{ij} = \sum_{n,m}\overline{e^{-i(E_n-E_m)t}}a_m^* a_n\langle m|c_i^\dagger c_j|n\rangle. \tag{6}$$

We take $t_0 = 10^5$ at which point the time evolution has reached a steady state. For a nondegenerate system, the phases in (6) are random and sum to zero if $n \neq m$; therefore

$$\bar{\rho}_{ij} \approx \sum_n |a_n|^2\langle n|c_i^\dagger c_j|n\rangle \equiv \rho_{ij}^{\mathrm{diag}}. \tag{7}$$

It is important to contrast the time-averaged density matrix with the instantaneous occupations in Fig. 1. The ordering of eigenvalues does not generally commute with time averaging, in particular if there is an interchange of occupations in the time evolution. This can be expected to occur in the MBL phase, where the eigenvalues correspond to local quantities separated in space and consequently do not couple. From now on, we therefore first time average the density matrix as in (5) and only then determine and order its eigenvalues, denoted by $\bar{n}_\alpha$, in descending order. This is also the experimentally relevant procedure in many experiments. The occupations $\langle\bar{n}_\alpha\rangle$ are plotted in Fig. 2 as a function of L and for three different values of W. In particular, we compare $\langle\bar{n}_\alpha\rangle$ with the ordered eigenvalues obtained directly from the diagonal ensemble (7), denoted with $\langle n_\alpha^{\mathrm{diag}}\rangle$; both are plotted in Fig. 2(a) as a function of L for $W = 8$, with excellent agreement. In the ergodic phase, we further find good agreement with the eigenvalues of the thermal OPDM, see Fig. 2(c), obtained from

$$\rho_{\mathrm{TH}} = \mathrm{tr}\left(\rho_c c_i^\dagger c_j\right), \tag{8}$$

where we use the density matrix of the canonical ensemble $\rho_c = e^{-\beta H}/\mathrm{tr}\,(e^{-\beta H})$, with inverse temperature β set by the requirement that the energy of the state be

$$E = \langle\Psi_0|H|\Psi_0\rangle = \mathrm{tr}\,(\rho_c H)\,. \tag{9}$$

The occupations obtained in the MBL phase are, in contrast, highly nonthermal as revealed by the comparison with the thermal occupation spectrum, plotted as stars in Fig. 2(a). The OPDM occupations tend to exhaust the full range of values between 0 and 1, similar to the occupations in eigenstates [8, 9], but with a discontinuity that goes exponentially to zero in the thermodynamic limit, see the inset in Fig. 2(a). This main result of our work suggests that a global quantum quench from a product state of local densities results in partial quasiparticle occupations and thus a continuous occupation spectrum. This behavior is similar to the effect of a finite temperature in a Fermi liquid.

The absence of the discontinuity is best understood in the diagonal ensemble. With the initial state being

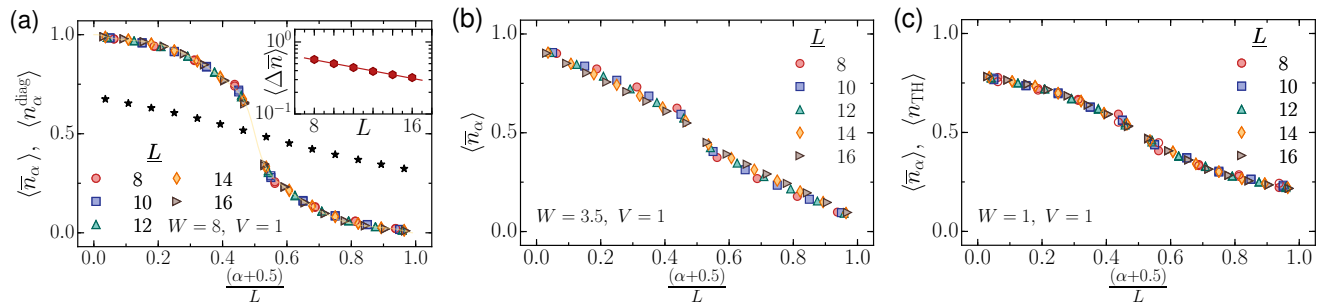

FIG. 2. Infinite-time and disorder-averaged distribution of occupations $\langle \overline{n}_\alpha \rangle$ as a function of system size L, for disorder strengths: (a) $W = 8$, (b) $W = 3.5$ and (c) $W = 1$. The horizontal axis is scaled to $(\alpha + 0.5)/L$ such that it runs from 0 to 1 in the thermodynamic limit. Additionally, (a) shows the diagonal-ensemble distribution $\langle n_\alpha^{\rm diag} \rangle$ for all L (open symbols), the thermal ensemble $\langle n_{\rm TH} \rangle$ for $L = 14$ (stars) and the inset contains the discontinuity $\langle \Delta \overline{n} \rangle$ as a function of L and a fit to an exponential $\sim e^{-0.6L}$. Figure (c) also contains the thermal distribution $\langle n_{\rm TH} \rangle$ for all L (open symbols).

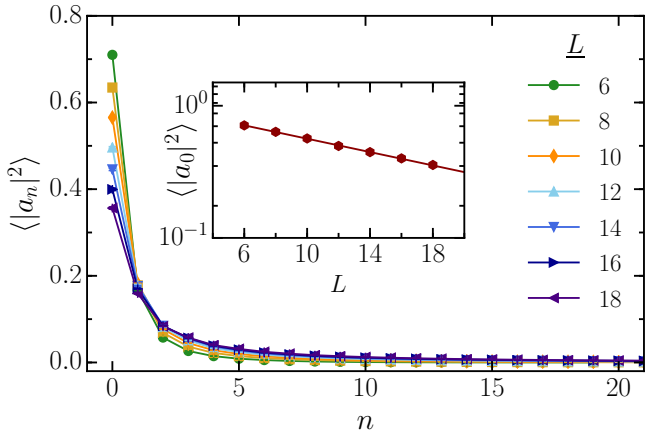

FIG. 3. Disorder-averaged overlap between the initial state $|\Psi_0\rangle$ and the many-body eigenstates $|n\rangle$, $\langle |a_n|^2 \rangle$, plotted in decreasing order $|a_0| > |a_1| > \ldots$ as a function of n for $W = 8$ and different system sizes L. Inset: disorder-averaged largest weight $\langle |a_0|^2 \rangle$ (see Eq. (7)) as a function of L as well as an exponential fit to $\exp(-bL)$, with $b = 0.06$.

a product state of single-site occupations, it has a large overlap with the eigenstates that have a large weight on these sites. The quenched state will, to first order in perturbation theory, inherit the step function from this eigenstate, while all the other states provide smearing of the step. To support this argument, we order the many-body eigenstates $|n\rangle$ according to their overlap with the initial state such that $|a_0| \geq |a_1| \geq \cdots \geq |a_n|$, and in Fig. 3, we plot the disorder-averaged overlap $\langle |a_n|^2 \rangle$ as a function of n. This function decays quickly with n and the largest overlap also decays exponentially with L, consistent with eigenstates built from N quasiparticles each with an overlap with absolute value $c < 1$ with a given site density, and therefore, a total overlap that scales like $|a_0| \propto c^N$. The maximum-overlap eigenstate $|0\rangle$ has an OPDM $\rho^{(0)}$ with a zero-temperature Fermi-liquid-like step function. The unitary transformation that diagonalizes $\rho^{(0)}$ approximately diagonalizes the OPDM $\rho^{(n)}$ of the higher eigenstates $|n\rangle$, but with random ordering such that the disorder average $\langle n_\alpha^{(n)} \rangle$ becomes a smooth function without any discontinuity (see [54] for detailed calculations supporting this picture). The resulting prediction of the diagonal ensemble for the discontinuity is then

$$\langle \Delta n^{\rm diag} \rangle \equiv \langle n_N^{\rm diag} \rangle - \langle n_{N+1}^{\rm diag} \rangle \approx \langle |a_0|^2 \Delta n^{(0)} \rangle. \qquad (10)$$

This indeed goes to zero exponentially with L since $\langle |a_0|^2 \rangle \sim e^{-bL}$.

Imbalance and connection to experiments.—The density imbalance $\mathcal{I} = (N_{\rm e} - N_{\rm o})/N$ between the number of physical particles $N_{\rm e}$ on even sites and $N_{\rm o}$ on odd sites is experimentally shown to relax to zero in the ergodic phase whereas in the localized phase it exhibits a fast relaxation towards a nonzero value, reflecting the absence of thermalization [46]; similar conclusions were obtained numerically in Ref. 55. From the occupation spectrum, we define a related imbalance between the occupied and unoccupied halves of the spectrum as

$$\mathcal{I}_{\rm OPDM}(t) = \frac{\langle N_+(t) \rangle - \langle N_-(t) \rangle}{N}, \qquad (11)$$

where $N_+(t) = \sum_{\alpha=1}^{N} n_\alpha(t)$ and $N_-(t) = \sum_{\alpha=N+1}^{L} n_\alpha(t)$. This imbalance $\mathcal{I}_{\rm OPDM} = 1$ for any product state, thus also for our initial density-wave state. We can view $\mathcal{I}_{\rm OPDM}$ as a measure of how close a state is to a step-function occupation spectrum with imbalance one, or to a completely flat occupation spectrum where its value is zero. The quantities $\mathcal{I}(t)$ (unfilled symbols) and $\mathcal{I}_{\rm OPDM}(t)$ (filled symbols) are plotted in Fig. 4. Both saturate at large times at nonzero values but the relaxation for the density imbalance is much faster. The reason for this is that $\mathcal{I}$ only captures the ballistic expansion part of the relaxation, while $\mathcal{I}_{\rm OPDM}$ also captures the dephasing mechanism coming from interactions between quasiparticles. As a second main result of our work, we have thus demonstrated that the OPDM occupation spectrum can

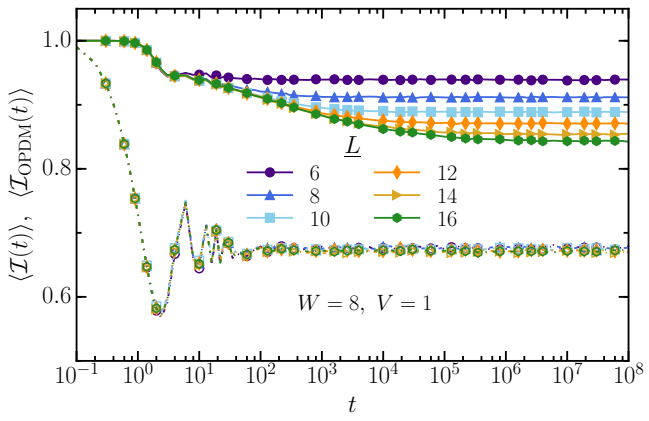

FIG. 4. Time evolution of the disorder-averaged density imbalance $\langle \mathcal{I}(t) \rangle$ and its analog in the OPDM basis, $\langle \mathcal{I}_{\rm OPDM}(t) \rangle$, as a function of system size L for $W = 8$.

be directly connected to lack of ergodicity and experimentally accessible quantities.

Conclusions.—In this work we demonstrated that in the many-body localized phase, the steady state reached after long times after a quench from a perfect density-wave state has one-particle density matrix occupations with a reduced discontinuity that goes exponentially to zero with system size. The shape of the occupation spectrum remains highly nonthermal, in contrast to the ergodic phase. This is consistent with the picture of local conserved quantities which have a significant overlap with the initial state. The approach towards the steady state is consequently a power law, reflecting dephasing via interactions between quasiparticles. We have also defined an occupation imbalance, similar to the density imbalance used in experiments, that captures the main effect of dephasing and absence of thermalization.

Our discussion suggests that the continuous occupation spectrum is phenomenologically similar to that of a finite-temperature Fermi liquid. The finite temperature is provided by the energy difference between the initial state and the closest eigenstates, which serve as reference states with a (zero-temperature) Fermi-liquid like occupation spectrum. This is not thermalization in the conventional sense since the many-body localized phase is manifestly nonergodic and there is no eigenstate thermalization. Nevertheless, the observation that the steady state OPDM spectrum is continuous may hint at the possibility of describing it with an emergent temperature, to be defined in a suitable way. It thus remains an interesting future research direction to establish whether such an emergent temperature corresponds to some thermal-like ensemble, necessarily different from eigenstate thermalization, and then how one can characterize it.

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