Many-Body Localization and Quantum Nonergodicity in a Model with a Single-Particle Mobility Edge

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We investigate many-body localization in the presence of a single-particle mobility edge. By considering an interacting deterministic model with an incommensurate potential in one dimension we find that the single-particle mobility edge in the noninteracting system leads to a many-body mobility edge in the corresponding interacting system for certain parameter regimes. Using exact diagonalization, we probe the mobility edge via energy resolved entanglement entropy (EE) and study the energy resolved applicability (or failure) of the eigenstate thermalization hypothesis (ETH). Our numerical results indicate that the transition separating area and volume law scaling of the EE does not coincide with the nonthermal to thermal transition. Consequently, there exists an *extended nonergodic phase* for an intermediate energy window where the many-body eigenstates violate the ETH while manifesting volume law EE scaling. We also establish that the model possesses an infinite temperature many-body localization transition despite the existence of a single-particle mobility edge. We propose a practical scheme to test our predictions in atomic optical lattice experiments which can directly probe the effects of the mobility edge.

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Thermalization, a commonplace phenomenon in various physical settings, can naturally fail in isolated disordered quantum interacting systems, making standard concepts of quantum statistical mechanics invalid. The fundamental theoretical underpinning of thermalization in quantum systems has been postulated in the form of the eigenstate thermalization hypothesis (ETH) [1,2]. Recently, it has been shown using perturbative arguments that the presence of interaction and disorder in a closed quantum system could lead to many-body localization (MBL) [3] with such an interacting quantum MBL state being nonthermal.

A hallmark of MBL is its violation of the ETH [2], where a local subsystem fails to thermalize with its environment [4]. MBL has now been established nonperturbatively in lattice models with finite energy density, where numerical evidence points towards the existence of MBL all the way to infinite temperature [5,6]. Further numerical work [7–9] and a rigorous mathematical proof [10] for the existence of the MBL phase have mounted compelling evidence for the existence of such a "finite-temperature" MBL phase which eventually gives way to an extended phase at strong enough interaction. Although much of the MBL work has focused on the interacting one-dimensional (1d) fermionic Anderson model with random disorder [11] (and closely related spin models), it turns out that MBL also exists without any disorder [8,12,13] for the Aubry-Andre-Azbel-Harper (AAAH) model [14–16], which is a nonrandom 1d model with a quasiperiodic on-site potential. We emphasize that neither the 1d Anderson model nor the AAAH model manifests a single-particle mobility edge (SPME).

In the absence of a SPME, interactions act on the Fock space of Slater determinants of either completely localized or delocalized single-particle eigenstates. Therefore, introducing a SPME allows one to study how localized and delocalized eigenstates will interact, thus introducing qualitatively new physics. There are several deterministic 1d incommensurate models with SPMEs in the literature [17–23], which can be adapted for studying MBL in the presence of a SPME.

We consider a recent generalization [23] of the 1d AAAH model with an analytical expression for the SPME, which enables us to study the interplay of many-body effects and the SPME in a controlled fashion. Since the MBL phase is a property of all eigenstates, the presence of a mobility edge adds a new dimension to the problem as both localized and delocalized single-particle orbitals are now present in the problem. Using exact diagonalization we find for certain parameter regimes of the model the following: (1) The existence of a many-body mobility edge (E_L) characterized by the area to volume law scaling of entanglement entropy (EE). (2) A distinct energy scale (E_T) that separates a thermal (i.e. ergodic) and nonthermal region in energy, which is established by directly considering an ETH violation based on the criterion in Refs. [1,2,24]. (3) Our results suggest $E_T \neq E_L$ and consequently the existence of a nonergodic regime with volume law EE scaling between E_T and E_L. All three of our findings are completely novel differing drastically from previous studies suggesting a sharp many-body mobility edge [9,25,26]. To guide future experiments that could probe our predicted mobility-edge physics, we present a realistic scheme with a straightforward modification to the existing experimental setup [27–29].

The model we consider is a generalized Aubry-Andre (GAA) model [23], $H = H_0 + H_{\rm int}$,

$$H_0 = -t\sum_{j=1}^{L}(c_j^\dagger c_{j+1} + {\rm H.c.}) + 2\lambda\frac{\cos(2\pi q j + \phi)}{1-\alpha\cos(2\pi q j + \phi)}n_j,$$
$$H_{\rm int} = V\sum_j n_j n_{j+1}, \tag{1}$$

where c_j is a fermionic annihilation operator, $n_j = c_j^\dagger c_j$, and the tunneling t is the energy unit throughout. We focus only on the fermionic case here. We consider $\alpha \in (-1, 1)$, with the AAAH model corresponding to $\alpha = 0$. In the noninteracting limit, the GAA model with an irrational wave number q [we fix $q = 2/(1+\sqrt{5})$, with no loss of generality], has a SPME [23] at $\alpha\epsilon = 2{\rm sgn}(\lambda)(|t| - |\lambda|)$ [30]. In this model, the particle number $\sum_j n_j = N$ is conserved.

Interaction effects on localization and thermalization in the presence of SPME.—We study interaction effects on localization and thermalization for the model Hamiltonian H using exact diagonalization. In the AAAH model ($\alpha = 0$), the noninteracting many-body wave function is a Slater determinant of all localized or all extended single-particle orbitals. This results in the interacting AAAH model having all many-body states either localized and nonthermal or extended and thermal [8].

However, for the noninteracting GAA model (with $\alpha \neq 0$), there are more possibilities originating from the SPME, where the Slater determinant can be composed of both localized and extended single-particle orbitals. Adding interactions to such a system may result in richer many-body states where the localization and thermalization properties may be qualitatively different from the $\alpha = 0$ case. To this end, we employ separate diagnostics to study localization and ergodicity without making the common assumption that thermalization and delocalization must necessarily be intrinsically connected in an interacting system. To investigate the localization properties, we cut the lattice at site l, which divides it into two subsystems A and B; we then calculate the energy resolved Rényi entropy $S_2(l) = -\log({\rm Tr}\rho_A^2)$ of A involving lattice sites $1, 2, \ldots, l$, whose reduced density matrix is obtained by tracing out region B at the other sites $(l+1, l+2, \ldots, L)$ [31]. The EE scaling reliably tracks the localization transition, where localized and delocalized many-body states are quantified by the area law ($S_2 \sim L^{d-1}$) and volume law scaling ($S_2 \sim L^d$), respectively [4,8]. To understand the thermalization features we calculate the observable $\mathcal{O}(E)$,

$$\mathcal{O}(E) = \sum_{j=1}^{L/2}\langle\Psi_E|n_j|\Psi_E\rangle, \tag{2}$$

with $|\Psi_E\rangle$ a many-body eigenstate. The large fluctuation in $\mathcal{O}(E)$ among eigenstates that are nearby in energy is a signature for the violation of the ETH [24].

We begin by focusing on the MBL transition as a function of energy for fixed model parameters. In Fig. 1 we show the energy resolved $S_2(l = L/2)$ for various system sizes. We find eigenstates with an energy below a certain value E_L are localized with an EE that obeys area law scaling ($S_2(L/2) \sim L^0$) [4], whereas the eigenstates with an energy above E_L exhibit a volume law scaling of the EE [$S_2(L/2) \sim L$] and are thus extended. We define E_L where $S_2(L/2)$ splays out in system size as shown in Fig. 1(b). Thus E_L defines the many-body mobility edge, which separates states with an area law scaling from extended states with volume law scaling. Although the existence of the many-body mobility edge E_L in our model is already a significant result, below we discuss the key issue of whether E_L also defines the ergodic properties of the interacting system.

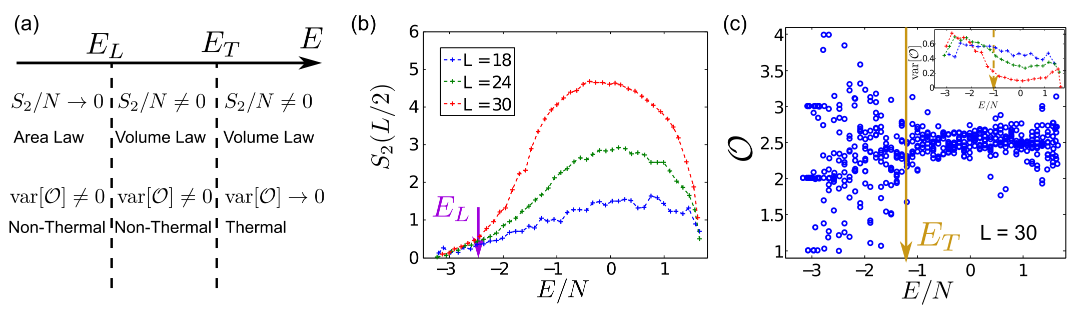

FIG. 1 (color online). Energy dependent ergodicity for interacting fermions. (a), A scenario for many-body mobility edge physics as we have found for the GAA model. (b) The bipartite Rényi entropy. The eigenstates above E_L have extensive EE, and are thus extended; whereas the states below E_L exhibit EE of area law scaling and are localized. (c) The energy dependence of an observable $\mathcal{O}(E)$ [Eq. (2)] with $L = 30$. The inset shows the fluctuation var[$\mathcal{O}$] (see main text) for different system sizes, using the same plot scheme as in (b). The fluctuation of $\mathcal{O}$ for states $E > E_T$ is small and gets significantly larger for states $E < E_T$. The system is expected to be thermal (nonthermal) above (below) E_T. (The slight increase of var[$\mathcal{O}$] near $E/N \approx 1.2$ is an artifact from the small number of states close to the spectra edge.) Our numerical results suggest $E_L < E_T$. In this plot, the filling is fixed at 1/6, and we use $\lambda/t = 0.3$, $V/t = 1$, and $\alpha = -0.80$, and we average over ϕ for better statistics [30]. In the calculation for system size $L = 30$, we use inverse Lanczos and target 500 interior eigenstates.

We now come to the thermalization properties, which are captured by the energy resolved observable $\mathcal{O}(E)$ as shown in Fig. 1(c). The fluctuations of $\mathcal{O}(E)$ within a narrow energy window are quantified by their variance, denoted as var[$\mathcal{O}$] [30]. As shown in Fig. 1(c) there is a clear energy threshold E_T that separates two qualitatively different regimes. In the energy window ($E > E_T$), the fluctuations of $\mathcal{O}$ among nearby eigenstates are small, for which the ETH is satisfied and the eigenstates are thermal [24]. The spread of the observable broadens out for energies $E < E_T$, where the fluctuations are significantly larger, leading to a violation of ETH [24]. We emphasize here that the thermal to nonthermal transition is unique to interacting systems, and is absolutely absent without interactions [24,32].

Our numerical results suggest that the MBL and thermal transitions in energy do not coincide, $E_L \neq E_T$ (see Fig. 1). In particular, our numerics imply that $E_T > E_L$, and as a result there exists an energy window ($E_L < E < E_T$) where the many-body states are nonergodic (violate the ETH) but remain extended (volume law scaling of EE). Therefore, we conclude that in this interacting many-body system with SPME two critical energy scales E_L and E_T exist, which is qualitatively different from the scenario of a sharp many-body mobility edge [26]. We emphasize that our results are completely distinct from the model in the absence of a SPME ($\alpha = 0$), which has no many-body mobility edge and all of the eigenstates are either thermal and delocalized or nonthermal and localized [30]. Thus our numerical results point to the existence of a nonergodic extended regime defined as $E_L < E < E_T$. The possible existence of a nonergodic extended (i.e. metallic) phase in the vicinity of the MBL transition has been speculated in the literature with no concrete examples [33–35].

Noninteracting many-body states.—In the following, we develop a physical intuition for the observed many-body mobility edge. The noninteracting many-body states are trivially nonergodic and violate ETH [36], as shown in Fig. 2(c) for $V = 0$ where the energy dependence of $\mathcal{O}(E)$ manifests large fluctuations among eigenstates that are nearby in energy [24]. We will discuss the noninteracting limit to gain insight into the emergence of the nonergodic extended phase in the interacting case.

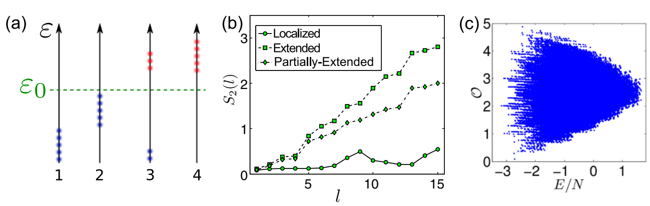

FIG. 2 (color online). Localization and nonthermalization of noninteracting fermions with a SPME. Here we simulate 5 particles in 30 sites. We take the GAA model with $\lambda/t = 0.3$, $\alpha = -0.8$, with mobility edge $\epsilon_0/t = -1.75$. (a) Different possibilities of many-body states. As shown the partially extended state as marked by 3 could have approximately the same energy as the localized one marked by 2. (b) Entanglement scaling for the three types of states, localized, extended and partially extended. The partially extended states exhibit extensive EE, similar to the extended ones. In (c) we show the energy dependence of $\mathcal{O}$ [Eq. (2)].

Without interactions, the many-body eigenstate of N fermions is a product state of N single-particle orbitals. In the presence of SPME, there are three different ways of constructing many-body states [Fig. 2(a)]: (i) all particles put in localized single-particle orbitals, (ii) all particles put in extended orbitals, and (iii) some particles put in localized and others in extended orbitals, which respectively give localized, extended, and partially extended many-body states. The partially extended states have extensive EE [Fig. 2(b)]. (We mention that the partially extended states would appear localized [30] from the perspective of the normalized participation ratio [8].) Such partially extended many-body states lead to important consequences. Consider a model with single-particle energies $\epsilon_1 < \epsilon_2 < \ldots < \epsilon_L$ having a SPME $\epsilon_{m^\star}$, such that the states with $\epsilon_{m \leq m^\star}$ ($\epsilon_{m > m^\star}$) are localized (extended). The lowest energy for a fermionic many-body partially extended state is $E_A = \epsilon_{m^\star + 1} + \sum_{m=1}^{N-1} \epsilon_m$. The highest energy of a localized state is $E_B = \sum_{m=m^\star - N+1}^{m^\star} \epsilon_m$. For a general Hamiltonian, $E_B > E_A$ is the most typical scenario [37]. The many-body states with energy $<$ ($>$) E_A are completely localized (extended, partially extended, or localized); the states above E_B are extended or partially extended. In the energy regime $E_B > E > E_A$, however, localized and partially extended states are coexisting by virtue of the SPME in the spectrum which enables the existence of this mixed intermediate energy regime.

Putting the noninteracting and interacting results all together, a physical picture naturally emerges. Interaction effects on the extended many-body states lead to thermal behavior, whereas for localized states, interactions make them nonthermal. The most interesting case is the coexistence of partially extended and localized states, where interactions could stabilize a nonthermal extended phase. Such a physical scenario is possible and seems to be consistent with our numerics.

The MBL phase in the GAA model.—Past studies have established the existence of a MBL phase (with all eigenstates localized) in the AAAH model [8,12] at *infinite temperature*. The infinite temperature limit is defined by averaging observables over all energy eigenstates (i.e. with a thermal weighting factor equal to unity). For the noninteracting GAA model with a SPME, the average is performed over localized, extended, and partially extended states, thus leading to extended behavior; e.g., the averaged EE obeys volume law. For the interacting case, in contrast to MBL studies in the absence of SPME where interactions make the system more extended, we find that interactions could actually stabilize the infinite temperature MBL phase in a considerable parameter region of the model in Eq. (1).

To capture the MBL transition at infinite temperature, in addition to the EE scaling (averaged over all eigenstates), we present the level statistics, an established diagnostic for MBL [5,8]. We consider the dimensionless adjacent gap ratio,

$$r_n = \min(\delta_n, \delta_{n+1}) / \max(\delta_n, \delta_{n+1}),$$

where $\delta_n = E_{n+1} - E_n$. We calculate its average $\bar{r} = (1/V_H)\sum_n r_n$ (V_H is the Hilbert space dimension), to locate the MBL phase [5].

As shown in Fig. 3, when the incommensurate potential strength λ is weak, the EE is extensive, a signature for the system being extended. The average adjacent gap ratio is $\bar{r} \approx 0.53$, which implies that the energy spectra satisfy Gaussian orthogonal ensemble level statistics, and the many-body phase is delocalized [5,8,38]. When λ is above a certain threshold $\lambda_c(\alpha, V)$, the model undergoes the MBL transition. In this parameter regime, the EE obeys area law scaling [Fig. 3(c)], and the gap ratio becomes $\bar{r} = 0.39$ [Fig. 3(f)], which is consistent with eigenstates satisfying a Poisson distribution, and the model is in the MBL phase [4,5,8,38]. We emphasize that for $\lambda > \lambda_c$ in the presence of delocalized single-particle orbitals, the MBL phase can still be stabilized by interactions. For example, with $\lambda/t = 1.5$ and $\alpha = -0.80$, although the noninteracting case is not completely localized due to the SPME, the interacting system is completely localized as implied by the EE [Fig. 3(a)], adjacent gap ratio [Fig. 3(d)], and their system size dependence [Figs. 3(c) and 3(f)]. In addition, starting from $\alpha = 0$ (with no SPME) as $\alpha \to -0.99$, where more localized orbitals are mixed in, we find both $S_2(L/2)$ and $\bar{r}$ decrease as displayed in Figs. 3(b) and 3(e). To conclude, we have established the existence of an MBL phase at infinite temperature in the presence of SPME.

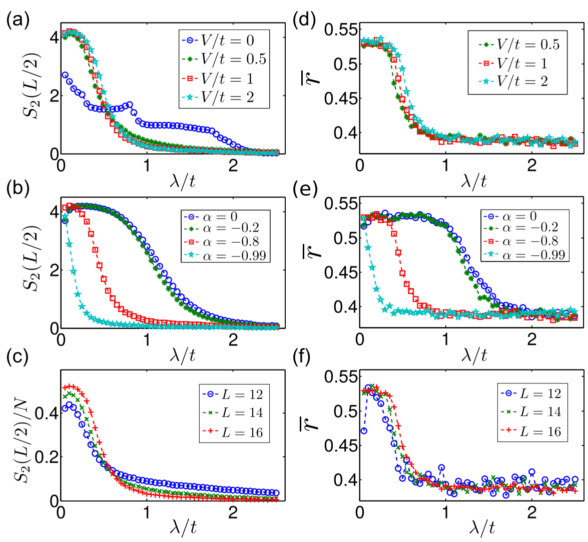

FIG. 3 (color online). MBL phase at half-filling and infinite temperature. (a), (b), and (c) show the Rényi entropy versus the incommensurate potential strength. (d), (e), and (f) show the averaged adjacent gap ratio. In (a) and (d), we show the interaction dependence with $\alpha = -0.8$. The numerical results indicate the interacting system is in the MBL phase (all states localized) when λ is larger than a certain critical value ($\lambda_c \approx 0.8$). In particular (a) explicitly shows that interaction effects make the GAA model more localized. (b) and (e) show the α dependence with $V/t = 1$. As we increase α, λ_c becomes smaller. In (c) and (f), we show the system size dependence with $V/t = 1$ and $\alpha = -0.8$.

Experiment.—To study the MBL phase in the AAAH model, a two-component Fermi gas of K^{40} atoms has been recently confined in a 1d superlattice with optical potential, $V_0\cos^2(kx) + V_1\cos^2(k'x)$ [27], with k' incommensurate to k. To investigate our predicted mobility edge physics, we propose to add an additional potential, $V_2\cos^2(2k'x)$. Choosing $V_0 = 5E_r$, $V_1 = 0.13E_r$, and $V_2 = 0.026E_r$ (E_r is the single-photon recoil energy) [39], the noninteracting model in Eq. (1) with $\lambda/t = 1$, and $\alpha = 0.2$ is approximately realized [30], and its localization properties are described in Ref. [23]. Preparing an initial state with its average energy in the nonthermal extended region, its unitary evolution would provide direct observation of nontrivial relaxation of an interacting many-body state in the presence of SPME [24,40]. As the numerical simulations on classical computers are limited in terms of system size, the quantum simulator, atoms in the optical lattice, would clarify the thermodynamic limit of our proposed nonergodic and MBL phenomena.

Conclusions.—In summary, we have shown the single-particle mobility edge and interactions result in a many-body mobility edge. A central new result here is the existence of two characteristic many-body energies (i.e. E_L and E_T) in general in a system with a corresponding SPME, which separate localized and extended states (E_L) and nonergodic and thermal states (E_T). Our numerical results (within our numerical accuracy and within the finite size limitations) suggest $E_L < E_T$, which allows for the possibility of nonergodic delocalized many-body states (i.e. a nonergodic metal) as a strange new intermediate phase of quantum matter. We expect our findings to generically apply to systems with SPME, specifically, to the three-dimensional interacting disordered Anderson model.

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Note added.—After completing our work we became aware of a complementary and independent recent study [42] of many-body localization in systems with mobility edges.

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[37] This follows since the many-body states with energy above E_B (below E_A) are all extended or partially extended (localized) by definition. If $E_B < E_A$, no states are allowed between E_B and E_A, and the (partially) extended and localized states are thus separated by an energy gap $E_A - E_B$. Such an energy gap closes when $E_B = E_A$. When $E_B > E_A$, states are allowed between E_A and E_B. We can reasonably assume for the model we consider that there is no single-particle energy gap near the single-particle mobility edge or at least, any such gap is nongeneric and negligibly small. Then the many-body energy spectrum is typically dense and does not involve a gap at finite energy density. It follows then that $E_B > E_A$ is most typical.
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