Nucleation of Ergodicity by a Single Mobile Impurity in Supercooled Insulators

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We consider a disordered Hubbard model and show that, at sufficiently weak disorder, a single spin-down mobile impurity can thermalize an extensive initially localized system of spin-up particles. Thermalization is enabled by resonant processes that involve correlated hops of the impurity and localized particles. This effect indicates that Anderson localized insulators behave as “supercooled” systems, with mobile impurities acting as ergodic seeds. We provide analytical estimates, supported by numerical exact diagonalization, showing how the critical disorder strength depends on the particle density of the localized system. In the $U \rightarrow \infty$ limit, doublons are stable excitations, and they can thermalize mesoscopic systems by a similar mechanism. The emergence of an additional conservation law leads to an eventual localization of doublons. Our predictions apply to fermionic and bosonic systems and are readily accessible in ongoing experiments simulating synthetic quantum lattices with tunable disorder.

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Introduction.—Relaxation of a many-body system towards thermal equilibrium, driven by the interaction between its elementary constituents, is the cornerstone of statistical physics. Classically, thermalization is explained by the ergodic hypothesis, stating that isolated many-body systems forget their initial conditions, exploring all possible configurations allowed by global conservation laws, such as energy conservation. The equivalent of the ergodic hypothesis in the quantum realm is the eigenstate thermalization hypothesis (ETH) [1–4].

It is of particular interest to find quantum systems avoiding thermalization. A generic mechanism to violate ETH is provided by many-body localization (MBL) [5–8], which can be viewed as a generalization of the celebrated phenomenon of Anderson localization (AL) [9,10] to interacting systems, such as disordered Hubbard-type models studied experimentally with cold atoms [11–13]. In MBL, the breakdown of thermalization stems from the emergence of local integrals of motion (LIOMs) [14–16]. They underlie surprising dynamical properties of MBL, which set it apart from AL, such as slow entanglement growth [17–19] and relaxation without thermalization [20].

In stark contrast to AL, which exists in dimensions $d = 1, 2$ at any disorder, MBL has been firmly established only at strong disorder in $d = 1$. It is an open question how the transition from MBL to the ergodic phase occurs when disorder strength is reduced. Recent theories [21–23] argued that this transition is driven by the formation of rare thermal “bubbles”. These theories build on a set of phenomenological assumptions regarding the interplay of bubbles and nearby, initially localized regions. It was shown that the bubbles can grow by including nearby localized degrees of freedom [24–27], which may destabilize certain localized systems, albeit at times that scale exponentially with the system size. However, these effects have not yet been observed in experiments with quantum simulators, which can access local, time-dependent observables in localized systems [11–13,28,29]. It is therefore crucial to identify simple, realizable mechanisms for the generation and spreading of thermal bubbles through an (initially) nonergodic system.

In this study, we consider a paradigmatic correlated system—disordered Hubbard model—and uncover a novel effect of interactions on localization. We consider a single spin-down impurity immersed in a spin-polarized background. We show that, similarly to seed crystals in supercooled liquids, at sufficiently weak disorder, a single impurity can act as “ergodic nucleus” that thermalizes the entire, initially Anderson localized system. For moderate on-site interaction strength $U$ of the order of the hopping $t$, mobile impurities take advantage of a finite density $\rho$ of single particles in adjacent localized states to propagate, destroying localization below a critical disorder strength $W_C(\rho)$. In the infinite interaction limit, $U \rightarrow \infty$, a single doublon, which is a composite excitation made of two particles (two identical bosons or two fermions with opposite spin), stabilized by strong interactions [30–34], can thermalize via a similar mechanism mesoscopic systems much larger than the single-particle localization length. The doublon is eventually localized due to the emergence of an additional conservation law.
The mechanism proposed here applies to fermionic and bosonic systems and differs qualitatively from that of Ref. \[24\], which considered a static, well-thermalized bosonic systems and differs qualitatively from that of region coupled to a localized system. In particular, we examine the conditions under which a mobile impurity may induce resonances that involve nearby localized particles.

Analysis of resonances for a mobile impurity.—We first examine the conditions under which a mobile impurity may induce resonances that involve nearby localized particles. We argue that for sufficiently weak disorder the impurity can propagate, thermalizing the entire system. We consider the Fermi-Hubbard model:

$$\mathcal{H}_{FH} = \sum_{j, \sigma} \varepsilon_j n_{j, \sigma} + U \sum_j n_{j, \uparrow} n_{j, \downarrow} + t \sum_{j, \sigma} \left[ c_{j, \sigma}^\dagger c_{j+1, \sigma} + \text{H.c.} \right]$$

where the operators $c_{j, \sigma}$ annihilate spin-$\sigma$ fermions on site $j$, $n_{j, \sigma} = c_{j, \sigma}^\dagger c_{j, \sigma}$, and the on site energies $\varepsilon_j$ are uniformly distributed in the energy box $[-W, W]$. As an impurity, we introduce a single spin-down fermion, $N_\uparrow = 1$, into an environment of $N_\downarrow$ spin-up fermions (particles) on $L$ sites, with $\rho_\uparrow = N_\downarrow/L$ being their density.

In the noninteracting limit ($U = 0$), on site disorder induces AL. It is convenient to switch to the basis of single-particle localized orbitals described by operators $a_{l, \sigma}$ related to lattice operators via $c_{l, \sigma} = \sum_j \psi_l(j) a_{l, \sigma}$. Here eigenfunctions $\psi_l(j) \sim e^{-|j-l|/\xi} \sqrt{\xi}$ are exponentially localized around site $l$. The localization length $\xi$ scales as $t^2/W^2$ at $W \ll t$ \[35-37\]. The Hamiltonian (1) becomes

$$\mathcal{H}_{FH} = \sum_l \mathcal{E}_l a_{l, \sigma}^\dagger a_{l, \sigma} + U \sum_{j, \sigma} \psi_l(j) \psi_m(j) \psi_p(j) \psi_q(j) a_{l, \uparrow} a_{m, \uparrow} a_{p, \downarrow} a_{q, \downarrow},$$

where $\{\mathcal{E}_l\}$ are the eigenenergies of the states $a_{l, \sigma}$.

The interaction of the impurity with the particles may induce resonances between initially fully localized configurations. To estimate the resonance probability, we study the matrix elements of the interaction term between an initial state $|\psi\rangle$ in which the impurity occupies orbital $l$, while spin-up fermions randomly occupy $N_\uparrow$ orbitals, and a final state $|\psi'\rangle$ in which the impurity moved to an orbital $l'$, and one spin-up fermion moved from orbital $p$ to $p'$. The corresponding matrix element reads

$$\langle \psi' | \mathcal{H}_{FH} | \psi \rangle = U \sum_j \psi_{p'}^*(j) \psi_p(j) \psi_{l'}^*(j) \psi_l(j).$$

We focus on processes where $l, l', p, p'$ all lie within one localization length $\xi$, for such processes the matrix element is largest. Assuming that $\psi_l(j)$ are oscillating functions of amplitude $1/\sqrt{\xi}$ within the localization volume, the matrix element (3) can be estimated as $V_{\text{typ}} \sim U \xi^{-3/2}$. Further, we note that a given state $|\psi\rangle$ is connected to $n(\xi, \rho_\uparrow) \sim \rho_\uparrow (1 - \rho_\uparrow)^{\xi^{-1}}$ states $|\psi'\rangle$, since any of the $\rho_\uparrow \xi$ spin-up fermions can be moved to any of the $(1 - \rho_\uparrow) \xi$ empty orbitals, while $l'$ can be chosen in $\sim \xi$ ways. The corresponding energy mismatch is a random quantity with a variance of order $\delta E \approx 2W$. Thus, the level

![FIG. 1. Spectral-statistics parameter $r$ (bottom panels) for a system with a Hamiltonian (1) with one spin-down impurity, shown as a function of disorder strength $W/t$ and renormalized energy $\epsilon = (E - E_{\text{min}})/(E_{\text{max}} - E_{\text{min}})$. Panel (a) illustrates the case of moderate interaction $U = t$, while (b), (c) show large-$U$ values, when a doublon can form. The upper panels show the many-body density of states (DOS) at $W = 1.6t$, which exhibits a clear separation between sectors with and without doublon at large $U$. At all values of $U$, a transition of Wigner-Dyson statistics (blue regions) at moderate disorder to Poisson statistics (yellow regions) is observed. At large $U$, this transition occurs in the doublon band, while the singlon band is AL. Averaging was performed over 2000 different disorder realizations, $L = 12$ sites, $N_\uparrow = 6$, and $N_\downarrow = 1$.](image)
We first focus on moderate interactions (estimate the critical disorder strength presented in Figs. 1, 2, for the Fermi-Hubbard model iterations with exact diagonalization numerical results on-site potential, subject to AL. tight-binding model for a single spin-down with random signalling localization. In both limits, Eq. (1) maps onto a tight-binding model for a single spin-down with random on-site potential, subject to AL.

Numerical calculations.—We support the above considerations with exact diagonalization numerical results presented in Figs. 1, 2, for the Fermi-Hubbard model (1). We focus on moderate interactions (\(U = t\)), and the large-\(U\) limit is discussed below. In this case a clear transition from Wigner-Dyson (WD) to Poissonian (P) spectral statistics is observed as disorder is increased, in which the ratio of consecutive level spacings \(\delta E/n(\xi, \rho^\uparrow)\), being the occupation of even/odd sites (see experiments [11,41]), as well as the averaged evolution of the local spin-up imbalance \(I = \langle \rho^\uparrow \rangle \). The resonance condition, \(V_{\text{typ}} \gtrsim \delta E\), then yields

\[
W < W_C, \quad 2W_C = U\rho^\uparrow(1 - \rho^\uparrow)^{3/2}(W_C).
\]

Thus, a single impurity efficiently induces many-body resonances in an initially localized system for \(W < W_C\). \(W_C\) is strongly sensitive to the precise dependence of the localization length \(\xi\) on the disorder strength \(W\), and on the spin-up density \(\rho^\uparrow\). In particular, \(W_C\) is the largest for \(\rho^\uparrow \approx 1/2\), and it is zero in the \(\rho^\uparrow \to 0\) and \(\rho^\uparrow \to 1\) limits, signalling localization. In both limits, Eq. (1) maps onto a tight-binding model for a single spin-down with random on-site potential, subject to AL.

The estimate (4) relies on the assumptions of weak interactions and that the localization length is a few lattice sites. Remarkably, the numerics show that a single impurity is able to induce ergodicity up to large disorder strengths \(W_C \approx 4t\), in which the single-particle localization length is of the order of 2/3 sites.

Dynamical properties.—Next, we focus on dynamical properties and study impurity propagation and its effect on the initially localized spin-up particles. We consider a quantum quench protocol, with an initial state chosen to be a product state of a spin-down particle located on a lattice site 0, and a density wave, with a spin-up fermion occupying every second lattice site, Fig. 3. We study the evolution of the spin-up imbalance \(I = (N_{\uparrow,0} - N_{\uparrow,0}^\uparrow)/(N_{\downarrow,0} + N_{\downarrow,0}^\uparrow), N_{\uparrow,0}\), being the occupation of even/odd sites (see experiments [11,41]), as well as the averaged evolution of the local spin-down (impurity) occupation \(\langle n_{\downarrow,0} \rangle\).

The results for \(W = 1.5t\), which lies below \(W_C\) for \(U = t\), and \(\rho^\uparrow = 1/2\), are illustrated in Fig. 3. In the noninteracting case (\(U = 0\)), neither of the quantities \(\langle n_{\downarrow,0} \rangle, I\) thermalizes because of AL, saturating to a value that depends weakly on the system size. At \(U \neq 0\), both quantities show a more pronounced decay as the system size is increased. In particular, the relaxation of \(\langle n_{\downarrow,0} \rangle\) towards \(1/L\) signals uniform spreading of the mobile impurity across the entire system. The suppression of the imbalance \(I\) is correlated in time with the impurity spreading across the system. Measurements of the imbalance decay and impurity position can be readily performed in ongoing experiments [11,28,41] and would provide a smoking-gun signature of the nucleation mechanism.

Mesoscopic nucleation and doublons in the \(U \to \infty\) limit.—Figure 1(c) shows that the condition \(U \gg N_{\uparrow} \cdot \max[\ell, W]\) induces a mesoscopic gap between two different many-body bands with distinct spectral properties. Such two bands are distinguished by the number of doublons present in the system. A doublon is formed when two fermions of opposite spin occupy the same site, with an energy cost \(U\). In the limit \(U \to \infty\), doublons are stable.
strength is observed in the single doublon sector for Anderson-localized free fermions, see Fig. 1(c). and spin-down fermions, which then behave as indistinguishable, \( U \rightarrow \infty \), are localized, as indicated by the Poisson unique spin-down fermion cannot occupy sites hosting spin-up fermions, is localized, as indicated by the Poisson level statistics. Similar to bosons in the Tonks-Girardeau gas [42–46] (see the Supplemental Material for details [39]), the \( U \rightarrow \infty \) limit induces a Pauli-like exclusion between spin-up and spin-down fermions, which then behave as indistinguishable, Anderson-localized free fermions, see Fig. 1(c).

A pronounced WD-P transition as a function of disorder strength is observed in the single doublon sector for \( U = 100t \). Figure 2(c) shows that the step in \( r \) is sharper than the one observed for moderate interactions (\( U = t \)); moreover, \( r \) reaches \( r_{WD} \) for accessible sizes \( L \) on the ergodic side of the step. Figure 2(d) shows that the WD-P transition depends on the spin-up density \( \rho_\uparrow \), but \( W_C(\rho_\uparrow) \) is less symmetric around \( \rho_\uparrow = 1/2 \). In the Supplemental Material [39], a similar transition is demonstrated for indistinguishable bosons described by the Bose-Hubbard model when a single doublon is stabilized by large \( U \rightarrow \infty \).

The emergence of WD statistics shows that, at sufficiently weak disorder, a single doublon can efficiently induce many-body resonances. The underlying processes are illustrated in Fig. 4 and are described in detail in the Supplemental Material [39]. In the \( U \rightarrow \infty \) limit, the doublon hopping is impossible in the absence of particles nearby. In this case, it involves a virtual transition through states without doublons, and therefore has an amplitude \( O(t^2/U) \) that vanishes for \( U \rightarrow \infty \). On the other hand, the hopping of the unique spin-down fermion on a nearby site already occupied by a spin-up particle is allowed. It has an amplitude \( t \) and conserves the doublon number. This constrained dynamics, summarized in Fig. 4(a), may induce resonances between localized configurations, as those shown in Fig. 4(b), favoring ergodicity for weak enough disorder. The analysis of the resonances induced by such correlated hopping is carried out in the Supplemental Material [39] to the leading order in \( t \). It is similar to the argument underlying Eq. (4), with the difference that \( \delta E \sim 3W \) (the impurity and two particle are displaced), and the number of connected states is estimated as \( \sim \rho_\uparrow(1-\rho_\uparrow)\xi^2 \) (the doublon moves by one site and only one particle-hole pair is rearranged in a localization volume \( \xi \)). This yields [39]

\[
3W \leq t \rho_\uparrow(1-\rho_\uparrow)\sqrt{\xi(W)}. \tag{5}
\]

Thus, the hopping amplitude \( t \) substitutes the interaction strength \( U \) in Eq. (4), and the existence of resonances is controlled by a single parameter \( W/t \), the only one left in the \( U \rightarrow \infty \) limit. The condition (5) explains the observation of the WD-P transition in Figs. 1(c) and 2(c), which is a consequence of the fact that the doublon is able to induce many-body resonances if a finite density of particles is present nearby. We attribute the observed deviations from particle-hole symmetric scaling \( \propto \rho_\uparrow(1-\rho_\uparrow) \) to finite-size effects, observing that the numerical results drift towards the dependence predicted by Eq. (5) as the system size is increased, see the Supplemental Material [39]. Nevertheless, a single doublon cannot spread over the entire system in the thermodynamic limit. In a strict \( U \rightarrow \infty \) and \( d = 1 \) limit, doublons cannot cross the holes present in the system. As shown schematically in Fig. 4(b), doublons and particles exchange positions through processes of amplitude \( t \), but the same process triggers the accumulation of holes on one side of the doublon and will eventually block its propagation. This effect becomes dominant after repeated hopping events of order \( t \), exchanging particle and doublons, and is apparent in the real-time evolutions shown in Fig. 3. In particular, the stationary long-time value of \( \langle r_{1,0} \rangle \) at \( U = 100t \) shows no convergence towards \( 1/L \). In the Supplemental Material [39], we compare the doublon spreading for periodic and open...
boundary conditions, showing that it is significantly suppressed in the latter case. The reason is that, for open boundary conditions, the number of empty sites on the left and on the right of the initial doublon position is a conserved quantity in the $U \to \infty$ limit, which quenches the doublon propagation, even in the absence of many-body localization. The doublon is thus able to take advantage of the doublon propagation, even in the absence of many-body localization; in which case there is no mechanism blocking the propagation of the interacting impurity at weak disorder across the entire system.

Conclusions.—In this work, we showed that a single impurity may thermalize an initially Anderson localized system at sufficiently weak disorder; such system is therefore a “supercooled insulator” that stays localized only until a suitable ergodic seed is introduced. Crucially, the associated thermalization time is expected to scale as a power-law in system size, while the static bubbles of Ref. [24], which are expected to trigger the ergodic-to-MBL transition, lead to much slower, exponential in size relaxation, difficult to attain in experiments.

On the contrary, the nucleation mechanism can be observed with current experimental capabilities, e.g., by studying dynamical signatures and impurity-induced decay imbalance. In the future work, it would be interesting to extend the analysis to the case of a finite impurity density. This may provide an insight into the results of a recent experiment [47], which reported MBL-thermal transition as a function of impurity density. Finally, several open questions regarding the doublon dynamics in the $U \to \infty$ limit remain; in particular, doublon dynamics in $d > 1$ is expected to be qualitatively different from $d = 1$ case, since no additional conservation law exists. In particular, we expect that, for $d > 1$, the doublon surrounded by its ergodic cloud will preserve its ability to propagate across the whole, initially localized, system.

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[40] For a discussion of uncertainties in extracting value of $W_C$, see the Supplemental Material [39].