Nucleation of ergodicity by a single doublon in supercooled insulators

Ulrich Krause\textsuperscript{1}, Théo Pellegrin\textsuperscript{2}, Piet W. Brouwer\textsuperscript{1}, Dmitry A. Abanin\textsuperscript{2,3}, and Michele Filippone\textsuperscript{2}

\textsuperscript{1}Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany and

\textsuperscript{2}Department of Quantum Matter Physics and \textsuperscript{3}Department of Theoretical Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland

We illustrate a remarkably simple mechanism in which single doublon excitations in interacting lattice systems with large on-site interaction $U$ trigger the generation of ergodic bubbles, which thermalize extensive localized systems. Such phenomenon shows how localized insulators behave as supercooled systems, in which doublons act as ergodic seeds. We provide analytical estimates showing how the critical disorder strength for such mechanism depends on singlon densities, which are supported by numerical exact-diagonalization simulations. Our predictions apply to both fermionic and bosonic systems and are readily accessible in ongoing experiments simulating synthetic quantum lattice systems with tunable disorder.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Delocalization of an initially localized system by a single doublon. Under certain conditions, doublons induce resonances between localized configurations. They thus diffuse without dissolving, simultaneously scrambling the localized system.}
\end{figure}

\textbf{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) \cite{1–3}.

It is of particular interest to find quantum systems which avoid thermalization. A generic mechanism for violating ETH is provided by many-body localization (MBL) \cite{4–7}, which can be viewed as a generalization of the celebrated phenomenon of Anderson localization (AL) \cite{8} to interacting systems, such as disordered Hubbard-type models studied experimentally with cold atoms \cite{9, 10}. In MBL systems, the breakdown of thermalization stems from the emergence of local integrals of motion (LIOMs) \cite{11–13}. They underlie surprising dynamical properties of MBL, which set it apart from AL, such as slow entanglement growth \cite{14} and relaxation without thermalization \cite{15}.

In a 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 \cite{16} argued that this transition is driven by the formation of rare thermal “bubbles”, which can grow and proliferate, establishing a thermal bath. A key object of this picture is a static bubble forming in rare regions with weak disorder potential. Its growth by absorbing nearby localized particles into a thermal bath has been studied \cite{17}, and it was conjectured that it may destabilize certain localized systems, albeit very slowly. However, these effects have not yet been observed in experiments with ultracold atom quantum simulators, which have been able to access local, time-dependent observables in localized systems\cite{9, 10, 18}. It is therefore crucial to identify simple mechanisms for the generation and spreading of thermal bubbles through an (initially) non-ergodic system.

In this study, we consider a paradigmatic example of a correlated system – disordered Hubbard model – and uncover a novel unexpected effect of interactions on localization. We show that, similarly to seed crystals in supercooled liquids, single doublons act as “ergodic nuclei” that can thermalize entire initially localized systems at sufficiently weak disorder, see Fig. 1. Doublons are composite excitations made of two particles (two identical bosons or two fermions with opposite spin), stabilized by strong local interactions of strength $W$. We initially focus on the $U \rightarrow \infty$ limit, and show that the presence of a single doublon activates an ergodic avalanche, below a critical disorder threshold $W_C$. We then show that this mechanism survives at a finite interaction strength $U$. We argue below that doublons can take advantage of a finite density $\rho$ of single particles (singlons) in adjacent localized states to diffuse, destroying localization. We establish the conditions for doublon-mediated de-

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We argue below that doublons can take advantage of a finite density $\rho$ of single particles (singlons) in adjacent localized states to diffuse, destroying localization. We establish the conditions for doublon-mediated de-
localization analytically, and support them by exact-diagonalization (ED) calculations. The energy separation between ergodic/localized states with/without doublons provides a clear example of a mesoscopic “mobility gap”, which enters and thermalizes the singlon sector in the thermodynamic limit. Our predictions equally apply to doublons in fermionic and bosonic systems, and they can be readily tested by ongoing experiments simulating disordered quantum lattices [9, 10, 18].

**Effective doublon model** — We first derive the effective model describing doublon motion among localized singlons. We then argue that a doublon thermalizes the entire system for disorder weaker than a critical value \( W_C \), which depends on the singlon density. We initially consider the Fermi-Hubbard model, with Hamiltonian that we separate into on-site/tunneling parts, \( \mathcal{H}_{O/T} \):

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

where the operators \( c_{j,\sigma} \) annihilate spin-\( \sigma \) fermions on site \( j \), \( n_{j,\sigma} = c_{j,\sigma}^+ c_{j,\sigma} \), and the onsite energies \( \varepsilon_j \) are uniformly distributed in the energy box \([-W, W] \). To show how a doublon can thermalize localized singlons, we consider a single spin-down fermion, \( N_\uparrow = 1 \), and \( N_\downarrow \) spin-up fermions on \( L \) sites, with \( \rho_\uparrow = N_\uparrow/L \) their density.

In the absence of tunneling between sites \( (t = 0) \), a doublon \( |\uparrow\downarrow\rangle \) is formed when two fermions of opposite spin occupy the same site, with energy cost \( U \). For simplicity, we first consider the limit \( U \to \infty \), which ensures that a doublon remains a stable excitation at \( t \neq 0 \), as the energy \( U \) released by doublon decay cannot be absorbed by bands without doublons [19]. In this limit, the low-energy band without doublons, where the unique spin-down fermion cannot occupy sites hosting spin-up fermions, is localized. Similar to bosons in the Tonks-Girardeau gas [20, 21] (see Supplementary Material (SM) for details [22]) the \( U \to \infty \) limit induces an effective Pauli-like exclusion between spin-up- and down fermions, which then behave as indistinguishable, Anderson-localized free fermions, see Fig. 3c.

To describe a system with a doublon, we introduce the composite doublon annihilation operator \( d_j = c_{j,\uparrow} c_{j,\downarrow} \) and then recast the on-site term in Eq. (1) as \( \mathcal{H}_O = \sum_j \varepsilon_j n_{j,\uparrow} n_{j,\downarrow} + 2 \sum_j \varepsilon_j d_j^\dagger d_j \) [23], in which \( h_{j,\uparrow} = 1 - n_{j,\downarrow} \). We then project the hopping \( \mathcal{H}_T \) onto the single doublon sector. As sketched in Fig. 2a, the hopping of the unique spin-down fermion on sites already occupied by singlons (spin-up fermions) does not change the doublon number, and this process remains of amplitude \( t \). Nevertheless, the \( U \to \infty \) limit totally quenches the doublon displacement in the absence of singlons nearby. These processes are second order in \( t \) and involve virtual singlon states. They are thus of order \( O(t^2/U) \) and disappear for \( U \to 0 \). This constrained dynamics, summarized in Fig. 2a, is described by the effective hopping

\[
\mathcal{D} = t \sum_j \left[ h_{j,\uparrow} c_{j,\uparrow}^\dagger c_{j+1,\uparrow} h_{j+1,\downarrow} + d_j^\dagger c_{j,\uparrow}^\dagger c_{j+1,\uparrow} d_{j+1} + \text{h.c.} \right],
\]

where \( h_{j,\uparrow} \) acts as a projector preserving the doublon number during singlon hopping. The detailed derivation of Eq. (2), using a Schrieffer-Wolff transformation, is provided in the SM [22]. Expression (2) clearly shows that, for \( U \to \infty \), doublons can still hop with an amplitude of order \( t \), only if singlons are present nearby. Such correlated hopping competes with localization, favoring ergodicity for weak enough disorder, as we discuss below.

**Analysis of resonances** — The correlated hopping (2) efficiently induces resonances between initially fully localized configurations, below a critical disorder strength \( W_C \). To analyze this effect for moderate disorder, we make two simplifying assumptions: (i) doublons and singlons are independent particles that correspond to \( d \) and \( c_\uparrow \) annihilation operators acting on separate Fock spaces and (ii) we identify \( h_{j,\uparrow} = 1 \) in Eq. (2). The first approximation applies in the \( U \to \infty \) limit. The second one neglects all local change of potential seen by singlons, following doublon displacements. Such processes can be neglected to leading order in \( t \), in which the doublon acts as an infinite barrier between two AL systems composed of free singlons. These assumptions lead to an effective Hamiltonian describing the single doublon sector

\[
\mathcal{H}_{\text{eff}} = \mathcal{H}_T + \sum_j \left[ 2 \varepsilon_j d_j^\dagger d_j + t d_j^\dagger c_{j,\uparrow}^\dagger c_{j+1,\uparrow} d_{j+1} + \text{h.c.} \right],
\]

in which \( \mathcal{H}_T = \sum_j \varepsilon_j n_{j,\uparrow} + t \sum_j [c_{j,\uparrow}^\dagger c_{j+1,\uparrow} + \text{h.c.}] \) is a single-particle nearest-neighbor hopping Hamiltonian in which onsite disorder leads to AL. It is thus convenient to switch to the basis of single-particle localized orbitals denoted by operators \( a_l \), such that \( c_{j,\uparrow} = \sum_l \psi_l(j) a_l \), where \( \psi_l(j) \sim e^{-i(j-l)/\xi}/\sqrt{\xi} \) are eigenfunctions localized around site \( l \), with a typical exponential decay. The localization length \( \xi \) scales as \( t^2/W^2 \) for \( W \ll t \) [24]. The effective
Hamiltonian (3) becomes
\[
H_{\text{eff}} = \sum_i \varepsilon_i a_i^\dagger a_i + 2 \sum_j \xi_j d_j^\dagger d_j
+ t \sum_{j,l,m} \psi_l(j) \psi_m(j+1) \left[ d_j^\dagger a_m^\dagger d_{j+1}^\dagger + \text{h.c.} \right],
\]
in which \(\{\varepsilon_i\}\) are the eigenenergies corresponding to AL states with Poissonian level-spacing distribution.

We inspect the matrix elements between typical states \(|\psi\rangle\) and \(|\psi'\rangle\), sketched in Fig. 2b, with a doublon and \(N_\uparrow\) localized orbitals randomly occupied by spin-up fermions. To leading order, the correlated hopping term in Eq. (4) couples \(|\psi\rangle\) to any state \(|\psi'\rangle\) in which the doublon is displaced by one site and a particle-hole pair is created. For typical initial(final) states, the probability of occupied or empty localized single-particle orbitals is \(\rho_\uparrow\) and \(1 - \rho_\uparrow\) respectively, thus we can estimate the matrix element between these two states as
\[
\langle \psi' | H_{\text{eff}} | \psi \rangle \simeq -t \psi_l(j) \psi_m(j+1) \rho_\uparrow (1 - \rho_\uparrow).
\]

Notice that this matrix element is suppressed, signaling doublon localization, both in the \(\rho_\uparrow \to 0\) and \(\rho_\uparrow \to 1\) limits. The nature of localization in such two limits is slightly different. For \(\rho_\uparrow \to 0\), localization is caused by the impossibility for doublons to hop in the absence of singlons nearby. For \(\rho_\uparrow \to 1\), Eq. (3) maps onto a tight-binding model for a single spin-down with random on-site potential and hopping, subject to AL. Notice that the matrix element (5) is maximum at half-filling \(\rho_\uparrow = 1/2\).

We compare now the matrix element (5) with the relevant level spacing. To leading order, the number of states connected to \(|\psi\rangle\) is roughly given by the number of ways particle-hole excitations can be arranged in a localization volume \(\xi\), thus \(\propto \xi^2\). As a consequence, the average level spacing is given by \(\delta \varepsilon = \delta E/\xi^2\), in which \(\delta E \approx 3W\) is the typical energy difference between the states \(|\psi\rangle\) and \(|\psi'\rangle\). By assuming that \(\psi_l(j) \sim 1/\sqrt{\xi}\) within a localization volume, the resonance condition reads
\[
3W \leq t \rho_\uparrow (1 - \rho_\uparrow) \xi.
\]

This result shows how, surprisingly, a single doublon efficiently induces many-body resonances in a localized system below a critical disorder strength \(W_C\) – defined by setting the equality in Eq. (6) – which strongly depends on the singlon density \(\rho_\uparrow\). Notice that the transition to the MBL phase for strong disorder is controlled by a single parameter \(W/t\), the only one left in the \(U \to \infty\) limit.

**Numerical calculations** – We support the above considerations with ED numerical results presented in Figs. 3, 4, for the Fermi-Hubbard Hamiltonian (1), with both \(U \gg t\) and \(U \gtrsim t\). Figure 3 shows that the condition \(U \gg N_\uparrow \cdot \max[t,W]\) ensures that many-body states with different doublon number are separated in energy. For large interactions (\(U = 100t\)), a clear transition from Wigner-Dyson (WD) to Poissonian (P) spectral statistics is observed in the single doublon sector, in which the ratio of consecutive level spacings \(r_n = \min(\delta_n, \delta_{n+1})/\max(\delta_n, \delta_{n+1})\) with \(\delta_n = E_n - E_{n-1}\) goes from \(r_{\text{WD}} \sim 0.53\) to \(r_{\text{P}} \sim 0.39\) [6, 25]. Fig. 4a reports finite-size scaling of the WD-P spectral transition, suggesting persistence of thermalization induced by a single doublon in the thermodynamic limit.

A similar transition is observed for \(U \sim t\), in which doublon and singlon bands merge. In the SM [22], we analyze this case in detail, showing that (i) the WD-P transition takes place at larger disorder strengths, but (ii) the average gap ratio \(r\) only shows a tendency towards
Figure 4. a) Finite-size scaling of the average spectral-statistics parameter $r$ as function of disorder strength $W/t$, for $U = 100t$. We consider $r$ for energies in the middle of the many-body band involving one doublon. b) WD-P transition as a function of $W/t$ and increasing $\rho_t$. c) Critical disorder $W_C$, at which the average level spacing $r = r_{TT}$, as function of $\rho_t$ for different system sizes $L$. The curve follows towards his estimate (6) in the thermodynamic limit. For all plots, disorder averaged were performed over 4000, 2000, 1000 realizations for $L = 8, 10$ and $12$. For $L = 14$ averaging performed for 100 to 1000 disorder realizations, depending on $N_{\uparrow}$.

$r_{WD}$ as $L$ is increased. We attribute (i) to the smaller level spacing caused by merging the doublon and singlon sectors, which allows resonance formation at larger disorder strengths. We consider (ii) to be a consequence of the fact that the singlon band – which always localizes, as apparent in Fig. 3b,c – merges with the one hosting doublons, reducing its distinct ergodic properties, see SM [22].

Figure 4b presents the evolution of the WD-P spectral transition as function of the spin-up density $\rho_t$. We assume that WD-P transition takes place at such $W = W_C$ that $r_C = (r_{WD} + r_{TP})/2 \sim 0.46$. In qualitative agreement with the estimate (6), WD level-repulsion is enforced up to larger disorder strength the more $\rho_t$ approaches 1/2. We attribute the observed deviations from particle-hole symmetric scaling $\propto \rho_t(1 - \rho_t)$ to higher order processes in $t$, which violate the assumption $h_{j,j+1} = I$, under which Eq. (6) was derived. Nevertheless, the numerical results show a drift towards the dependence predicted by Eq. (6), as the system size is increased.

As a concluding study, Fig. 5 shows how the emergence of WD statistics is accompanied by diffusive behavior. Following Refs. [9, 26], we consider the evolution of the spin-up imbalance $I = (N_{\uparrow, e} - N_{\uparrow, o})/(N_{\uparrow, e} + N_{\uparrow, o})$ in the presence of a single doublon, in which $N_{\uparrow, e/o}$ is the total occupation of even/odd sites by spin-up fermions. We time-evolve an initial state with a spin-up fermion in every even site and one doublon. We also monitor the averaged evolution of the local spin-up occupation $\langle n_{\uparrow, i} \rangle$ as a function of time, different system sizes and disorder $W < W_C$. In the non-interacting case ($U = 0t$), both quantities do not thermalize and show weak size dependence because of AL. In the presence of a doublon, both quantities show stronger decay, as size of the systems is increased. The suppression of the imbalance $I$ is clearly correlated in time with the doublon spreading across the system. We also emphasize that, for weaker interactions ($U \sim t$), analogous behavior is expected, but the decay dynamics is slower, see SM [22].

Conclusions – In this work, we described a striking effect arising from the interplay of interactions and disorder: a single doublon acting as an ergodic nuclei that can thermalize an initially localized system of singlons; such system is therefore a “supercooled insulator” that stays localized only until a suitable ergodic seed is introduced. Our predictions apply regardless of particle statistics: while here we focused on fermions, in SM [22], we studied doublon-mediated delocalization in Bose-Hubbard models.

Thanks to its simplicity and direct experimental relevance, this effect offers a new approach to better understand quantum-classical transition between MBL and ergodic phases [16]. In contrast to Ref. [27], the processes described in our work do not require a finite density of ergodic bubbles to destroy localization, but only a single spin-down fermion [17]. Moreover, the effects that we described are straightforward to observe using currently available experimental capabilities, by tracking the position of doublon and singlons. Crucially, doublon-induced thermalization is expected to occur on time scales scaling as power-laws in system size, while the thermalization induced by a static bubble of Ref. [17] requires exponent-
tially long times in the system size.

Finally, even though our analytical arguments assumed the infinite-$U$ limit, where doublons are stable in finite-size systems, we expect the mechanism of doublet-mediated delocalization at $W < W_C$ to be effective also in the thermodynamic limit $L \to \infty$ at finite, but large $U$. The stability of doublon in this case is ensured by its parametrically long life-time, which has the same origin as prethermalization phenomena in periodically driven systems [28].

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Supplementary Material of “Ergodic nucleation activated by single doublons”
Ulrich Krause, Théo Pellegrin, Piet W. Brouwer, Dmitry A. Abanin, and Michele Filippone
Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany and Department of Quantum Matter Physics and Department of Theoretical Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland

In this Supplemental Material, we provide details concerning the derivation of Eq. (2) in the main text. We provide additional and detailed information concerning the numerical calculations presented in the main text for the Fermi-Hubbard model and U = 100t. We equally provide a detailed numerical study of the U = 1t case, for which we also provide analytical estimates explaining the slower setting in of a ergodicity, but up to larger disorder strengths. We conclude showing how the ergodic bubble generation by single doublons equally emerges in bosonic systems, by carrying an analog numerical study on the Bose-Hubbard model.

DETAILS OF THE DERIVATION OF THE EFFECTIVE SINGLE DOUBLON HAMILTONIAN.

We provide here details concerning the derivation of the correlated hopping Eq. (2) in the main text. We consider the case of large interaction U \gg N_t t. This condition guarantees that many-body bands with and without doublon do not overlap in energy, see Fig. 3. In the main text. We focus on the situation in which a doublon is formed and simplify Eq. (1). We first separate the hopping term in Eq. (1) in two parts H_T = t(D + V), in which the operator D(V) = \sum_j |D_j(V_j)| + h.c. preserves changes the number of doublons [S1, S2]

\[ D_j = h_{j,\sigma} c_{j,\sigma}^{\dagger} c_{j,\sigma} + n_{j,\sigma} c_{j,\sigma}^{\dagger} c_{j,\sigma} n_{j+1,\sigma} + n_{j,\sigma} c_{j,\sigma}^{\dagger} c_{j+1,\sigma} n_{j+1,\sigma} \]

\[ V_j = h_{j,\sigma} c_{j,\sigma}^{\dagger} c_{j+1,\sigma} n_{j+1,\sigma} + n_{j,\sigma} c_{j,\sigma}^{\dagger} c_{j+1,\sigma} h_{j+1,\sigma} \]

\[ \Phi \]

in which n_{j,\sigma} = c_{j,\sigma}^{\dagger} c_{j,\sigma} and h_{j,\sigma} = 1 - n_{j,\sigma} are projectors controlling whether fermion hoppings change or preserve the doublon number. The effective doublon-conserving Hamiltonian is obtained by eliminating \Phi to leading order, which is achieved via a unitary Schrieffer-Wolff transformation \Phi = e^{iS} \Phi e^{-iS} [S3]

\[ \mathcal{H}' = \mathcal{H}_O + D + i \frac{1}{2} \left( S, \mathcal{V} \right) + \mathcal{O}(S^2) \]

where S is chosen to satisfy \Phi + i \left( S, \mathcal{H}_O + D \right) = 0. In the particular case N_\uparrow = 1, \mathcal{V} only connects states |\Psi_{1/0}\rangle with one/zero doublons. Such states are of the form |\phi_1\rangle = |\ldots, \uparrow\downarrow, \ldots\rangle and |\phi_0\rangle = |\ldots, \uparrow\downarrow, \ldots\rangle, in which we use the notation |\uparrow\downarrow\rangle for the doublon at site j and |0\rangle for no particle at site j. They differ in energy by U + \varepsilon_j - \varepsilon_{j+1} \sim U, in the large U limit. By evaluating the matrix element between such states for \Phi, we find

\[ \langle \phi_0 | \mathcal{V} | \phi_1 \rangle + iU \langle \phi_0 | S \phi_1 \rangle + \langle \phi_0 | \left( S, D \right) | \phi_1 \rangle = 0 . \]

\[ \Phi \]

As \langle \phi_0 | S | \phi_1 \rangle is of order \mathcal{O}(t/U), the last term in the above expression is of order \mathcal{O}(t/U)^2, and we can neglect it in a first approximation. Accordingly, also the commutator \left[ S, \mathcal{V} \right] = \mathcal{O}(t^2/U), therefore \mathcal{H}' = \mathcal{H}_O + D + \mathcal{O}(t^2/U). We can also write \mathcal{H}_O = \sum_j \varepsilon_j n_j + \mathcal{O}(t^2/U), where we introduce the composite doublon annihilation operator \mathcal{O_{j}} = c_{j,\uparrow} c_{j,\downarrow}. Further, the doublon-conserving operator D in Eq. (S1) can be considerably simplified in the single doublon sector: we can neglect operators of the form \mathcal{O_{j}} c_{j,\uparrow} c_{j+1,\downarrow} h_{j+1,\uparrow} (no site occupied exclusively by a spin-down) and \mathcal{O_{j}} c_{j,\uparrow} c_{j+1,\uparrow} n_{j+1,\downarrow} . One thus obtains the residual hopping Eq. (2) given in the main text.

ADDITIONAL DETAILS ON NUMERICAL DENSITY- AND FINITE-SIZE SCALING

In this section, we provide additional plots showing how Wigner-Dyson statistics is induced by the presence of a single doublon for different spin-up densities \rho_\uparrow = N_\uparrow / L and system sizes L. Figure S1, reports analogous plot to Fig. 3 in the main text. We consider only large interactions (U = 100t), different system sizes and different \rho_\uparrow. Notice that we inverted the axes and switched to a different scale for the vertical axis. Instead of the energy of the state, we consider its position in the many-body spectrum. This choice has limited physical meaning, for instance it does not
make apparent the “mobility gap” in energy between doublon and singlon bands. Nevertheless, it allows to clearly
distinguish many-body bands with and without doublons and better appreciate the transition from Wigner-Dyson to
Poisson level-spacing statistics. We remind that, for the Fermi-Hubbard model with \( N_{\uparrow} \) and \( N_{\downarrow} \) spin-up and -down
fermions on \( L \) sites, the Hilbert space dimension is \((\binom{L}{N_{\uparrow}}) \times (\binom{L}{N_{\downarrow}})\). For the specific case in which \( N_{\downarrow} = 1 \), the singlon and
doublon bands feature \( L \times (\binom{L-1}{N_{\uparrow}}) \) and \( L \times (\binom{L-1}{N_{\uparrow}-1}) \) states respectively.

Figure S1. Density plot of the averaged gap-ratio \( r \) as function of disorder strength \( W/t \) and state label (see text). The black
horizontal lines signal the state in the middle of the doublon bands and give the cuts along which the lines in Fig. S2 are taken.
The red regions appearing on the bottom correspond to the AL bands with only singlons. All features there are artifacts of
the numerical averaging procedure. Disorder averages were performed over 4000, 2000, 1000 realizations for \( L = 8, 10 \) and 12.
For \( L = 14 \) averages over disorder range from 1000 to 100 differen disorder realizations depending on \( N_{\uparrow} \).
Figure S2 reproduces the analog of Fig. 4.b in the main text for different system sizes and a wider range of $\rho^\uparrow$. The plots collected in Fig. S2 show how the transition from Wigner-Dyson to Poissonian statistics moves as function of $\rho^\uparrow$ and they were used to construct Fig. 4.c in the main text.

In this section, we explore the thermalization induced by a single spin-down fermion for weaker interactions $U = 1t$. Figure S3 is the analog of Fig. 4 in the main text, but for $U = 1t$ instead of $U = 100t$. As visible in Fig. 3 in the main text, in this case it is not possible to distinguish between many-body bands characterized by their doublon number, as they are mixed. This case better illustrates the situation in the thermodynamic limit with fixed interactions. We remind here that the condition $U \gg N^\uparrow \cdot (t, W)$ was necessary to avoid the mixing of singlon and doublon bands. Figure S3.a shows the finite-size scaling of the average gap ratio $r$ in the middle of the many-body spectrum as function of disorder. Also in this case, the transition from Wigner-Dyson to Poisson statistics becomes sharper for larger system sizes, showing that the thermalization of a localized systems by a single spin-down fermion persists in the thermodynamic limit. Nevertheless, we notice that the crossing of the curves happens at a different $r_C \sim 0.425$. We consider this point as the transition point of critical disorder $W_C$ at which the transition between the ergodic and the MBL phase takes place. Two further differences with the case with a stabilized doublon addressed in the main text are i) for equivalent disorder strength $W$, full Wigner-Dyson statistics takes longer to enforce as function of system size and ii) the WD-P spectral transition takes place at a larger disorder strength $W_C$. The coexistence of these two facts is somehow surprising. If it may not appear surprising that weaker interactions require a larger system sizes to fully enforce Wigner-Dyson spectral statistics, one would consequently expect that MBL would be enforced for weaker disorder strengths, which is not the case.

This surprising fact can be explained by recurring to a similar approach to that used to derive the estimate (6) in the main text for systems with stable doublons at large interactions. The main difference in the following discussion is that we consider the weak interacting limit $U \rightarrow 0$. In this case, we keep the Fermi-Hubbard model, Eq. (1) in the
Figure S3. Analog of Fig. 4 in the main text, but for $U = 1t$. a) Finite-size scaling of the average gap-ratio $r$ as function of disorder strength $W/t$. We consider $r$ for energies in the middle of the many-body band. b) WD-P transition as function of $W/t$ and increasing $\rho^\uparrow$. c) Critical disorder $W_C$, at which the average level spacing $r = r_C \sim 0.425$, as function of $\rho^\uparrow$ for different system sizes $L$, supporting the validity of the estimate (S5) in the thermodynamic limit. Disorder averages were performed over 4000, 2000, 1000 realizations for $L = 8, 10$ and 12.

In this section we consider the Bose-Hubbard model, which is the bosonic version of the Fermi-Hubbard model we considered in Eq. (1) in the main text. It reads

$$H_{BH} = \sum_j [b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j] + U \sum_j n_j(n_j - 1) + \sum_j \varepsilon_j n_j, \quad (S6)$$

in which we adopted the same notations as those used in Eq. (4) in the main text, with the only difference that we did not introduce any doublon annihilation operator $d$, but kept the spin flavor of fermions $\sigma$. The resonance condition between localized states can be derived in an analogous fashion as in the main text. In this case, the main differences are that the change in energy between states connected by the interaction $U$ is of order $\delta E \sim 2W$, the matrix element between such states in a localization volume is of order $U/\xi^2$. The number of states which this matrix element connects is of order $\xi^3$. By repeating the estimate carried in the main text the resonance condition reads

$$2W \leq U \rho^\uparrow (1 - \rho^\uparrow) \xi. \quad (S5)$$

Notice that this resonance condition is analogous to Eq. (6) derived for the case involving doublons in the main text. The main difference is that now the interaction strength $U$ takes the place of the hopping strength $t$ and a smaller prefactor (2 instead fo 3) is in front of the disorder strength $W$. This smaller prefactor hints why resonances can be induced by interactions for larger disorder strengths, thus pushing the transition to MBL at larger disorder strengths.

We attribute the fact that ergodicity sets in much slower than in the $U \rightarrow \infty$ for increasing system sizes, to the intrinsically localized nature of singlon states. As a further evidence, we also consider, as in the main text, the evolution of an initial state with a spin-up fermion in every even site and one doublon. Figure S4 is the analog of Fig. 5 in the main text, but for $U = 1t$. Also in this case, we compare with the non-interacting case ($U = 0$). One notices that decay of local observables is slower than in the large $U$ limit.

**ERGODIC BUBBLE GENERATION BY SINGLE DOUBLONS IN BOSONIC SYSTEMS**

In this section we consider the Bose-Hubbard model, which is the bosonic version of the Fermi-Hubbard model we considered in Eq. (1) in the main text. It reads

$$H_{BH} = t \sum_j \left[ b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right] + U \sum_j n_j(n_j - 1) + \sum_j \varepsilon_j n_j, \quad (S6)$$
in which the operators $b_{j,\sigma}$ annihilate bosons on site $j$, $n_{j,\sigma} = b_{j,\sigma}^\dagger b_{j,\sigma}$, and the onsite energies $\varepsilon_j$ are uniformly distributed in the energy window $[-W, W]$. Notice that for boson, doublon formation does not need to add any internal degree of freedom, like spin, as the bosonic statistics allows for the multiple occupation of a single site, thus permitting the formation of doublons, even triplons and so forth.

Figure S5 is the analog of Fig. 3 in the main text, but derived for Eq. (S6). As for Fig. S1, also in this case, it is practical to exchange the axes and consider the state position in the many-body spectrum instead of its energy. This choice allows to better observe the WD-P transition in sectors with different numbers of doublons. The phase diagram is totally analogous to the one derived for fermions in the main text. The main difference resides in the fact that more than one doublon and even triplons can be formed in the Bose-Hubbard model, being all bosonic particles indistinguishable. We remind here that, in our study concerning the Fermi-Hubbard model, we considered only a single spin-down fermion, thus allowing for the formation of a single doublon at most. For instance, the black lines drawn in Fig. S5 for $U = 10t$ and $100t$ sit exactly at $(\frac{L}{N})$ and $(\frac{L}{N}) + L \cdot (\frac{L-1}{N-2})$. Thus, as in the fermionic case, it is possible to isolate the section of the Hilbert space with a single doublon and observe that its presence leads to
Wigner-Dyson statistics also in bosonic systems. The similarity between the fermionic and bosonic case shows the generality of the mechanism discussed in the main text, that is the importance of doublon formation for the activation of thermalization in localized system.

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