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Disorder enhanced quantum many-body scars in Hilbert hypercubes

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We consider a model arising in facilitated Rydberg chains with positional disorder which features a Hilbert space with the topology of a $d$-dimensional hypercube. This allows for a straightforward interpretation of the many-body dynamics in terms of a single-particle one on the Hilbert space and provides an explicit link between the many-body and single-particle scars. Exploiting this perspective, we show that an integrability-breaking disorder enhances the scars followed by inhibition of the dynamics due to strong localization of the eigenstates in the large disorder limit. Next, mapping the model to the spin-1/2 XX Heisenberg chain offers a simple geometrical perspective on the recently proposed Onsager scars [Phys. Rev. Lett. 124, 180604 (2020)], which can be identified with the scars on the edge of the Hilbert space. This makes apparent the origin of their insensitivity to certain types of disorder perturbations.

Introduction. The understanding of thermalization and relaxation dynamics is at the forefront of research on quantum many-body systems out of equilibrium. Since the formulation of the eigenstate thermalization hypothesis [1–3], predicting fast thermalization following a quench from most many-body states, many exceptions to this behavior have been identified. The prominent examples are integrable [4,5] and many-body localized (MBL) systems [6–14]. A recently added category is quantum many-body scars (QMBS) [15,16], which are particular eigenstates responsible for slow decay and oscillatory behavior of observables following a quantum quench from certain initial states, typically close to a product state, as observed in Ref. [17] realizing the so-called PXP model [18]. This has triggered a great interest in QMBS in settings ranging from constrained to driven [19–64], and recently also disordered systems [65,66].

QMBS owe their name to the single-particle quantum scars [67,68] which were in turn inspired by particle motion in classical billiards. In both the quantum and classical cases, it is the shape of the billiard boundary, such as the celebrated Bunimovich stadium or cardioid shape [69,70], which causes the motion of the particle to be generically ergodic. The exception to this rule is a set of periodic trajectories, around which the density of certain wave functions—the scars—is enhanced in the presence of disorder, naturally emerging from the positional disorder of the atoms. Finally, exploiting the mapping of the present model to the Heisenberg spin-1/2 XX chain [78], we identify the recently proposed Onsager scars [65,79] with scars corresponding to sparse eigenstates residing at the “edge” of the Hilbert space. This provides intriguing connections between QMBS and single-particle scars and highlights the utility of a graph-theoretical approach to many-body dynamics, which has been advocated also in the studies of quantum chaos [80–84], integrability [85], QMBS [86], and fermionic and exchange models [87,88].

The model. We consider a one-dimensional chain of $M$ Rydberg atoms along the $z$ axis, with open boundaries and spaced by $r_0$. We denote the ground and excited (Rydberg) states as $|\downarrow\rangle, |\uparrow\rangle$. The corresponding Hamiltonian reads

$$H_{\text{Ry}} = \sum_k \frac{\Omega}{2} \sigma^z_k + \Delta n_k + \sum_{l>k} V(|r_k - r_l|) n_k n_l, \quad (1)$$

where $\sigma^z_k = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|$, $n_k = |\uparrow\rangle\langle\uparrow|$, and $V(r) = C_a/r^2$, $r = |r|$. $C_a$, which we take to be positive, is the interaction strength coefficient with $a = 3 (6)$ for dipole-dipole (van der Waals) interaction. The positions of the atoms are $r_k = (0,0,(k-1)r_0) + \delta r_k$, where $\delta r_k$ describes the positional disorder which induces the disorder in energy. Denoting $V_{NN} = V(r_0)$ and $V_{NNN} = V(2r_0)$, we define an energy shift for a pair of nearest neighbors $\delta V_k = V_{NN} - V(|r_{k+1} - r_k|)$.

It has been shown in [71] that under the facilitation condition $\Delta = -V_{NN}$ and in the regime $V_{NN} \gg \Omega$, $\delta V_k$ the Hamiltonian (1) effectively reduces to

$$H_{\text{eff}} = \Delta N_{cl} + \sum_k \frac{\Omega}{2} \sigma^z_k P(k) + \delta V_k n_k n_{k+1} + V_{NNN} n_k n_{k+2}, \quad (2)$$

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The occupation Eq. (9) with (of basis states constituting a specific sparse eigenvector (a scar), momenta $p$ is specified in Eq. (10).

Next we will be particularly focusing on the $N_{cl} = 1$ sector for which the Hilbert space can be represented as a square lattice with a triangular boundary. Each site $(\bar{x}, \bar{y})$ of this lattice corresponds to a state

$$|\bar{x}, \bar{y}\rangle = |\downarrow, \uparrow, \uparrow, \downarrow\rangle.$$

Here, $|\downarrow\rangle$ labels a string of consecutive down spins of length $\ell$. The boundaries are determined by the natural conditions $x \geq 0, y \geq 0$, and $x + y < M$ [cf. Fig. 1(a)].

$H_{dis}$ projected on the $N_{cl} = 1$ sector can be written as

$$H = H_0 + H_{pot} + H_{dis},$$

$$H_0 = \frac{\Omega}{2} \sum_{\bar{x}\in\mathbb{L}/h} |\bar{x}\rangle \langle \bar{x} + 1| + |\bar{x} + 1\rangle \langle \bar{x}| + H.c.,$$

$$H_{pot} = V_{NNN} \sum_{\bar{x}\in\mathbb{L}} \max (0, M - 2 + (\bar{x} + \bar{y})|\bar{x}\rangle \langle \bar{x}| + \bar{y}\rangle$$

$$H_{dis} = \sum_{\bar{x}\in\mathbb{L}} |\bar{x}\rangle \langle \bar{x}| \delta V_k,$$

where $1_{k,\ell}$ is a unit vector in the direction $\bar{x}, \bar{y}, H = (|\bar{x}\rangle |\bar{x} + 1| + (\bar{x} + 1)|\bar{x}\rangle + H.c.$, and $\delta V_k$ is specified in Eq. (10).

$H_0$ can be solved exactly [89] with eigenenergies

$$2\Omega^{-1}E_{m,n} = 2 \cos \left( \frac{m\pi}{M + 2} \right) + 2 \cos \left( \frac{n\pi}{M + 2} \right)$$

and eigenvectors

$$|u_{m,n}\rangle = \sum_{x,y} u_{m,x}(y) - u_{m,y}(x)|x, y\rangle.$$
methods such as exact diagonalization to few sites and small phonon number [96]. To proceed, we treat the atomic motion $\mathbf{r}_i(t)$ as that of a classical particle in a harmonic motion with coordinates $\mathbf{r}_i(t) = C_{\nu,k} \cos(\omega_i t + \phi_{\nu,k})$, where $C_{\nu,k} = \sqrt{\nu/(2m)}$ and $\phi_{\nu,k} \equiv \arccos[C_{\nu,k} C_{\nu,k}]/C_{\nu,k}$, which are fully specified by the initial position $\mathbf{r}_i(0) = \delta_{\nu,k}(t = 0)$ and momentum $p_{\nu,k}(0)$. Here, the latter is drawn from an isotropic Boltzmann distribution $\rho(p_{\nu,k}) \propto \exp[-\beta p_{\nu,k}^2/(2m)]$.

The third and final comment is that for $V \propto 1/\rho^2$, the distribution $\rho(\delta_{\nu,k})$ leads to the energy probability distribution $\rho(\delta)$ with undefined moments, a consequence of rare events when two atoms come arbitrarily close to each other [93]. This is an artifact, not expected to occur under realistic experimental conditions, of the algebraic form of $V$. For this reason and in order to gain analytical control, we use a small-displacement approximation

$$\delta V_k = \sum_{k=1}^{M-1} \left[ \frac{C_{\nu,k}}{r_{k+1} - r_k} - V_{NN} \right].$$

where $\delta_{\nu,k} = (v_{k+1} - v_k)/r_0$. In order to get the occupation (9) with the time-dependent Hamiltonian (4a), we solve the corresponding Schrödinger equation for the wave function. In particular, we are interested in the properties of the occupation as a function of the disorder. The results for $|\psi(0)\rangle = |\psi_G\rangle$ are shown in Figs. 2(a) and 2(f) with examples of $\langle \psi(0)|\langle \psi|\rangle$ for three different values of disorder shown in Figs. 2(c)–2(e).

The solid blue line in Fig. 2(f) corresponds to a quantity $F_r$, which characterizes the overlap of the occupation with the occupation $\langle n_0(\bar{x})\rangle$ generated by the idealized Hamiltonian $H_0$, Eq. (4b). It is defined as $F_r = (F_r - \bar{F}_0)/(1 - \bar{F}_0)$, where $F = \sum_k \langle \langle \bar{n}_0(\bar{x})\rangle \rangle_{\psi}$. $\bar{F}_0$ is given by $F$ with the replacement $\langle \langle \bar{n}_0(\bar{x})\rangle \rangle_{\psi} \rightarrow \sqrt{2/(M+1)\mu}$. The tilde denotes the occupations normalized as $\sum_x \langle \langle \bar{n}_0(\bar{x})\rangle \rangle_{\psi}^2 = 1$, and the double angular brackets denote the averaging over disorder realizations (initial conditions). The rationale behind $F_r$ is that $F_r = 1$ when the occupation is that of the idealized scenario of Fig. 1(b) and $F_r = 0$ for a featureless uniform occupation. For comparison, the orange solid line shows the level statistics $r = \min\{\Delta_{E_{i-1}},\Delta_{E_{i+1}}\}$ taking the initial conditions, i.e., quenched positional disorder, where the average is taken over all energy differences $\Delta E_i = E_i - E_{i-1}$ of adjacent ordered eigenenergies $E_i \geq E_{i-1}$ of $H$. The values $r \approx 0.39, 0.53$ corresponding to the Poisson and Wigner-Dyson statistics are indicated by the horizontal dashed lines. It is apparent from Fig. 2 that increasing the disorder enhances the many-body scars appearing in the occupation, which can be explained in terms of the eigenstate localization: as the disorder is increased from zero, the eigenstates of $H$ become more and more localized on the Hilbert space square lattice. This initially enhances their overlap with the initial state along the scar path. We observe similar enhancement also for other initial states and values of disorder and discuss quantitatively the energy landscape of the Hilbert space in [89].

**Thermalization.** Next we investigate how the scars affect the capacity of the system to thermalize. To this end we consider the time evolution of the (second Rényi) entanglement entropy (EE) $S(t) = -\log \text{Tr}[\rho_A(t)^2]$, where $\rho_A(t)$ is the reduced density matrix of subsystem $A$, which we choose to be a half-chain of length $M/2$. In Fig. 3(a) we plot the time evolution of EE for a quench in the nonintegrable regime $d = 0.12$ from the Gaussian state $|\psi_G\rangle$ (blue), a midspcetrumtrs (green), and $|\psi_{\text{random}}\rangle$ (orange). The vertical dashed lines indicate the (scaled) times $t_{0}, t_\text{f}$ used in Fig. 2 and the inset shows the detail of the late-time evolution. (b) The standard deviation of the saturated $S$ vs $d$. Data obtained with 10 realizations of the initial conditions (a) and 300 realizations (b), where static disorder was considered for numerical reasons, yielding a value of the average saturated entropy compatible with (a) within std$[S \to \infty]$.

**FIG. 2.** (a) An example of the autocorrelation $A(t) = \langle |\psi_G(\langle \psi|\rangle)^2 \rangle$ for $M = 11$. (b) The threshold time $t_c$ vs disorder strength for various system sizes $M$. (c)–(e) Examples of the occupation Eq. (9) for various disorder strengths indicated by circle, cross, and triangle, respectively, in panel (f). (f) $F_r$ (blue) and the $r$ statistics (orange) vs disorder strength $d$ [here $\alpha = 6$, $\nu_0 = 0.03$, $\epsilon = 9$, $(\bar{\nu}, \bar{\nu}) = (50, 250)$ and $V_{NN}/\bar{\nu} = 4$].
states which we attribute to superscarring, i.e., the fact that each basis state either belongs to a scar in the Hilbert space or is adjacent to it. We also note the initial rise for the Gaussian state for the magnetic moment a ≈ 0.3 corresponds to the transition from nonintegrable to integrable as quantified by r [13,75,97] and hints towards a possible MBL-like phase [78].

Relation to Onsager scars. It has been shown in [78] that the spin flip part of $H_{\text{eff}}$, Eq. (2), can be mapped to the spin-1/2 XX Heisenberg spin chain of length $M + 1$

$$\sum_k \sigma_k^z \rho(k) \rightarrow H_{\text{XX}} = \sum_{k=1}^M \mu_k^x \mu_{k+1}^x + \mu_k^y \mu_{k+1}^y,$$

where $\mu^{x,y,z}$ are the Pauli matrices in a {$|0\rangle$, $|1\rangle$} basis. It is related to the {$|\uparrow\rangle$, $|\downarrow\rangle$} basis through the mapping $\uparrow\uparrow \rightarrow 0$, $\uparrow\downarrow \rightarrow 1$, where the ambiguity is lifted by including fictitious boundary spins ($\downarrow$) to the left and right ends of the chain. Consequently, $\sigma_0^x = \mu_0^x \mu_1^x$, $\sigma_0^y = (-1)^k \sum_{\mu=1}^k \mu_k^x \mu_{k+1}^y$, $\sigma_0^z = (-1)^k \prod_{\mu=1}^k \mu_\mu^z$, and $\Delta V$ of Eq. (2) maps to nonlocal disorder given by a string of $\mu^z$ operators [78].

Crucially, the structure of the Hilbert space (connectivity between the basis states) remains unchanged as it is given solely by the spin flip terms [89]. Recently, Ref. [65] proposed a class of spin models with $n$ spin components featuring so-called Onsager scars, which are states with perfect revivals of the integrated autocorrelation subject to certain types of the integrability-breaking disorder. The simplest instance $n = 2$ of this class is $H_{\text{XX}}$, Eq. (11), with the Onsager state $|\psi(\beta)\rangle \propto \exp[\beta Q^+ Q^z] |0\ldots0\rangle = \sum_{n=0}^{(M+1)/2} (\beta Q^+ Q^z)_{n\bar{n}} |0\ldots0\rangle$ and $Q^+ = \sum_{\mu=1}^{M+1} (-1)^{\mu+1} \mu_{\mu}^+ \mu_{\mu+1}^z$. We have intentionally indexed the sum-summation of $|\psi(\beta)\rangle$ by $n \equiv \bar{n}$ as each term corresponds to a superposition of $\mathcal{N}_d$ pairs $|\ldots1_k \downarrow k \ldots1\rangle$, i.e., single Rydberg spins $\uparrow$. The projection of $|\psi(\beta)\rangle$ on the $\mathcal{N}_d = 1$ sector is nothing but the scar indicated in Fig. 1(a).

This allows for the following identifications: (i) The $|\mathcal{N} + 1/2\rangle$ eigenstates which form the special band in the eigenstates’ EE [cf. Fig. 2(a) in [65]] correspond to different cluster sectors of $H_{\text{eff}}$. (ii) The projection of $|\psi(\beta)\rangle$ on the $\mathcal{N}_d = 1$ sector is the scar corresponding to the $0, (M - 1) - (M, 0)$ diagonal, i.e., the edge of the Hilbert space [cf. Fig. 1(a)], which is comprised only of single Rydberg spin excitations. This interpretation applies to other $\mathcal{N}_d$ as well. Furthermore, the simple structure of the Hilbert space allows for a straightforward visualization of why certain types of the integrability-breaking disorder do not affect the Onsager scars, such as Eq. (13) in [65]. Another example naturally realized in the Rydberg systems is the disorder of Eq. (2), which affects all but the isolated Rydberg spins.

Experimental considerations. We have simulated the time evolution with the assumption that the atomic trajectories are that of classical particles in a harmonic potential, independent of their internal state. To estimate the effect of the Rydberg interactions on the atomic motion and hence the disorder energies, we consider $\Delta V(\langle n_{NN}\rangle)$ to be the expectation value of $\delta V$, Eq. (10), corresponding to basis state $|\bar{n}\rangle$ containing $n_{NN}$ nearest neighbors and evaluated using $p(\delta r_k)$. Analogously, we define $\Delta V(\langle n_{NN}\rangle)_{\text{int}}$ where the equilibrium positions of the atoms are taken in the presence of the interactions [89].

The difference between the two provides an estimate for a threshold timescale beyond which the atomic motion cannot be treated as independent of the internal state and we define $t_c \equiv 2\pi \hbar/(\Delta V(M - 1)_{\text{int}} - \Delta V(M - 1))$. The plot of $t_c$ vs $d$ is shown in Fig. 2(b) with an example of $t_c$ indicated in Fig. 2(a). Thus, for $d \approx 0.1$, the present analysis holds for $\Omega t = O(100)$ for $M$ of few tens, sufficient to capture the behavior of the time-averaged occupation in a realistic experimental setting.

Outlook. In this work we have highlighted how the structure of the Hilbert space, resembling that of a hypercubec, provides useful insights in the nonequilibrium dynamics in spin chains. This allowed us to identify quantum many-body scars as single-particle scars in the Hilbert space, link them to the Onsager scars, and show how their signature is enhanced by disorder. This provides a number of interesting openings, such as the interpretation of the disordered Heisenberg XXZ spin chain as that of an Anderson model on a hypercubic lattice, which is relevant to the ongoing discussion about the scaling of the Thouless time in many-body systems [98,99]. It would also be interesting to explore the role of sparse eigenvectors, which play an important role in various applications, such as in the signal analysis of networks [100,101], in the context of many-body Hamiltonians and their graph-theoretic representations [85,87,88,102]. Finally, to describe the entangling dynamics between the motional and internal degrees of freedom, new approaches, such as the variational ansatz based on non-Gaussian states [103], need to be investigated.

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[89] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.103.L220301 for (i) diagonalization of $H_0$, (ii) the computation of disorder energy expectation values, (iii) the energy landscape, (iv) comments on the numerical treatment of the atomic motion, and (v) the structure of the Hilbert space and Refs. [104–114].