Disorder enhanced quantum many-body scars in Hilbert hypercubes

Van Voorden, B.; Marcuzzi, M.; Schoutens, K.; Minář, J.

DOI
10.1103/PhysRevB.103.L220301

Publication date
2021

Document Version
Final published version

Published in
Physical Review B

Citation for published version (APA):
Disorder enhanced quantum many-body scars in Hilbert hypercubes

Bart van Voorden,1 Matteo Marcuzzi,2 Kareljan Schoutens,1,3 and Jiří Minář1,3
1Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands
2School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom
3QuSoft, Science Park 123, 1098 XG Amsterdam, The Netherlands

(Received 11 December 2020; revised 4 May 2021; accepted 17 May 2021; published 3 June 2021)

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.

DOI: 10.1103/PhysRevB.103.L220301

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 quantum case.

Here we analyze a model of spins-1/2, which describes a chain of Rydberg atoms with open boundaries under a facilitation condition [71]. Representing the Hilbert space as a graph, we show that it corresponds to a truncated hypercube with the dimension given by the number of spin clusters (cf. below for definition).

This allows us to identify the QMBS as single-particle scars on the Hilbert space [16]. Building on the graph representation of the Hilbert space, an approach also exploited in the studies of MBL [6,7,32,72–77], we demonstrate that the scar signatures are 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 $|↓\rangle$, $|↑\rangle$. The corresponding Hamiltonian reads

$$H_{\text{Ry}} = \sum_k \Omega/2 \sigma_k^z + \Delta n_k + \sum_{l \neq k} V(|r_k - r_l|) n_k n_l,$$

where $\sigma_k^z = |↑\rangle\langle↓| + |↓\rangle\langle↑|$, $n_k = |↑\rangle\langle↑|$, and $V(r) = C_o/r^6$, $r = |r|$. $C_o$, which we take to be positive, is the interaction strength coefficient with $\alpha = 3 (6)$ 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

$$H_{\text{eff}} = \Delta N_{\text{cl}} + \sum_k \Omega/2 \sigma_k^z P_{(k)} + \delta V_k n_k n_{k+1} + V_{\text{NNN}} n_k n_{k+2},$$

where $P_k = |↑\rangle\langle↓| + |↓\rangle\langle↑|$. This Hamiltonian describes a model of spins-1/2, which is integrable 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.
The occupation Eq. (9) with (a) blocks of consecutive spin excitations (e.g., the configuration contains two clusters highlighted by boxes). The projector or disappear and hence their number represents a conserved charge, \( N_3, H_{\text{eff}} \equiv 0 \). For each \( N_3 \), the topology of the Hilbert subspace of (2) is that of a truncated hypercube of dimension \( d = 2N_3 \) [89].

In what follows we will be particularly focusing on the \( N_3 = 1 \) 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

\[
|\bar{\Psi}\rangle \equiv |\bar{x}, \bar{y}\rangle = |\downarrow\rangle_{\bar{x}} \uparrow \cdots \uparrow |\downarrow\rangle_{\bar{y}}.
\]

Here, \([\downarrow]\) 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)].

The projected on the \( N_3 = 1 \) sector can be written as

\[
H = H_0 + H_{\text{pot}} + H_{\text{dis}},
\]

\[
H_0 = \frac{\Omega}{2} \sum_{\bar{k} \in \mathbb{H}} |\bar{\Psi}\rangle \langle \bar{\Psi}| + H_{\text{c},0},
\]

\[
H_{\text{pot}} = V_{\text{NNN}} \sum_{\bar{k} \in \mathbb{H}} \text{max}[0, M - 2 - (\bar{x} + \bar{y})] |\bar{\Psi}\rangle \langle \bar{\Psi}|,
\]

\[
H_{\text{dis}} = \sum_{\bar{k} \in \mathbb{H}} |\bar{\Psi}\rangle \langle \bar{\Psi}| \delta V_{\bar{k}},
\]

where \( \delta V_{\bar{k}} \) are unit vectors in the direction \( \bar{x}, \bar{y}, \mathcal{H} = |\bar{\Psi}\rangle [0 \leq (\bar{x}, \bar{y}) < M \land \bar{x} + \bar{y} < M], b = |\bar{\Psi}\rangle [\bar{x} + \bar{y} = M - 1], \) and \( \delta V_{\bar{k}} \) 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

\[
|u_{m,n}\rangle = \sum_{x,y} |u_m(x)u_n(-y) - u_m(-y)u_n(x)|x,y\rangle,
\]

where

\[
u_m(x) = \sqrt{\frac{2}{M + 2}} \sin \left[ \frac{m \pi}{M + 2} \left( x + 1 + \frac{M}{2} \right) \right].
\]

In Eqs. (6) and (7) we have used the shifted variables \( x = \bar{x} - M/2, m, n \in \{1, 2, \ldots, M + 1\}, m > n, \) and \( \bar{x} \in \mathcal{H} \). All energies are nondegenerate, except for \( [M/2] \) zero-energy states for which \( m + n = M + 2 \). It can be shown that the zero-energy subspace is spanned by eigenvectors, which are sparse in the basis Eq. (3) [89]. Due to its simple structure, these states can be identified as scars in the Hilbert space [cf. Fig. 1(a)]. Consequently, one can directly apply the single-particle perspective used in quantum scars on discrete lattices [90]. In what follows we examine the dynamics following a quantum quench. Motivated by the use of Gaussian wave packets as probes for single-particle scars [67, 68, 91, 92], we introduce effective “Gaussian” initial states defined as (up to normalization)

\[
|\psi_{\bar{k}}^{p,w}(t = 0)\rangle \propto P \sum_{x} e^{-|\bar{k} - \bar{x}|^2/2w^2} e^{-ip\bar{x}} |\bar{k}\rangle,
\]

where \( p = (p_x, p_y) \) are the phases specifying the initial direction of propagation of the “wave packet” and for simplicity we project the state by \( P \) on four basis states with maximal weight. For future convenience, we define \( |\psi_{G}\rangle \equiv |\psi_{\bar{k}}^{p=(\pi/2,\pi/2),w=2}\rangle \). We also define the time-averaged occupation of the basis states in the Hilbert space as

\[
\langle n_{\bar{k}}(\bar{k})\rangle = \frac{1}{t_f - t_0} \int_{t_0}^{t_f} dt \langle \bar{k}|\psi(t)|\bar{k}\rangle^2,
\]

where \( |\psi(t)\rangle \) is the time evolved initial state.

In Figs. 1(b) and 1(c) we show \( \langle n_{\bar{k}}(\bar{k})\rangle \) for different initial states Eq. (8). It is apparent that the occupation reveals the scar behavior in the Hilbert space in exact analogy to the single-particle case.

**Disorder:** Since \( H_0 \) is integrable, a natural way to break the integrability is provided by positional disorder of the atoms. Denoting \( \delta r = (\delta x, \delta y, \delta z) \), the initial position of the 4th atom is drawn from a Gaussian probability distribution \( \rho(\delta r) = (2\pi)^{-3/2}\prod_{x,y,z} \exp[-\sum_{x,y,z} (\frac{\delta r}{\sigma_0})^2] \) [71, 93, 94].

While the primary focus of this Letter is the analysis of the model (2), (1), to provide a description applicable to a realistic experimental realization, the time dependence of the atom motion \( \mathbf{r}_i(t) \) has to be taken into account. To set the stage, a few remarks are in order.

First, we consider both the ground and the Rydberg states to be subject to the same harmonic trapping potential \( H_u = \sum_{x} \sum_{x,y,z} \omega_0^2 r_{xy}^2/2 \) [95], where \( \omega_0 \) are the trap frequencies which determine, together with the inverse temperature \( \beta = 1/k_B T \), the disorder through \( \sigma_0 = \sqrt{1/\langle \beta \omega_0^2 \rangle} \), and \( M \) is the atom mass. We parametrize the trap frequencies as \( \omega = (\epsilon^{-1}, 1, 1)\omega_0/d \), which leads to the dimensionless disorder \( s = (s_x, s_y, s_z) \equiv (\epsilon, 1, 1)d\sigma_0 \), where \( s_0 = \sigma_0/r_0 \) for some \( s_0 \) and motivated by [71] we choose \( s_0 = 0.03 \). Here \( \epsilon \) and \( d \) tune the shape and the overall strength of the trapping potential where typically \( \epsilon > 1 \) in a tweezer experiment [71, 78, 93].

Second, we note that the interaction \( V(|\mathbf{r}_i - \mathbf{r}_j|) \) leads to dynamics entangling the motional and internal degrees of freedom necessitating a fully quantum treatment. This is a difficult problem limiting the applicability of
methods such as exact diagonalization to few sites and small phonon number [96]. To proceed, we treat the atomic motion \( \mathbf{r}_k(t) \) as that of a classical particle in a harmonic potential with coordinates

\[
V_{\text{pot}}(r_k) = \sum_{\alpha=1}^{N} \frac{1}{2} \alpha \beta \delta_{\nu, k}^2,
\]

where \( \tilde{\phi}_\nu = (v_k - v_k)/r_0 \). 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 \( |\langle \psi(0) | = |\psi_G \rangle \) are shown in Figs. 2(a) and 2(f) with examples of \( \langle \psi_0 (\tilde{x}) \rangle \)

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 \( \langle \psi_0 (\tilde{x}) \rangle_0 \) generated by the idealized Hamiltonian \( H_0 \), Eq. (4b). It is defined as

\[
F_r = \frac{F_r^+ (F_r^- (1 - F_r))}{1 - F_r^+ (1 - F_r^-)},
\]

where \( \tilde{F}_r = (F_r^+ - F_r^-)/(1 - F_r^+ - F_r^-) \), \( F_r^+ \) is given by \( F \) with the replacement \( \langle \tilde{\psi}_0 (\tilde{x}) \rangle \rightarrow \sqrt{2/(M + 1)} \langle \tilde{\rho}_{\text{mid}} \rangle \). The tilde denotes the occupations normalized as \( \sum_k (\langle \tilde{\psi}_0 (\tilde{x}) \rangle)^2 = 1 \), 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 \( \varrho = (\min(F_r^+ (F_r^- (1 - F_r)))/(\max(E_{\text{mid}}, E_{\text{mid}}) \rangle \langle \tilde{\rho}_{\text{mid}} \rangle \rangle \rangle \) taking the initial conditions, i.e., quenched positional disorder, where the average is taken over all energy differences \( E_i = E_i - E_{i-1} \) 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) \( S(t) = -\log Tr(\rho_A(t)^2) \), where \( \rho_A(t) \) is the reduced density matrix of subsystem \( A \), which we choose to be a half-chain of length \( \lfloor N/2 \rfloor \). 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 midspectrum positional disorder, where the average is taken over all energy differences \( \Delta \) 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) \( S(t) = -\log Tr(\rho_A(t)^2) \), where \( \rho_A(t) \) is the reduced density matrix of subsystem \( A \), which we choose to be a half-chain of length \( \lfloor N/2 \rfloor \). 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 midspectrum positional disorder, where the average is taken over all energy differences \( \Delta \) 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) \( S(t) = -\log Tr(\rho_A(t)^2) \), where \( \rho_A(t) \) is the reduced density matrix of subsystem \( A \), which we choose to be a half-chain of length \( \lfloor N/2 \rfloor \). 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 midspectrum positional disorder, where the average is taken over all energy differences \( \Delta \) 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) \( S(t) = -\log Tr(\rho_A(t)^2) \), where \( \rho_A(t) \) is the reduced density matrix of subsystem \( A \), which we choose to be a half-chain of length \( \lfloor N/2 \rfloor \). 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 midspectrum positional disorder, where the average is taken over all energy differences \( \Delta \) 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].
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 basis state either belongs to a scar in the Hilbert space or each \( \text{Eq. (13)} \) in [65]. Another example naturally realized in the Rydberg systems is the disorder of Eq. (2), which affects all but the isolated Rydberg spins.

\[ R = \frac{\hbar}{2 V (M - 1)} \text{ and Eq.} \langle \delta V (M) \rangle \rangle \text{ shown in Fig. 2(b) with an example of} \langle t \rangle \text{ indicated in Fig. 2(a).} \text{ Thus, for} \langle d \rangle \approx 0.1, \text{ the present analysis holds for} \Omega r = O(100) \text{ for} \langle M \rangle \text{ of few tens, sufficient to capture the behavior of the time-averaged occupation in a realistic experimental setting.} \]

\[ \text{Outlook.} \text{ In this work we have highlighted how the structure of the Hilbert space (connectivity between the basis states) remains unchanged as it is given solely by the spin flip terms [89].} \text{ Recently, Ref. [65] proposed a class of spin models with} \langle \rangle \text{ on non-Gaussian states [103], need to be investigated.} \]

\[ \text{Acknowledgments.} \text{ We are very grateful to V. Gritsev, Neil J. Robinson, W. Buijsman, W. Vleeshouwers, A. Urech, V. Alba, T. Iadecola, Y. Miao, and O. Gamayun for fruitful discussions. This work is part of the Delta ITP consortium, a program of the Netherlands Organisation for Scientific Research (NWO) that is funded by the Dutch Ministry of Education, Culture and Science (OCW). M.M. gratefully acknowledges funding from the University of Nottingham under a Nottingham Research Fellowship scheme.} \]

\[ \text{[4] B. Sutherland, Beautiful Models: 70 Years of Exactly Solved Quantum Many-Body Problems (World Scientific, Singapore, 2004).} \]


[87] 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].


