Periodic Orbits, Entanglement, and Quantum Many-Body Scars in Constrained Models: Matrix Product State Approach

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Periodic orbits, entanglement and quantum many-body scars in constrained models: matrix product state approach

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We analyze quantum dynamics of strongly interacting, kinetically constrained many-body systems. Motivated by recent experiments demonstrating surprising long-lived, periodic revivals after quantum quenches in Rydberg atom arrays, we introduce a manifold of locally entangled spin states, representable by low-bond dimension matrix product states, and derive equations of motions for them using the time-dependent variational principle. We find that they feature isolated, unstable periodic orbits, which capture the recurrences and represent nonergodic dynamical trajectories. Our results provide a theoretical framework for understanding quantum dynamics in a class of constrained spin models, which allow us to examine the recently suggested explanation of 'quantum many-body scarring' [Nature Physics **14**, 745-749 (2018)], and establish a possible connection to the corresponding phenomenon in chaotic single-particle systems.

Introduction. — Understanding non-equilibrium dynamics in closed quantum many-body systems is of fundamental importance. In ergodic systems, the eigenstate thermalization hypothesis (ETH) provides a means to describe their late-time, steady-state behavior by equilibrium statistical mechanics [1–5]. The few known exceptions to this paradigm include exactly solvable, integrable systems [6–8], and strongly disordered, many-body localized systems, which feature extensive number of conservation laws [9–12]. At the same time, the dynamics of equilibriation and thermalization is not as well understood. Concepts such as the ETH, while providing requirements for a system to eventually relax, do not unambiguously prescribe the mechanism nor the timescales on which this occurs; interesting transient dynamics like prethermalization can occur [6–8, 13–21]. Such non-equilibrium phenomena are generally challenging to analytically analyze & simulate, and much progress has thus been spurred by quantum simulation experiments in well-isolated, controllable many-body systems [22–34].

Recently, experiments on Rydberg atom arrays demonstrated surprising long-lived, periodic revivals after quantum quenches [28], with strong dependence of equilibriation timescales on the initial state. Specifically, quenching from some unentangled product states, quick relaxation and thermal equilibriation of local observables was observed, typical of a chaotic, ergodic many-body system. Conversely, quenching from certain other product states, coherent revivals with a well-defined period were instead observed, which were not seen to decay on the experimentally accessible timescales, a distinctively nonergodic dynamical behavior. Most surprisingly, these strikingly different behavior resulted from initial states that are all highly excited with similar, extensive energy densities, and are hence indistinguishable from a thermodynamic standpoint. The apparent simplicity of the special, slowly thermalizing initial states' dynamics – *periodic, coherent many-body oscillations* – therefore brings to question whether they can be understood in a simple, effective picture. In fact, recent theoretical work [35] suggested an intriguing analogy of the oscillations with the phenomenon of quantum scarring in chaotic single-particle systems, where a quantum particle shows similarly long-lived periodic revivals when launched along weakly unstable, periodic orbits of the underlying classical model [36]. However, to date, a firm connection to the theory of single-particle quantum scars [36] has not been established.

In this Letter, we develop a theoretical framework to analyze the quantum dynamics of a family of constrained spin models, which display similar phenomenology of long-lived periodic revivals from certain special initial states. Specifically, we introduce a manifold of simple, locally entangled states respecting the constraints, representable by a class of low bond dimension matrix product states (MPS), and derive equations of motions (EOMs) for them using the time-dependent variational principle (TDVP) [38, 39]. We find that these EOMs support isolated, unstable, periodic orbits. By quantifying the accuracy of this effective description, we show that these closed orbits indeed capture the persistent recurrences, and hence signal slow relaxation of local observables, a form of weak ergodicity breaking in dynamics, see Fig. 1(a,b). Furthermore, since the TDVP generates a Hamiltonian flow in the phase space parametrizing this (weakly entangled) manifold, one can associate our approach with a generalized "semiclassical" description of many-body dynamics in constrained Hilbert spaces. Our finding of periodic orbits in this description is therefore suggestive in establishing the connection to the theory of quantum scarring of single-particle systems of Heller [36].

Kinetically constrained spin models. — We consider a family of interacting, constrained spin models and demonstrate that they show atypical thermalization behavior for certain initial states. Consider a chain of L

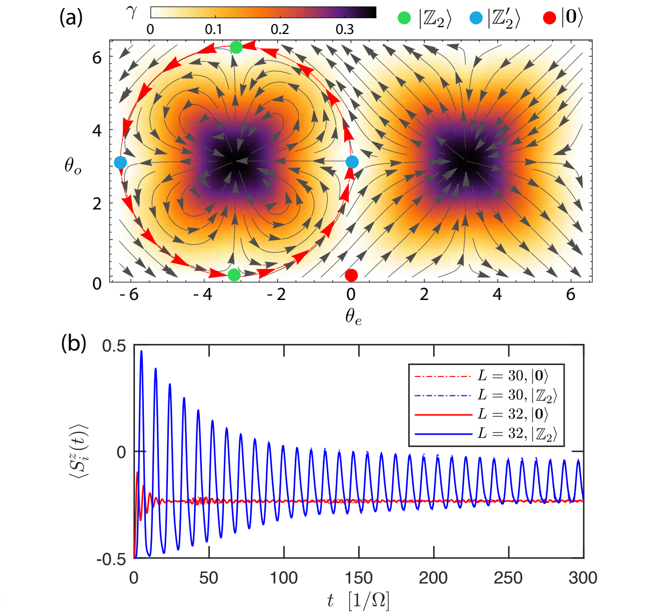

Figure 1. (a) Flow diagrams of $\dot{\theta}_e(t), \dot{\theta}_o(t)$ for the model (1) with $s=1/2$. The color map gives the error γ, (5). There is an isolated, unstable periodic orbit (red curve) describing oscillatory motion between $|\mathbb{Z}_2\rangle$ (green dot) and $|\mathbb{Z}_2'\rangle$ (blue dot), with numerically extracted period $T \approx 2\pi \times 1.51\,\Omega^{-1}$. Conversely, motion from $|\mathbf{0}\rangle$ (red dot) proceeds towards a saddle point where the error is large. (b): Dynamics of local observable $S_i^z(t)$. There are persistent, coherent oscillations in the local observable for $|\mathbb{Z}_2\rangle$ with similar period, while $|\mathbf{0}\rangle$ instead shows quick relaxation and equilibriation towards a thermal value predicted by ETH [37].

spin-s particles on a ring, with Hamiltonian

$$H = \Omega \sum_i \mathcal{P} S_i^x \mathcal{P}. \tag{1}$$

Here, a basis on each site i is spanned by eigenstates $|n\rangle_i$ of $S_i^z + s\,\mathbb{I}_i$, with $n = 0, \cdots, 2s$, and S_i^x is the spin-s operator in the x-direction. The projector $\mathcal{P} = \prod_i \mathcal{P}_{i,i+1}$ is a product of commuting local projectors $\mathcal{P}_{i,i+1} = \mathbb{I}_i \otimes \mathbb{I}_{i+1} - Q_i \otimes Q_{i+1}$, with $Q_i = \mathbb{I}_i - P_i$ and $P_i = |0\rangle_i \langle 0|_i$, and constrains dynamics to a subspace where at least one of two neighboring spins is in the state $|0\rangle$, which has dimensionality $d \sim ((1+\sqrt{8s+1})/2)^L$. When $s=1/2$, Eqn. (1) effectively models the experimental setup of [28], where the constraint stems from the Rybderg blockade mechanism (see also [40–44]).

The Hamiltonian (1) has a simple interpretation: each spin rotates freely about the x-axis if both its neighbors are in the state $|0\rangle$, while its dynamics is frozen otherwise. Despite its apparent simplicity, the Hamiltonian is nonintegrable and quantum chaotic, as seen in Fig. 2(a) from level repulsion in the energy eigenspectrum. The chaotic nature of the system is expected to govern the nonequilibrium dynamics arising from a quantum quench. For example, consider “simple”, unentangled initial states, specifically product states in the z-basis that satisfy the constraints. All these states have the property that they have the same energy density under (1), corresponding to that of the infinite-temperature thermal state, and are hence thermodynamically indistinguishable. Under time evolution, one would expect a quick relaxation of local observables (on the timescale $t_r \sim \Omega^{-1}$) to infinite-temperature ensemble values [37], in accordance with ETH predictions [1–3, 47–50]. This behavior is indeed observed generically, as demonstrated previously [41–44], and also in Fig. 1(b) for the local observable $S_i^z(t)$ from the initial state $|\mathbf{0}\rangle = \otimes_{i=1}^L |0\rangle_i$ ($s=1/2$). However, time evolution of the initial state $|\mathbb{Z}_2\rangle \equiv \otimes_{i=1}^{L/2} |0\rangle_{2i-1} |2s\rangle_{2i}$ does not follow this expectation. As shown in Fig. 1(b), the same observable instead unexpectedly exhibits long-lived, coherent oscillations with a well-defined period $T \approx 2\pi \times 1.51\,\Omega^{-1}$. Furthermore, it does not relax to, nor oscillate about, the thermal value expected from ETH, at least on numerically accessible timescales and system sizes.

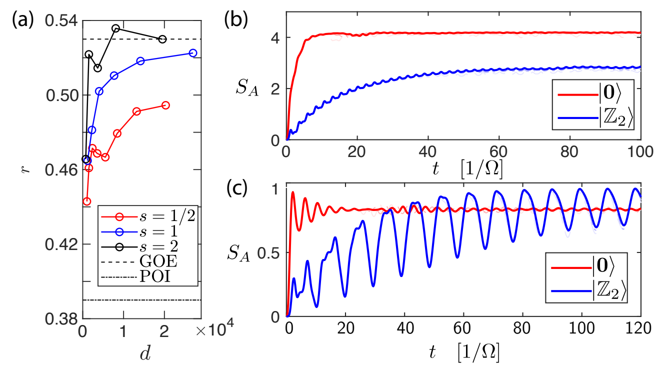

Figure 2. (a) Level spacing statistics in the momentum-zero, inversion-symmetric sector. Plotted is the r-statistics defined by the average of $r_n = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}$ where $s_n = E_{n+1} - E_n$. There is a clear albeit slow trend with Hilbert space dimension d towards Wigner-Dyson statistics in the GOE class, indicated by $r \approx 0.53$, away from the integrable Poissonian (POI) limit of $r \approx 0.39$ (for discussion of the slow convergence, see [45, 46]). (b,c) Growth of entanglement entropy S_A following quenches from the $|\mathbf{0}\rangle$ and $|\mathbb{Z}_2\rangle$ states, of subregions A being (b) six contiguous sites, (c) a single-site, for the $s=1/2$ model. Total system size is $L=30$.

This striking departure from generic behavior is also reflected in the growth of entanglement entropy (EE) (Fig. 2(b,c)). While for generic initial states EE essentially grows linearly and quickly saturates to that of a random state [37], this is not the case for $|\mathbb{Z}_2\rangle$. In particular, the single-site EE drops periodically, indicating that each spin is repeatedly partially disentangling itself from the rest of the chain. This tantalizingly hints that the motion for the $|\mathbb{Z}_2\rangle$ state lies within a low-entanglement manifold of the Hilbert space, thereby possibly allowing for a simple, effective description of dynamics.

Equations of motion from the TDVP. — Motivated

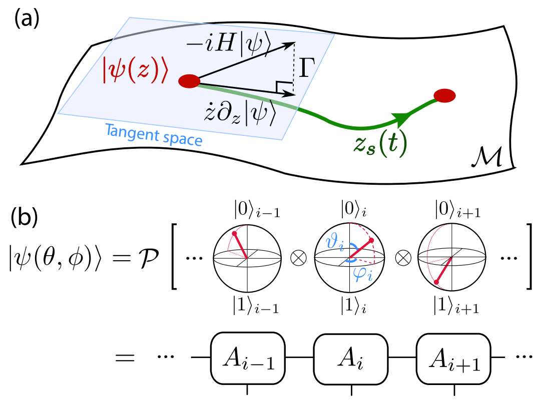

Figure 3. (a) Geometrical depiction of the TDVP over a manifold of states $|\psi(\boldsymbol{z})\rangle$ parameterized by $\boldsymbol{z}$. The instantaneous motion $-iH|\psi(\boldsymbol{z})\rangle$ is projected onto the tangent space at the point, leading to motion on the manifold (green trajectory). The norm of the vector orthogonal to the manifold, $\Gamma = \gamma\sqrt{L}$ (c.f. Eqn. (5)), is a measure of its accuracy. (b) MPS representation of states $|\psi(\boldsymbol{\theta},\boldsymbol{\phi})\rangle$ (c.f. Eqn. (3)) used.

by these considerations, we analyze the dynamics of the system using the TDVP on a suitable variational manifold of simple, low entanglement states. For concreteness, we focus first on $s=1/2$. Starting from classical spin configurations, i.e. products of unentangled coherent states $\otimes_i|\vartheta_i,\varphi_i\rangle := \otimes_i[\cos(\vartheta_i/2)|0\rangle_i - ie^{i\varphi_i}\sin(\vartheta_i/2)|1\rangle_i]$, we construct states that respect the constraints set by $\mathcal{P}$, by explicitly projecting out neighboring excitations,

$$|\psi(\boldsymbol{\vartheta},\boldsymbol{\varphi})\rangle = \mathcal{P}\bigotimes_i |(\vartheta_i,\varphi_i)\rangle, \tag{2}$$

which is akin to a Gutzwiller projection to the constrained subspace [37, 51], see Fig. 3(b). Importantly, (2) is weakly entangled, and can be written as a particular matrix product state (MPS) with bond dimension $D=2$ [37, 52]. We find it convenient to normalize (2) and change to new variables $(\boldsymbol{\vartheta},\boldsymbol{\varphi}) \to (\boldsymbol{\theta},\boldsymbol{\phi})$ via a non-linear mapping [37], such that $|\psi(\boldsymbol{\vartheta},\boldsymbol{\varphi})\rangle/||\psi(\boldsymbol{\vartheta},\boldsymbol{\varphi})|| = |\psi(\boldsymbol{\theta},\boldsymbol{\phi})\rangle$, so that the MPS repesentation is given by

$$\begin{aligned} |\psi(\boldsymbol{\theta},\boldsymbol{\phi})\rangle &= \mathrm{Tr}(A_1A_2\cdots A_L),\\ A_i(\theta_i,\phi_i) &= \begin{pmatrix} P_i|(\theta_i,\phi_i)\rangle & Q_i|(\theta_i,\phi_i)\rangle \\ |0\rangle_i & 0\end{pmatrix}, \end{aligned} \tag{3}$$

and $|(\theta_i,\phi_i)\rangle = e^{i\phi_i s}e^{i\phi_i S_i^z}e^{-i\theta_i S_i^x}|0\rangle_i$, which is normalized in the thermodynamic limit $L\to\infty$ (see too [53, 54]). The generalization of (3) to spin-s then simply consists of replacing the appropriate operators and states with the spin-s analogs.

The TDVP respects conservation laws, and in particular conserves the energy of the Hamiltonian (1) [37–39, 55]. On this general ground, we obtain that $\dot{\boldsymbol{\phi}}=0$, and can set $\boldsymbol{\phi}=0$, which is obeyed for initial product states in the z-basis [37]. Furthermore, to describe the motions of the $|\mathbf{0}\rangle$ and $|\mathbb{Z}_2\rangle$ states, it suffices to focus on the submanifold of states with a two-site translational symmetry, i.e. $\theta_i=\theta_{i+2}$. The TDVP-EOMs are obtained by projecting the instantaneous motion of the quantum system onto the tangent space of the variational manifold (Fig. 3(a)), and read $\sum_\mu \dot{\boldsymbol{\theta}}_\mu\langle\partial_{\boldsymbol{\theta}_\nu}\psi|\partial_{\boldsymbol{\theta}_\mu}\psi\rangle = -i\langle\partial_{\boldsymbol{\theta}_\nu}\psi|H|\psi\rangle$, for $\mu\in\{o,e\}$ (standing for even(e) and odd(o) sites). A lengthy but straightforward calculation [37] yields closed-form, analytic expressions: $\dot{\theta}_\mathrm{e}(t) = f(\theta_\mathrm{e}(t),\theta_\mathrm{o}(t))$ and $\dot{\theta}_\mathrm{o}(t) = f(\theta_\mathrm{o}(t),\theta_\mathrm{e}(t))$, with

$$\begin{aligned} f(x,y) = \Omega\Big[&1-\cos^{4s-2}\left(\frac{x}{2}\right)+\cos^{4s-2}\left(\frac{x}{2}\right)\cos^{2s}\left(\frac{y}{2}\right)\\ &+2s\sin\left(\frac{x}{2}\right)\cos^{6s-1}\left(\frac{x}{2}\right)\tan\left(\frac{y}{2}\right)\Big]. \end{aligned} \tag{4}$$

These EOMs are coupled, nonlinear equations. Yet, remarkably, we find that for each spin-s, there is an isolated, unstable, periodic orbit $\mathcal{C}$, as seen in the corresponding flow diagrams for $s=1/2$ in Fig. 1(a), and $s=1,2$, in Fig. 4(a,c). Furthermore, $\mathcal{C}$ includes the points $(\theta_e,\theta_o)=(\pi,0)$, and $(0,-\pi)$ (modulo 2π), corresponding to $|\mathbb{Z}_2\rangle$ and its counterpart $|\mathbb{Z}_2'\rangle = \otimes_{i=1}^{L/2}|0\rangle_{2i}|2s\rangle_{2i-1}$ respectively. Thus, the EOMs describe continual oscillations between these two product states (akin to a quantum Newton's cradle! [see also [22]]), which is manifestly an athermal, nonergodic behavior [56]. The periods of oscillations from the EOMs can be determined by numerical integration of Eq. (4), and the extracted values match excellently with those from numerical simulations of local observables such as $S_i^z(t)$, see Fig. 1(b) and Fig. 4(b,d). This already indicates that the variational manifold (3) is well suited to capture central aspects of the exact quantum dynamics.

To further corroborate this fact, we quantify the error in TDVP evolution as the instantaneous rate at which the state evolving under the full Hamiltonian leaves the variational manifold (see Fig. 3, [38, 39]), given by

$$\gamma(\boldsymbol{\theta}) = ||(iH+\dot{\boldsymbol{\theta}}\partial_{\boldsymbol{\theta}})|\psi(\boldsymbol{\theta})\rangle||/\sqrt{L}, \tag{5}$$

where we have normalized it to be an intensive quantity. The numerically integrated error rates around the closed orbits $\epsilon_\mathcal{C} = \oint_\mathcal{C}\gamma(\theta_e(t),\theta_o(t))dt$ yield $\epsilon_\mathcal{C}\approx 0.17, 0.32, 0.41$ for $s=1/2,1,2$ respectively, which are small values compared to neighboring trajectories [37], illustrating that $\mathcal{C}$ is indeed a good approximation to exact quantum dynamics. We stress that the ability to capture the key features of some dynamics of a chaotic many-body system within a low entanglement manifold is remarkable. This is in contrast to generic expectations; for example, the trajectory beginning at $(\theta_e,\theta_o)=(0,0)$ for $s=1/2$, (i.e. the $|\mathbf{0}\rangle$ state), instead traces out a path that terminates in a saddle point where γ is large (see Fig. 1(a)), indicating that this low entanglement manifold is unable to capture the large growth of entanglement from this state, as expected in a thermalizing system.

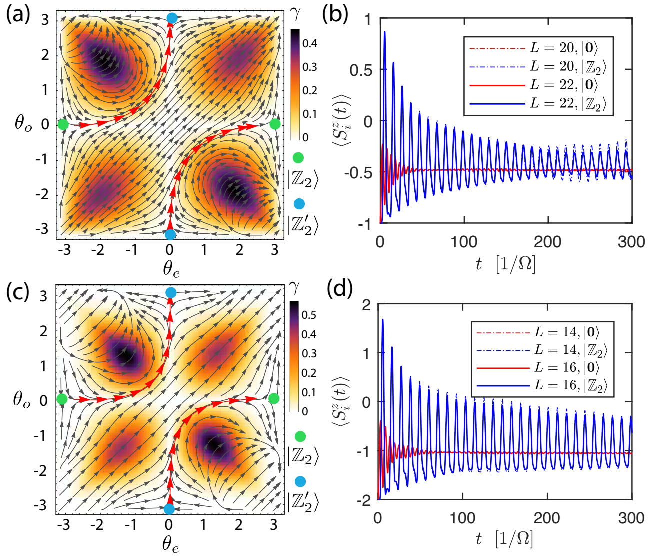

Figure 4. (a,c) Flow diagrams (4) and error γ for (a) $s=1$, (c) $s=2$. The indicated periodic orbits (red curves) have periods (a) $T \approx 2\pi \times 1.64\,\Omega^{-1}$, and (c) $T \approx 2\pi \times 1.73\,\Omega^{-1}$. Note that points $\theta_{o/e} = \theta_{o/e} \pm 2\pi$ are identified. (b,d) Relaxation of local observable $S_i^z(t)$ for (b) $s=1$, (d) $s=2$. One sees, similarly to Fig. 1, quick relaxation of the $|\mathbf{0}\rangle$ state toward a thermal value predicted by ETH [37], while persistent oscillations for $|\mathbb{Z}_2\rangle$, with similar periods in (a,c).

Discussion. — Our effective description of the persistent oscillations seen in the many-body systems (1), in terms of isolated, unstable orbits, provides a framework to analyze a possible connection with the phenomenon of quantum scarring in single-particle chaotic systems [36]. There, special, weakly unstable classical orbits of a single-particle, characterized by the condition $\lambda T < 1$ (where T is the period of the orbit and λ the average Lyapunov exponent about the orbit) play a central role: the persistent revivals and slow decay of a Gaussian wavepacket (a quatum particle) launched along such an orbit give rise to a statistically significant enhancement of certain wavefunctions' probability densities about these orbits, above that expected of Berry's conjecture [57]. Indeed, the apparent similarity between these phenomena, and atypical signatures in the ergodic properties of certain many-body eigenstates of the $s=1/2$ model (1) tied to the long-lived oscillations, motivated the recently proposed explanation in terms of quantum many-body scars [35, 46]. Our work provides a way to make such an analogy firmer: even though our variational manifold encompasses states that explicitly include quantum entanglement, the TDVP-EOMs describe a Hamiltonian flow in the corresponding phase space [38, 39, 58, 59], and thus offer a notion of a "semiclassical trajectory" through the many-body Hilbert space. A natural extension of the condition $\lambda T < 1$ characterizing the instability of orbits is then the leakage out of the manifold $\epsilon_{\mathcal{C}} = \oint_{\mathcal{C}} \gamma(\boldsymbol{\theta}) dt < 1$; it would be interesting to relate this quantity to the Lyapunov exponent of the EOMs [59]. Furthermore, the effect of these orbits on the nature of many-body eigenstates deserve further study; however this has to be done while contending with the thermodynamic limit, a notion absent in the single-particle scenario.

Finally, we note that the equations of motion we obtained can also be understood as the leading order, saddle-point evaluation of a path integral for the constrained spin systems (1). In particular, the manifold of states $|\psi(\boldsymbol{\theta}, \boldsymbol{\phi})\rangle$ is dense and supports a resolution of the identity on the constrained space, with an appropriate measure $\mu(\boldsymbol{\theta}, \boldsymbol{\phi})$ (see [37]), allowing the construction of a Feynman path integral [58, 60–63]. The TDVP EOMs extremize the action functional with the Lagrangian $\mathcal{L} = i\langle\psi|\partial_{\boldsymbol{\theta}}\psi\rangle\dot{\boldsymbol{\theta}} + i\langle\psi|\partial_{\boldsymbol{\phi}}\psi\rangle\dot{\boldsymbol{\phi}} - \langle\psi|H|\psi\rangle$, which evaluates (for $s=1/2$) to:

$$\mathcal{L} = \sum_i K_i(\boldsymbol{\theta})[\sin^2\left(\frac{\theta_i}{2}\right)\dot{\phi}_i + \frac{\Omega}{2}\cos\left(\frac{\theta_{i+1}}{2}\right)\sin(\theta_i)\cos(\phi_i)],$$

where $K_i(\boldsymbol{\theta})$ is given in [37]. This formulation provides a framework, which can be used to systematically recover quantum dynamics from the saddle-point limit, by including higher-order corrections, i.e. fluctuations.

Conclusion. — In this Letter, we introduced and analyzed the dynamics of a family of constrained spin models which show atypical thermalization behavior – long-lived, coherent revivals from certain special initial states, similar to recent quench experiments in a quantum simulator of Rydberg atoms. We derived an effective description of these systems in terms of equations of motion for dynamics of locally entangled spins and found that they host isolated, unstable, periodic orbits, which correspond to long-lived recurrences at the quantum many-body level. Our results establish a possible connection to quantum scarring in single-particle chaotic systems, and suggest a framework for a generalization of the theory of quantum scars by Heller [36], which is intimately tied to unstable periodic orbits, to the many-body case.

While our analysis demonstrates that the phenomenology of stable, long-lived oscillations from special initial states extends to a number of interacting, constrained models, one of the most important outstanding questions is related to their physical origin and the sufficient conditions for their existence. A complementary Letter [45] demonstrates that these models possess important features resembling ergodic systems that are close to integrability, and that these features can be enhanced by non-trivial deformations of the Hamiltonian. In [37], we show that our variational description of the periodic dynamics is able to capture the effect of these deformations by making the corresponding error γ smaller. While it is currently unclear if this near-integrable-like behavior is directly related to, required for, or follows from the existence of scar-like dynamics, these observations as well as the framework presented here provide both theoretical foundations and important physical insights on which future studies of quantum dynamics can be based upon.

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