Embedding Semiclassical Periodic Orbits into Chaotic Many-Body Hamiltonians

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Protecting coherent quantum dynamics from chaotic environment is key to realizations of fragile many-body phenomena and their applications in quantum technology. We present a general construction that embeds a desired periodic orbit into a family of nonintegrable many-body Hamiltonians, whose dynamics is otherwise chaotic. Our construction is based on time-dependent variational principle that projects quantum dynamics onto a manifold of low-entangled states, and it complements earlier approaches for embedding nonthermal eigenstates, known as quantum many-body scars, into thermalizing spectra. By designing terms that suppress "leakage" of the dynamics outside the variational manifold, we engineer families of Floquet models that host exact scarred dynamics, as we illustrate using a driven Affleck-Kennedy-Lieb-Tasaki model and a recent experimental realization of scars in a dimerized superconducting qubit chain.

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Introduction.—The dynamics of nonintegrable quantum many-body systems typically gives rise to rapid thermalization and scrambling of information. These hallmarks of quantum ergodicity can be traced to the properties of the system's midspectrum eigenstates, which are generally highly entangled and obey the eigenstate thermalization hypothesis (ETH) [1,2]. In recent years, there has been a flurry of activity aimed at understanding the conditions for *weak* breaking of the ETH to emerge, in particular, by devising ways of embedding nonthermalizing eigenstates into otherwise chaotic many-body spectra [3–5]. These eigenstates, referred to as quantum many-body scars (QMBSs), have been identified in prominent models of quantum magnets, such as the Affleck-Kennedy-Lieb-Tasaki (AKLT) model [6–8], and in Rydberg atom quantum simulators [9,10], where their signatures were first observed in quench experiments [11]. Potential applications of QMBSs have been explored in the context of controlling quantum-information dynamics in complex systems [12] and for quantum metrology [13–15].

Despite much interest in weak ergodicity breaking phenomena in different experimental platforms [16–18], the origin of QMBSs remains the subject of ongoing investigation. In much of theoretical work, QMBSs are studied by algebraic constructions of ergodicity-breaking eigenstates. In particular, the local projector approach by Shiraishi and Mori [19] embeds a few nonthermal eigenstates into the spectrum of a nonintegrable Hamiltonian. Other approaches construct families of eigenstates, representing condensates of quasiparticles evenly spaced in energy [8,20]. More recent proposals aim to unify these different constructions into a single framework [21–24]. All these approaches, however, differ dramatically from the case of single-particle scars in quantum billiards, which are understood as quantum remnants of classical unstable periodic orbits [25–28]. Nevertheless, for QMBSs observed in Rydberg atom experiments [11], the eigenstate constructions [10,20,29–31] were shown to be in harmony with a semiclassical limit of the dynamics, developed by Ho *et al.* [32], which identified a periodic orbit in the many-body Hilbert space that underpins the coherent QMBS dynamics. The notion of a semiclassical limit, introduced in Ref. [32] and adopted in this Letter, is based on projecting quantum dynamics to a variational manifold spanned by states with low entanglement.

In this Letter, we introduce a systematic method for embedding a desired periodic trajectory into the dynamics generated by a chaotic many-body Hamiltonian. The latter is understood to obey the ETH, apart from a vanishing fraction of states in the thermodynamic limit. Our method is based on decomposing the Hamiltonian into a component that generates an exact periodic orbit and a second component that vanishes upon taking the semiclassical limit. Thus, within a suitably defined semiclassical manifold, the projected dynamics is a periodic oscillation. However, the dynamics of the full model may deviate from the projection to the manifold and this deviation is quantified by the so-called quantum leakage [32,33]. Using the quantum leakage, we introduce driving terms to the model that cancel the distinction between the semiclassical and quantum dynamics, schematically depicted in Fig. 1, which results in exact Floquet QMBSs. We demonstrate the

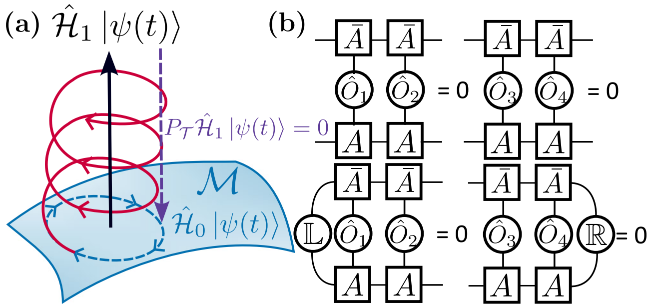

FIG. 1. (a) A periodic orbit can be embedded into a chaotic many-body Hamiltonian by decomposing the latter into two terms: $\hat{\mathcal{H}}_0$, which generates a periodic orbit in a semiclassical manifold $\mathcal{M}$, and $\hat{\mathcal{H}}_1$ that vanishes as the semiclassical limit is taken. (b) For an MPS manifold, $\hat{\mathcal{H}}_1$ takes a simplified form. The generic conditions for a four-site local $\hat{\mathcal{H}}_1$, valid for any system size and choice of boundary conditions, are illustrated (top). These conditions can be weakened for translation invariant MPSs in the thermodynamic limit (bottom).

utility of our approach using the AKLT model [6,8] and a recent superconducting circuit realization of QMBS [18] based on the Su-Schrieffer-Heeger (SSH) model [34].

Time-dependent variational principle (TDVP).—To avoid the exponential complexity of many-body quantum systems, the TDVP method [35,36] approximately solves the time-dependent Schrödinger equation (TDSE) by projecting it onto a manifold $\mathcal{M}$ spanned by ansatz wave functions that capture the most important features of the dynamics. In this Letter, we focus on one-dimensional lattice systems with a d-dimensional Hilbert space on each site, where $\mathcal{M}$ is spanned by wave functions $|\psi(\{z_n\})\rangle$, parametrized by a complex variable z_n for each site n. For example, in a simple manifold describing product states of spins-1/2, one can think of z_n parametrizing the orientation of each spin on the Bloch sphere. However, as pointed out by Haegeman *et al.* [37], a much larger class of dynamical behaviors can be described if we allow $\mathcal{M}$ to contain entangled states such as matrix product states (MPSs) [38]. For MPSs, the variables z_n on each site are $\chi\times\chi$-dimensional matrices A_n^s, labeled by a local basis vector $s = 1, 2, \ldots d$ and site index n. Increasing χ increases the power of the ansatz, representing states with larger amounts of entanglement between sites.

The time evolution within $\mathcal{M}$ is given by [36]

$$i\frac{d}{dt}|\psi(\{z_n\})\rangle = P_{\mathcal{T}}\hat{\mathcal{H}}|\psi(\{z_n\})\rangle, \tag{1}$$

where $P_{\mathcal{T}} = \sum_n |\partial_{z_n}\psi(\{z_n\})\rangle g^{-1}_{z_n\bar{z}'_n}\langle\partial_{\bar{z}'_n}\psi(\{\bar{z}'_n\})|$ is a projector onto the tangent space of $\mathcal{M}$ at the point $|\psi(\{z_n\})\rangle$. $g^{-1}_{\bar{z}_n z'_n}$ is the inverse of the metric tensor of $\mathcal{M}$, $g_{\bar{z}_n z'_n} = \langle\partial_{\bar{z}_n}\psi(\{\bar{z}_n\})|\partial_{z'_n}\psi(\{z'_n\})\rangle$. Because of the tangent-space projectors dependence on $\{z_n\}$, the TDVP dynamics typically deviate from that generated by the TDSE, becoming nonlinear. When $\mathcal{M}$ is a so-called Kähler manifold, it is a classical dynamical phase space with the TDVP equations being the corresponding Hamilton equations [39,40]. Additionally, when the states in $\mathcal{M}$ form an overcomplete basis, a Feynman path integral over $\mathcal{M}$ can be constructed [41]. The TDVP equations then correspond to the Euler-Lagrange equations of the path integral.

Semiclassical limit.—The deviation between TDVP and TDSE can be characterized using "quantum leakage" Γ [32]. The leakage is the norm of the difference between the full and approximate time-evolved wave functions, integrated around the orbit

$$\Gamma = \frac{1}{T}\oint \|(\mathbb{1} - P_{\mathcal{T}})\hat{\mathcal{H}}|\psi[\{z_n(t)\}]\rangle\| dt. \tag{2}$$

Typically, Γ^2 is extensive, i.e., asymptotically proportional to the system size N. By constraining the complexity of $\mathcal{M}$, the TDVP approach allows one to effectively *define* a semiclassical limit of the full quantum dynamics [32]: provided the full quantum dynamics are well approximated within the manifold, i.e., $\Gamma \ll \sqrt{N}$, and $\mathcal{M}$ is spanned by low bond dimension MPSs, we will refer to such dynamics as "semiclassical." Note that this definition admits a semiclassical limit that includes (short-range) quantum correlations, which is essential, e.g., for capturing the behavior of constrained systems [32].

Orbit embedding conditions.—We now focus on Hamiltonians $\hat{\mathcal{H}}_0$ that possess a periodic orbit from a certain initial state, $|\psi(t)\rangle = |\psi(t+T)\rangle$, for which it is possible to find a low-dimensional $\mathcal{M}$ that exactly captures the dynamics. Suppose the Hamiltonian is then perturbed, $\hat{\mathcal{H}}_0 \to \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_1$, so that the TDSE is altered, but Eq. (1) is not. A Hamiltonian that satisfies the following conditions along the trajectory will retain a semiclassical periodic orbit, despite its quantum dynamics being altered:

$$P_{\mathcal{T}}\hat{\mathcal{H}}_0|\psi(\{z_n\})\rangle = \hat{\mathcal{H}}_0|\psi(\{z_n\})\rangle, \tag{3}$$

$$\left[\hat{\mathcal{H}}_1 - \langle\psi(\{\bar{z}_n\})|\hat{\mathcal{H}}_1|\psi(\{z_n\})\rangle\right]|\psi(\{z_n\})\rangle \neq 0, \tag{4}$$

$$P_{\mathcal{T}}\hat{\mathcal{H}}_1|\psi(\{z_n\})\rangle = 0. \tag{5}$$

These conditions are illustrated in Fig. 1(a). Equations (4) and (5) require that $|\psi(\{z_n\})\rangle$ is a fixed point of the TDVP equations with respect to $\hat{\mathcal{H}}_1$, while not being an eigenstate. For Hamiltonians that satisfy the conditions (3)–(5), the leakage can be simplified,

$$\Gamma = \frac{1}{T}\oint \|\hat{\mathcal{H}}_1|\psi[\{z_n(t)\}]\rangle\| dt. \tag{6}$$

Periodic orbit for MPSs.—Restricting our discussion to MPSs as a variational ansatz, we can be more precise about the form $\hat{\mathcal{H}}_1$ must take in order to satisfy Eq. (5).

Suppose $\hat{\mathcal{H}}_1$ can be written as a sum of $2K$-local operators, $\hat{\mathcal{H}}_1 = \sum_n \hat{O}_1^n \otimes \hat{O}_2^{n+1} \otimes \cdots \otimes \hat{O}_{2K}^{n+2K-1}$, where $\hat{O}_k^n$ is the kth type of local term in $\hat{\mathcal{H}}_1$ acting on site n. For evaluating correlation functions with MPSs, it is useful to introduce the MPS transfer matrix, $\mathbb{E}_n(\hat{O}_k) = \sum_{s,\bar{s}'} \bar{A}_n^{s'} \hat{O}_{k,s,\bar{s}'}^n A_n^s$ [42]. In the Supplemental Material [43], we prove that Eq. (5) is satisfied for any system size and choice of boundary conditions if we impose

$$\prod_{k=1}^{K} \mathbb{E}_{n+k-1}(\hat{O}_k) = 0, \qquad \prod_{k=K+1}^{2K} \mathbb{E}_{n+k-1}(\hat{O}_k) = 0. \quad (7)$$

In the thermodynamic limit, these conditions can be significantly weakened. Let us assume that A_n^s is site-independent and $\mathbb{E}_n(\mathbb{1})$ possesses a unique dominant left and right eigenvector $(\mathbb{L}|$ and $|\mathbb{R})$, respectively. In this case, Eq. (1) will always begin with $(\mathbb{L}|$ and end with $|\mathbb{R})$, so Eq. (5) is satisfied, provided

$$(\mathbb{L}|\prod_{k=1}^{K} \mathbb{E}_{n+k-1}(\hat{O}_k) = 0, \qquad \prod_{k=K+1}^{2K} \mathbb{E}_{n+k-1}(\hat{O}_k)|\mathbb{R}) = 0. \quad (8)$$

These conditions are illustrated in Fig. 1(b) and below we demonstrate how they can be used to construct families of models that share the same periodic orbit, using SSH and AKLT chains as examples. We note that the above assumption about the form of $\hat{\mathcal{H}}_1$ can be straightforwardly lifted for Hamiltonians that are sums of local operators or feature long-range interactions.

SSH chain.—We now apply our approach to the dimerized SSH model of polyacetylene [34,48],

$$\hat{\mathcal{H}}_{\mathrm{SSH}} = \sum_{n=0}^{N/2-1} J_o \sigma_{2n+1}^+ \sigma_{2n+2}^- + \sum_{n=0}^{N/2-2} J_e \sigma_{2n+2}^+ \sigma_{2n+3}^- + \mathrm{H.c.}, \quad (9)$$

where $\sigma^\pm$ denote the Pauli raising and lowering spin operators, J_o and J_e are the hopping amplitudes on the odd and even sublattice, respectively, and we have assumed open boundary conditions. In Ref. [18], the SSH chain was used as a starting point to realize QMBS dynamics on a superconducting quantum processor when additional couplings between sites are added to break the integrability. In the absence of interdimer couplings, $J_e = 0$, the state $|\psi(0)\rangle = |10011001\cdots\rangle$, i.e., with dimers alternating between 10 and 01 local states, undergoes free precession, with frequency $2J_o$. The oscillations are no longer perfect at $J_e \approx 2J_o/3$ and instead exhibit a decaying envelope [18]. It was found that a translation invariant next-next-nearest-neighbor hopping enhances the QMBS oscillations. Indeed, such a term reduces leakage from the scarred subspace, but it does not lead to its total suppression [43]. However, using the above approach, we can identify a driving protocol that embeds an exact periodic trajectory into the model.

In order to embed the periodic trajectory into the SSH chain, we block together sites $\{2n, 2n+1\}$ and use a $d = 4, \chi = 1$ MPS ansatz. The SSH Hamiltonian in Eq. (9) then neatly fits into the form introduced above, with $\hat{\mathcal{H}}_0$ being the J_o term and $\hat{\mathcal{H}}_1$ the J_e term. It is straightforward to see that Eq. (4) is satisfied. To see that Eq. (5) is satisfied, we note that, because the variational parameters are localized to a single site, each term in the sum defining $P_{\mathcal{T}}$ differs from $|\psi(t)\rangle$ on just one site. $\hat{\mathcal{H}}_1$ acting on $|\psi(t)\rangle$ makes it orthogonal to $|\psi(t)\rangle$ on two sites, therefore $\hat{\mathcal{H}}_1|\psi(t)\rangle$ is annihilated by $P_{\mathcal{T}}$. In this sense, the SSH Hamiltonian for any J_e has the same semiclassical limit, corresponding to the quantum dynamics of the $J_e = 0$ model.

Suppose we modify the SSH chain by adding longer-range hopping terms of the form

$$\hat{\mathcal{H}} = \sum_n J_o \sigma_{2n+1}^+ \sigma_{2n+2}^- + J_e \sigma_{2n+2}^+ \sigma_{2n+3}^- + \Delta \sigma_{2n+1}^+ \sigma_{2n+4}^- + i\alpha(-1)^n (\sigma_{2n+1}^+ \sigma_{2n+3}^- - \sigma_{2n+2}^+ \sigma_{2n+4}^-) + \mathrm{H.c.} \quad (10)$$

The additional hopping terms introduced here all satisfy Eqs. (4) and (5). and therefore Eq. (10) defines a class of models that share the same semiclassical limit as the SSH chain. This form was chosen so the $\hat{\mathcal{H}}_1$ contributions all take $|\psi(t)\rangle$ to the same state. For this reason, the quantum leakage takes a simple form,

$$\Gamma = \frac{\sqrt{N-2}}{T} \int_{t=0}^{T=\frac{\pi}{J_o}} \left| \frac{J_e + \Delta}{2} \sin(2J_o t) + \alpha \right| dt. \quad (11)$$

When $\Gamma = 0$, the periodic TDVP trajectory becomes an exact trajectory in the full quantum dynamics. By fixing $\alpha = 0$ and $J_e = -\Delta$, we obtain a family of static Hamiltonians, Eq. (10), that admit exact periodic orbits. However, we can also make Γ vanish if we allow the coupling to vary with time, $\alpha(t) = -\frac{1}{2}(J_e + \Delta)\sin(2J_o t)$, as confirmed in Fig. 2(a). The latter Floquet model hosts the same periodic orbit as the static SSH model. However, unlike the static case, the tower of QMBS eigenstates are not preserved by the Floquet operator, see Fig. 2(c). This is reminiscent of Rydberg atoms with a modulated chemical potential [12], where the scarred initial state also has high overlap with only a few Floquet modes [49].

AKLT model.—Our construction can also embed trajectories that involve entangled states with nontrivial correlations. As a second example, we consider the AKLT model [50]—a paradigmatic model of symmetry protected topological (SPT) order,

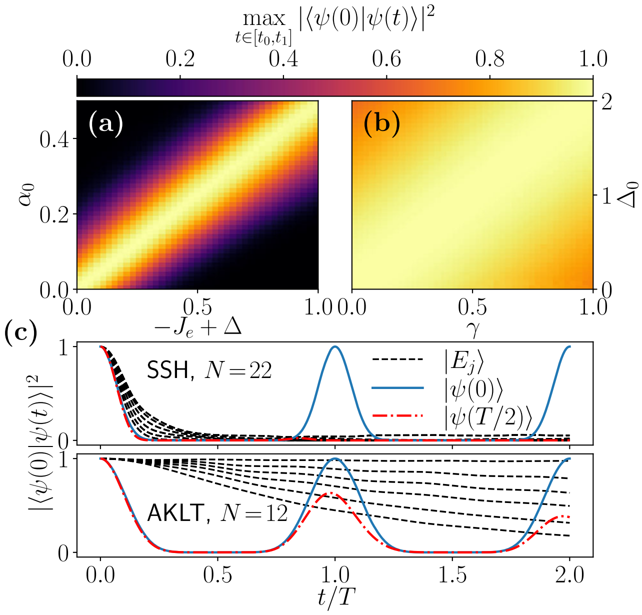

FIG. 2. (a) Maximum fidelity revival (between times $t_0 = 1$ and $t_1 = 2\pi$) for the driven SSH model in Eq. (10) with $\alpha(t) = -\alpha_0 \sin(2J_o t)$. The system size $N = 80$ and coupling $J_e = 2/3$ are fixed, while α_0 and Δ are varied. (b) Maximum fidelity revival (between $t_0 = 0.5$ and $t_1 = \pi$) for the driven AKLT model (14), with $\Delta(t) = \Delta_0 \sin(\epsilon t)$. Data are for the system size $N = 50$, varying Δ_0 and γ. In both (a) and (b), data are obtained using numerical implementation of the TDVP with bond dimension $\chi = 64$. (c) The scarred eigenstates $|E_j\rangle$ of the static model are destroyed by the Floquet operator; only the periodic orbit $|\psi(0)\rangle$ is preserved. Also shown is the periodic orbit shifted by $T/2$. Data for both models in (c) are obtained via exact diagonalization.

$$\hat{\mathcal{H}}_{\rm AKLT} = \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \frac{1}{3}(\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2, \tag{12}$$

where $\mathbf{S}_n$ is a spin-1 operator on lattice site n. Recently, there has been much interest in quantum simulations of this model [51–55]. For present purposes, it will be important that $\hat{\mathcal{H}}_{\rm AKLT}$ contains a tower of QMBS eigenstates, generated by repeatedly applying the π-momentum spin-raising operator, $Q^+ = \sum_n (-1)^n (S_n^+)^2$, to the ground state [8,56]. The QMBS towers were shown to allow signatures of SPT order, such as the fractionalized boundary excitations, to persist at high energies above the ground state [57].

To construct the AKLT periodic orbit, we use the following $\chi = 2$ initial state:

$$|\psi(0)\rangle = \bigotimes_n [\mathbb{1} + (-1)^n (S_n^+)^2/2] |\psi_{\rm GS}^{\rm AKLT}\rangle. \tag{13}$$

This state oscillates periodically at a constant entanglement entropy $S_E(t) = \log(2)$, with the period set by the level spacing in the scarred subspace, $\epsilon = 4$. Note that this choice of the initial state is not unique, e.g., a similar $\chi = 4$ state was considered in Ref. [21]. We construct $\hat{\mathcal{H}}_1$ that satisfies Eqs. (4) and (5) by noting that, for the AKLT ground state, no two neighboring sites can be in the state $|-\rangle$, a property inherited by $|\psi(t)\rangle$. As $P_{\mathcal{T}}$ differs from the MPSs $|\psi(t)\rangle$ on a single site, $\hat{\mathcal{H}}_1$ will satisfy Eq. (5) provided it maps at least four neighboring sites to $|-\rangle$. Therefore, introducing the state $|\chi_-\rangle \equiv |-,-,-,-\rangle$, a suitable Hamiltonian will be of the form $\hat{\mathcal{H}}_1 = \gamma \sum |\Phi\rangle\langle\chi_-| + \mathrm{H.c.}$, where $|\Phi\rangle$ is an arbitrary state on four sites, which needs to have a finite overlap with $|\psi(t)\rangle$ in order to satisfy Eq. (4). These perturbations to the AKLT model differ fundamentally from those that preserve the entire tower of QMBS eigenstates in Ref. [21]. Indeed, the QMBS eigenstates of the AKLT model are not contained within the manifold; therefore, even perturbations with a perfectly coherent scarred orbit are not required to preserve the eigenstates.

Using quantum leakage, we can construct a driven perturbation of the AKLT model with an exact Floquet scarred state. First, we introduce the local basis vectors $|\alpha_\pm\rangle = (|+\rangle \pm |-\rangle)/\sqrt{2}$. Using this basis, we examine the following two-parameter perturbation:

$$\hat{\mathcal{H}}_1 = \sum_n \gamma |\alpha_+, \alpha_-, \alpha_+, \alpha_-\rangle\langle\chi_-| + \gamma |\alpha_-, \alpha_+, \alpha_-, \alpha_+\rangle\langle\chi_-| + (-1)^n \Delta |0,+,0,+\rangle\langle\chi_-| + \mathrm{H.c.} \tag{14}$$

All of the terms in this $\hat{\mathcal{H}}_1$ map $|\psi(t)\rangle$ to the same state; therefore, the leakage takes the form

$$\Gamma \propto \sqrt{N} \int_{t=0}^{T=\frac{\pi}{2}} |\gamma \cos(\epsilon t) - \Delta/2| dt. \tag{15}$$

The leakage can be exactly canceled by setting $\Delta = 2\gamma \cos(\epsilon t)$, as confirmed in Fig. 2(b). The Floquet model once again destroys the underlying tower of QMBS states, as shown in Fig. 2(d).

While to the best of our knowledge, there is no general relation between QMBS states and SPT order, it is interesting to note that our periodic scarred trajectory exhibits a constant-in-time AKLT string order parameter [58]. This is surprising given that the Floquet model breaks the dihedral $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry that normally protects the SPT order in the AKLT model [59]. Thus, our construction can embed a trajectory with quantized SPT order parameter into a non-SPT model. In the Supplemental Material [43], we show that similar conclusions hold for the cluster model [60], which exhibits Majorana boundary modes [61,62].

Conclusions and discussion.—We have presented a method for constructing classes of quantum Hamiltonians with equivalent semiclassical dynamics. This construction results in models that possess approximate QMBSs associated with a semiclassical trajectory, reminiscent of scars in quantum billiards [25]. For the choice of Hamiltonians above, the calculation of the quantum leakage is tractable, allowing one to write down new Floquet models with exact QMBSs (see the Supplemental Material [43] for further examples). The choice of MPSs for defining the manifold $\mathcal{M}$ was due to many QMBS models previously studied in the literature using MPS methods. However, our approach can be extended to other classes of variational wave functions such as bosonic or fermionic Gaussian states [63] or projected entangled pair states [42].

The approach here complements recent works that construct exact QMBSs using cellular automata [64–66]. In particular, it furnishes a constructive realization of orbit "steering" by Ljubotina *et al.* [67]. In contrast to the latter, our approach yields exact Floquet QMBSs without the need for variational optimization. Furthermore, our method does not require that the periodic orbit be generated by QMBSs, e.g., it could result from other ergodicity-breaking mechanisms, such as integrability or Hilbert space fragmentation [68–70].

If the states in $\mathcal{M}$ form an overcomplete basis, then a Feynman path integral over the manifold can be constructed [41]. The saddle point equations of the path integral will correspond to the TDVP equations of motion, while additional perturbative corrections eventually reproduce the exact quantum dynamics. In particular, the quadratic corrections to TDVP equations of motion can be related to Lyapunov exponents that characterize the chaotic nature of mixed semiclassical phase space [33,71]. For Hamiltonians that can be decomposed in the manner introduced in this Letter, it may be possible to write analytic expressions for the Lyapunov exponents.

In some physical applications, one would wish to "invert" the above procedure, i.e., given a manifold $\mathcal{M}$ and a Hamiltonian $\hat{\mathcal{H}}$, describing some physical system which supports QMBSs, one would like to identify a decomposition into $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_1$, such that Eqs. (3)–(5) approximately hold. A notable example is the PXP model [72,73], which provides an effective description of QMBS in Rydberg atom arrays. In the PXP model, it is not obvious how to perform the decomposition into $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_1$, although it has been conjectured that a suitable deformation of the model could result in exact QMBSs [30,74,75]. In this context, we note that, while Eqs. (7) or (8) are sufficient conditions to satisfy Eq. (5), they are not necessary. Hence, it would be interesting to understand if there exist more general yet analytically tractable mechanisms for embedding periodic orbits into larger families of nonintegrable quantum Hamiltonians.

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