Schrieffer-Wolff Transformation for Periodically Driven Systems: Strongly Correlated Systems with Artificial Gauge Fields

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We generalize the Schrieffer-Wolff transformation to periodically driven systems using Floquet theory. The method is applied to the periodically driven, strongly interacting Fermi-Hubbard model, for which we identify two regimes resulting in different effective low-energy Hamiltonians. In the nonresonant regime, we realize an interacting spin model coupled to a static gauge field with a nonzero flux per plaquette. In the resonant regime, where the Hubbard interaction is a multiple of the driving frequency, we derive an effective Hamiltonian featuring doublon association and dissociation processes. The ground state of this Hamiltonian undergoes a phase transition between an ordered phase and a gapless Luttinger liquid phase. One can tune the system between different phases by changing the amplitude of the periodic drive.

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The Schrieffer-Wolff transformation (SWT) [1–4] is a generic procedure to derive effective low-energy Hamiltonians for strongly correlated many-body systems. It allows one to eliminate high-energy degrees of freedom via a canonical transform. The SWT has proven useful for studying systems with a hugely degenerate ground-state manifold, such as the strongly interacting limit of the Fermi-Hubbard model (FHM) [2], without resorting to conventional perturbation theory.

Treating interactions in such a nonperturbative way is difficult in periodically driven systems [5–10], which have received unprecedented attention following the realization of dynamical localization [11–15], artificial gauge fields [16–22], models with topological [23–28] and state-dependent [29] bands, and spin-orbit coupling [30,31]. In this Letter, we consider strongly interacting periodically driven systems and show how the SWT can be extended to derive effective static Hamiltonians of nonequilibrium setups. The parameter space of such models, to which we add the driving amplitude and frequency, opens up the door to new regimes. We use this to propose realizations of nontrivial Hamiltonians, including spin models in artificial gauge fields and the Fermi-Hubbard model with enhanced doublon association and dissociation processes.

SWT from the high-frequency expansion.—Intuitively, the high-frequency expansion (HFE) for periodically driven systems and the SWT share the same underlying concept: they allow for the elimination of virtually populated high-energy states to provide a dressed low-energy description, as illustrated in Fig. 1. For a system driven off resonantly [Fig. 1(a)], virtual absorption of a photon renormalizes tunneling. Similarly, nondriven fermions develop Heisenberg interactions via off-resonant (virtual) tunneling processes [Fig. 1(b)]. In this Letter we combine the HFE and SWT into a single framework allowing one to treat both resonantly and nonresonantly driven systems on equal footing. Let us illustrate the connection by deriving the SWT using the HFE. Consider the nondriven FHM:

$$H = -J_0 \sum_{\langle ij\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}, \tag{1}$$

where J_0 is the bare hopping and U is the fermion-fermion interaction. We are interested in the strongly correlated regime $J_0 \ll U$. Going to the rotating frame $|\psi^{\rm rot}(t)\rangle = V^\dagger(t)|\psi(t)\rangle$ with respect to the operator $V(t) = \exp(-iUt\sum_j n_{j\uparrow} n_{j\downarrow})$ eliminates the energy U in favor of fast oscillations. If $id_t|\psi^{\rm rot}\rangle = H^{\rm rot}(t)|\psi^{\rm rot}\rangle$, then

$$H^{\rm rot}(t) = -J_0 \sum_{\langle ij\rangle,\sigma} [g_{ij\sigma} + (e^{iUt} h^\dagger_{ij\sigma} + {\rm H.c.})],$$
$$h^\dagger_{ij\sigma} = n_{i\bar\sigma} c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j\bar\sigma}),$$
$$g_{ij\sigma} = (1 - n_{i\bar\sigma}) c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j\bar\sigma}) + n_{i\bar\sigma} c^\dagger_{i\sigma} c_{j\sigma} n_{j\bar\sigma}, \tag{2}$$

where $\bar\uparrow = \downarrow$ and vice versa. The first term $g_{ij\sigma}$ models the hopping of doublons and holons, while the second term $h^\dagger_{ij\sigma}$

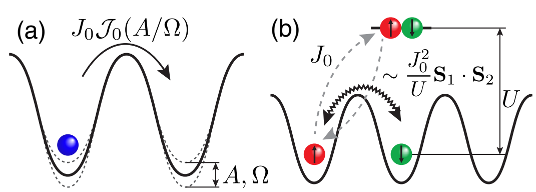

FIG. 1. Similarity between renormalization of tunneling, an interference effect induced virtually by an off-resonant drive (a), and Heisenberg interactions induced by virtual off-resonant interaction processes (b).

represents the creation and annihilation of doublon-holon pairs. Since $H^{\rm rot}(t)$ is time periodic with frequency U, we can apply Floquet's theorem [32]. Thus, the evolution of the system at integer multiples of the driving period $T_U = 2\pi/U$ (i.e., stroboscopically) is governed by the effective Floquet Hamiltonian $H_{\rm eff}$. If we write $H^{\rm rot}(t) = \sum_\ell H_\ell^{\rm rot} e^{i\ell U t}$, the HFE gives an operator expansion for $H_{\rm eff} = H_0^{\rm rot} + \sum_{\ell>0}[H_\ell^{\rm rot}, H_{-\ell}^{\rm rot}]/\ell U + O(U^{-2})$ [33–38]. The zeroth-order term $H_{\rm eff}^{(0)} = H_0^{\rm rot}$ is the period-averaged Hamiltonian (here the doublon-holon hopping g), while the first-order term is proportional to the commutator $H_{\rm eff}^{(1)} \sim J_0^2[h^\dagger, h]/U$, cf. Fig. 1(b):

$$H_{\rm eff} \approx -J_0 \sum_{\langle ij\rangle,\sigma} g_{ij\sigma} + \frac{4J_0^2}{U}\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{n_i n_j}{4}\right). \quad (3)$$

This effective Hamiltonian is in precise agreement with the one from the standard SWT [39]. At half filling, doublons and holons are suppressed in the ground state and this reduces to the Heisenberg model. Away from half filling this Hamiltonian reduces to the $t-J$ model [2,40].

Using the HFE to perform the SWT offers a few advantages: (i) the SW generator comes naturally out of the calculation, (ii) one can systematically compute higher-order corrections [33–38,41], and (iii) the HFE allows for obtaining not only the effective Hamiltonian but also the kick operator, which keeps track of the mixing between orbitals and describes the intraperiod dynamics [34,41]. This is important for identifying the fast time scale associated with the large frequency U in dynamical measurements [42] and expressing observables through creation and annihilation operators dressed by orbital mixing [41].

Generalization to periodically driven systems.—The HFE allows us to extend the SWT to time-periodic Hamiltonians. Related approaches have been used to study noninteracting Floquet topological insulators [43] and ultrafast dynamical control of the spin-exchange coupling [44] in fermionic Mott insulators [45]. Let us add to the FHM an external periodic drive:

$$H(t) = -J_0 \sum_{\langle ij\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_j n_{j\uparrow}n_{j\downarrow} + \sum_{j\sigma} f_{j\sigma}(t) n_{j\sigma}. \quad (4)$$

The driving protocol $f_{j\sigma}(t)$ with frequency Ω encompasses experimental tools such as mechanical shaking, external electromagnetic fields, and time-periodic chemical potentials, relevant for the recent realizations of novel Floquet Hamiltonians. In the following, we work in the limit $J_0 \ll U, \Omega$ and assume that the amplitude of the periodic modulation also scales with Ω [41].

Since both the interaction strength U and the driving amplitude are large, we go to the rotating frame with respect to $V(t) = e^{-i[Ut\sum_j n_{j\uparrow}n_{j\downarrow} + \sum_{j,\sigma} F_{j\sigma}(t) n_{j\sigma}]}$, where $F_{j\sigma}(t) = \int^t f_{j\sigma}(t')dt'$. The drive induces phase shifts to the hopping:

$$H^{\rm rot}(t) = -J_0 \sum_{\langle ij\rangle,\sigma}[e^{i\delta F_{ij\sigma}(t)} g_{ij\sigma} + (e^{i[\delta F_{ij,\sigma}(t)+Ut]} h_{ij\sigma}^\dagger + \text{H.c.})],$$

where $\delta F_{ij,\sigma}(t) = F_{i\sigma}(t) - F_{j\sigma}(t)$. Notice that now there are two frequencies in the problem: U and Ω. Hence, $H^{\rm rot}(t)$ is not strictly periodic in either. To circumvent this difficulty, we choose a common frequency Ω_0 by writing $\Omega = k\Omega_0$ and $U = l\Omega_0$, where k and l are co-prime integers. Then $H^{\rm rot}(t)$ becomes periodic with period $T_{\Omega_0} = 2\pi/\Omega_0$, and we can proceed using the HFE. Alternatively, before going to the rotating frame, we could decompose the interaction strength as $U = l\Omega + \delta U$, where δU acts as a detuning, and can continue without including the term proportional to δU in $V(t)$.

Nonresonant driving.—Let us first assume $k, l \gg 1$ such that resonance effects can be ignored. We begin by Fourier expanding the drive $e^{i\delta F_{ij\sigma}(t)} = \sum_\ell A_{ij\sigma}^{(\ell)} e^{i\ell\Omega t}$. If opposite spin species are driven out of phase, we have $A_{ij\bar\sigma}^{(\ell)} = (A_{ij\sigma}^{(-\ell)})^*$. Similarly, flipping the direction of the bond flips the sign of δF, so $A_{ji\sigma}^{(\ell)} = (A_{ij\sigma}^{(-\ell)})^*$. We now apply the generalized SWT with frequency Ω_0. At half filling and for off-resonant driving double occupancies are suppressed, and the dominant term in the effective Hamiltonian is $H_{\rm eff}^{(1)} = \sum_{\ell>0}[H_\ell^{\rm rot}, H_{-\ell}^{\rm rot}]/\ell\Omega_0$. Two types of commutators occur in this sum: the first comes from terms that have no oscillation with frequency U, giving commutators of the form $[\sum_{ij\sigma} A_{ij\sigma}^{(\ell)} g_{ij\sigma}, \sum_{i'j'\sigma'} A_{i'j'\sigma'}^{(\ell)} g_{i'j'\sigma'}]$; all of these commutators vanish. The second type are the same commutators relevant for the SWT, $[\sum_{ij\sigma} A_{ij\sigma}^{(\ell)} h_{ij\sigma}^\dagger, \sum_{i'j'\sigma'} A_{i'j'\sigma'}^{(-\ell)} h_{j'i'\sigma'}]$, but note the presence of all higher-order harmonics induced by the drive. These involve terms rotating with $e^{i(U+\ell\Omega)t}$, and thus will be suppressed by a $(U+\ell\Omega)$ denominator. The commutators are explicitly done in the Supplemental Material [46], giving

$$H_{\rm eff}^{(1)} = \sum_{\langle ij\rangle,\ell} \frac{J_0^2}{U+\ell\Omega}(\alpha_{ij}^{(\ell)} S_i^+ S_j^- + \alpha_{ij}^{(\ell)*} S_i^- S_j^+ + 2\beta_{ij}^{(\ell)} S_i^z S_j^z),$$

where $\alpha_{ij}^{(\ell)} \equiv A_{ij\uparrow}^{(\ell)} A_{ij\uparrow}^{(-\ell)}$ and $\beta_{ij}^{(\ell)} \equiv |A_{ij\uparrow}^{(\ell)}|^2$.

One can Floquet engineer the Heisenberg model with a uniform magnetic flux per plaquette $\Phi_\square$; see Fig. 2. To this end, we choose the spin-dependent driving protocol $f_{j,\sigma}(t) = \sigma[A\cos(\Omega t + \phi_j) + \Omega m]$ (cf. Fig. 2, inset), where $\phi_j = \phi_{mn} = \Phi_\square(m+n)$, $\sigma \in \{\uparrow,\downarrow\} \equiv \{1,-1\}$, and we denote the square-lattice position by $\mathbf{r}_j = (m,n)$. Such spin-sensitive drives are realized in experiments via the Zeeman effect using a periodically modulated [29] and static [19,20] magnetic-field gradients which couple to atomic hyperfine states. For this protocol,

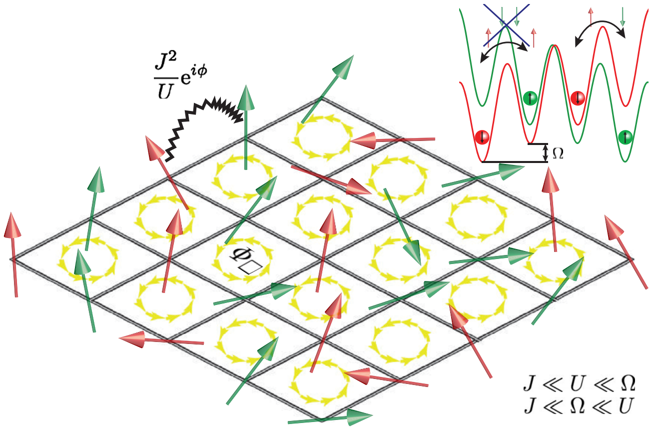

FIG. 2. In the presence of a spin-dependent drive off resonant with the interaction strength U (inset), the stroboscopic physics of the strongly driven, strongly correlated Fermi-Hubbard model is governed by an effective spin Hamiltonian in the presence of a gauge field.

$$A^{(\ell)}_{(m,n),(m,n+1)\uparrow} \equiv A^{(\ell)}_{y\uparrow} = e^{i\ell\phi_{mn}}\mathcal{J}_\ell(2\zeta_\Phi),$$
$$A^{(\ell)}_{(m,n),(m+1,n)\uparrow} \equiv A^{(\ell)}_{x\uparrow} = e^{i(\ell+1)\phi_{mn}}\mathcal{J}_{\ell+1}(2\zeta_\Phi),$$

where $\mathcal{J}_\ell$ is the Bessel function of the first kind, $\zeta = A/\Omega$ is the dimensionless driving strength, and $\zeta_\Phi = \zeta\sin(\Phi_\square/2)$ is the flux-modified strength [48].

There are two physically interesting limits. For $U \ll \Omega$, only $\ell = 0$ survives and we get

$$H^{U\ll\Omega}_{\text{eff}} = \sum_{m,n}\bigg(J^{\text{ex},x}_{\text{eff}}\bigg[S^z_{m+1,n}S^z_{mn} + \frac{1}{2}(e^{2i\phi_{mn}}S^+_{m+1,n}S^-_{mn} + \text{H.c.})\bigg] + J^{\text{ex},y}_{\text{eff}}\bigg[S^z_{m,n+1}S^z_{mn} + \frac{1}{2}(S^+_{m,n+1}S^-_{mn} + \text{H.c.})\bigg]\bigg),$$

where $J^{\text{ex},x/y}_{\text{eff}} = 4[J_0\mathcal{J}_{1/0}(2\zeta_\Phi)]^2/U$. For $\Omega \ll U$, we can set $U + l\Omega \to U$ and sum over l to obtain

$$H^{\Omega\ll U}_{\text{eff}} = \frac{4J_0^2}{U}\sum_{m,n}\bigg[S^z_{m+1,n}S^z_{mn} + \frac{\mathcal{J}_2(4\zeta_\Phi)}{2}(e^{2i\phi_{mn}}S^+_{m+1,n}S^-_{mn} + \text{H.c.}) + S^z_{m,n+1}S^z_{mn} + \frac{\mathcal{J}_0(4\zeta_\Phi)}{2}(S^+_{m,n+1}S^-_{mn} + \text{H.c.})\bigg].$$

The exchange strengths depend on Ω and U, but both limits give spin Hamiltonians with phases along x. This phase physically appears on the flip-flop and not the Ising term because the drive is spin dependent. Thus, a phase difference only occurs if the electron virtually hops as one spin and returns as the other.

Let us discuss the regime $J_0 \ll \Omega \ll U$ a bit more. This spin Hamiltonian can be identified with the Heisenberg model in the presence of an artificial gauge field with flux $\Phi_\square$ per plaquette. Whenever the S^zS^z interaction is small, the Hamiltonian reduces to the fully frustrated XY model in 2D, in which one cannot choose a spin configuration minimizing the spin-exchange energy for all XY couplings. In the classical limit, similarly to a type-II superconductor, the minimal energy configuration is known to be the Abrikosov vortex lattice [49,50]. The realization of the deep XY regime with this particular driving protocol is limited, since $|\mathcal{J}_2(4\zeta_\Phi)| < 1$, but, at finite S^zS^z interaction, a semiclassical study showed that vortices persist and can be thought of as half-Skyrmion configurations of the Néel field [51–53]. Another interesting feature of the spin Hamiltonian is that it exhibits a Dzyaloshinskii-Moriya interaction term [54–57], $\mathbf{D}_{mn}\cdot(\mathbf{S}_{m+1,n}\times\mathbf{S}_{mn})$. The Dzyaloshinskii-Moriya coupling is spatially dependent, polarized along the z direction $\mathbf{D}_{mn} = \sin(\phi_{mn})\mathcal{J}_2(4\zeta_\Phi)\hat{\mathbf{n}}_z/2$, and present only along the x-lattice direction.

Finally, let us mention that spin-1/2 systems are equivalent to hard-core bosons. In this respect, $H^{U\ll\Omega}_{\text{eff}}$ and $H^{\Omega\ll U}_{\text{eff}}$ model hard-core bosons with strong nearest-neighbour interactions in the presence of a gauge field. For a flux of $\Phi_\square = \pi/2$ the noninteracting model has four topological Hofstadter bands. If we then consider the strongly interacting model, and half fill the lowest Hofstadter band ($S^z_{\text{tot}} = -3N_{\text{site}}/8$), the Heisenberg model supports a fractional quantum Hall ground state [25,58–60]. Away from half filling of the fermions, doublon and holon hopping terms appear in the effective Hamiltonian, cf. Supplemental Material [46], and it would be interesting to study the effect of such correlated hopping terms [61] on this topological phase.

Resonant driving.—Novel physics arises in the resonant-driving regime $J_0 \ll U = l\Omega$. To illustrate this, we choose a one-dimensional system with the driving protocol $f_{j\sigma}(t) = jA\cos\Omega t$, which was realized experimentally by mechanical shaking [12–14]. Unlike off-resonant driving, resonance drastically alters the effective Hamiltonian by enabling the lowest-order term $H^{(0)}_{\text{eff}}$: on resonance, the doublon-holon (DH) creation or annihilation terms $h^\dagger$ survive the time averaging, and the leading-order effective Hamiltonian reads

$$H^{(0)}_{\text{eff}} = \sum_{\langle ij\rangle,\sigma}\{-J_{\text{eff}}g_{ij\sigma} - K_{\text{eff}}[(-1)^{l\eta_{ij}}h^\dagger_{ij\sigma} + \text{H.c.}]\}, \quad (5)$$

where $\eta_{ij} = 1$ for $i > j$, $\eta_{ij} = 0$ for $i < j$, $J_{\text{eff}} = J_0\mathcal{J}_0(\zeta)$, and $K_{\text{eff}} = J_0\mathcal{J}_l(\zeta)$. The first term, $g_{ij\sigma}$, is familiar from the static SWT, with a renormalized coefficient J_{eff}. The term proportional to $h^\dagger_{ij\sigma}$ appears only in the presence of the resonant periodic drive and is the source of new physics in this regime. By adjusting the drive strength, one can tune J_{eff} and K_{eff} to a range of values, including zeroing out either one. Starting from a state with unpaired spins, DH pairs are created via resonant absorption of drive photons.

Hence, holons and doublons become dynamical degrees of freedom governed by $H_{\rm eff}^{(0)}$, with the Heisenberg model as a subleading correction. The DH production rates and further properties of the system have been investigated both experimentally and theoretically [44,62–72]. A Dynamical Mean Field Theory (DMFT) study found that the ac field can flip the band structure, switching the interaction from attractive to repulsive [73].

Such correlated hopping models have been proposed to study high-T_c superconductivity [74–76]. To get an intuition about the effect of the new terms, we use the numerical tools Density Matrix Renormalization Group (DMRG) and Matrix Product States (MPS) from the open-source software Algorithms and Libraries for Physics Simulations (ALPS) [77,78] to calculate the ground state of $H_{\rm eff}^{(0)}$ at half-filling. The many-body gap in the thermodynamic limit Δ is extracted from simulations of even-length chains with open boundary conditions by extrapolation in the system size: $\Delta(L) = {\rm const}/L + \Delta$. We numerically confirm that the model features a transition between a symmetry-broken ordered phase and a gapless Luttinger liquid phase [74–76] as follows [79]. For $K_{\rm eff} > J_{\rm eff}$, the physics is dominated by the DH creation or annihilation processes. In this regime, fermions can hop along the lattice by forming and destroying DH pairs. Thus, for l *even*, the ground state exhibits bond-wave order with order parameter $B_j = \sum_\sigma c_{j+1,\sigma}^\dagger c_{j\sigma} +$ H.c., while the corresponding order parameter for l odd is not yet known. This order breaks translation invariance with a two-site unit cell, and thus yields a many-body gap for even-length chains with open boundary conditions (cf. Fig. 3). For $K_{\rm eff} < J_{\rm eff}$, renormalization group arguments show that bond ordering terms become irrelevant, leading to a gapless Luttinger liquid [81]. At $K_{\rm eff} = J_{\rm eff}$ and for l even, one surprisingly finds that the system is equivalent to free fermions. The existence of such a noninteracting point is rather striking, since it means that a strongly driven, strongly interacting system can effectively behave as if the fermions were free. This phenomenon can be understood by noticing that double occupancies, effectively forbidden in the absence of the drive by strong interactions, are reenabled by the resonant driving term. As a result, whenever the amplitude of the driving field matches a special value to give $K_{\rm eff} = J_{\rm eff}$, the matrix element for creation of doublons and holes becomes equal to their hopping rate and the effect of the strong interaction is completely compensated by the strong driving field. We emphasize that this is a highly nonperturbative effect since it requires a large drive amplitude, $A \sim U = l\Omega$.

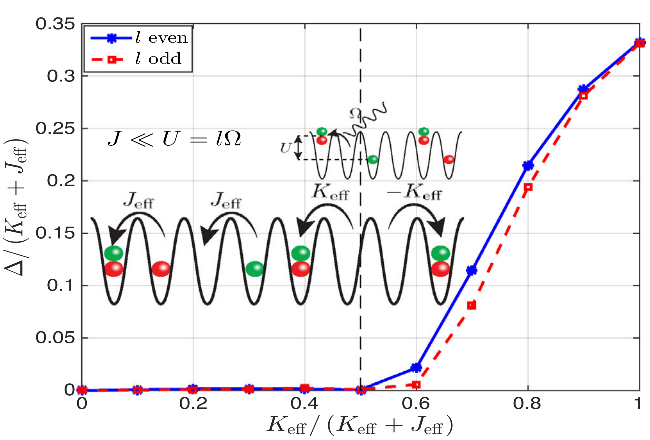

FIG. 3. Resonant driving of the Fermi-Hubbard model enables doublon creation and dissociation processes (inset). The many-body gap Δ shows a phase transition from a gapless Luttinger liquid to gapped translation-invariance-broken phase. The doublon-holon hopping and creation coefficients $J_{\rm eff}$ and $K_{\rm eff}$ are controlled by varying the driving amplitude.

It bears mentioning that all regimes of the model are accessible using present-day cold atoms experiments [66]. We propose a loading sequence into the ground state of $H_{\rm eff}^{(0)}$ in the Supplemental Material [46]. Moreover, by tuning the frequency away from resonance, one can write $U = \delta U + l\Omega$ and go to the rotating frame with respect to the $l\Omega$ term, keeping a finite on-site interaction δU in the effective Hamiltonian. This is required if one wants to capture important photon-absorption avoided crossings in the exact Floquet spectrum. Including artificial gauge fields is also straightforward in higher dimensions, see Supplemental Material [46], and expected to produce novel topological phases. By utilizing resonance phenomena, this scheme only requires shaking of the on-site potentials, which is easier in practice than other schemes that have suggested modulating the interaction strength to realize similar Hamiltonians [82,83].

Discussion and outlook.—It becomes clear from the discussion above how to generalize the SWT to arbitrary strongly interacting periodically driven models. First, we identify the large energy scale denoted by λ (e.g., $\lambda = U$) and write the Hamiltonian as $H = H_0 + \lambda H_1 + H_{\rm drive}(t)$. Second, we go to the rotating frame using the transformation $V(t) = \exp[-i\lambda t H_1 - i\int^t H_{\rm drive}(t')dt']$ to get a new time-dependent Hamiltonian with frequencies [84] λ and Ω: $H^{\rm rot}(t) = V^\dagger(t) H_0 V(t)$. Finally, depending on whether we want to discuss resonant or nonresonant coupling, we apply the HFE to obtain the effective Hamiltonian $H_{\rm eff}$ order by order in λ^{-1} and Ω^{-1}. This procedure will generally work if a closed-form evaluation of $H^{\rm rot}(t)$ is feasible. For instance, H_1 can be a local Hamiltonian or can be written as a sum of local commuting terms. The method also works if the interaction strength is periodically modulated [82,83,85].

Although isolated interacting Floquet systems are generally expected to heat up to infinite temperature at infinite time [5–9,86], the physics of such systems at experimentally relevant time scales is well captured by the above effective Hamiltonians; indeed, it was recently argued that typical heating rates at high frequencies are suppressed exponentially [87–90], and long-lived prethermal Floquet steady states have been predicted [88,90–92]. In particular, rigorous mathematical proofs [88–90] supported by numerical studies [10] showed that the mistake in the dynamics due to the approximative character of the HFE is under control for the large frequencies and the experimentally relevant times considered. Our work paves the way for studying such strongly driven, strongly correlated systems. Both the resonant and nonresonant regimes that we analyze for the FHM yield systems directly relevant to the study of high-temperature superconductivity. More generally, we show that by using the generalized SWT, one can Floquet engineer additional knobs controlling the model parameters of strongly correlated systems, such as the spin-exchange coupling. Our methods are readily extensible to strongly interacting bosonic systems, as well as many other systems under active research.

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