

# Quantum Floquet engineering with an exactly solvable tight-binding chain in a cavity

Christian J. Eckhardt,<sup>1,2,\*</sup> Giacomo Passetti,<sup>1,\*</sup> Moustafa Othman,<sup>3</sup> Christoph Karrasch,<sup>3</sup> Fabio Cavaliere,<sup>4,5</sup> Michael A. Sentef,<sup>2</sup> and Dante M. Kennes<sup>1,2,†</sup>

<sup>1</sup>*Institut für Theorie der Statistischen Physik,  
RWTH Aachen University and JARA-Fundamentals of  
Future Information Technology, 52056 Aachen, Germany*

<sup>2</sup>*Max Planck Institute for the Structure and Dynamics of Matter,  
Luruper Chaussee 149, 22761 Hamburg, Germany*

<sup>3</sup>*Technische Universität Braunschweig, Institut für Mathematische Physik,  
Mendelssohnstraße 3, 38106 Braunschweig, Germany*

<sup>4</sup>*Dipartimento di Fisica, Università di Genova, 16146, Genova, Italy*

<sup>5</sup>*SPIN-CNR, 16146, Genova, Italy*

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## SUPPLEMENTARY INFORMATION

### SUPPLEMENTARY NOTE 1: COLLECTIVE STRONG COUPLING IN THE CASE OF $N$ IDENTICAL MODES

In this supplementary we show that coupling electrons to  $N$  identical modes with a coupling constant  $\frac{g}{\sqrt{L}}$ , in a setup as described in the Model subsection under Results of the main text, effectively results in a single mode coupling with enhanced strength  $\frac{g\sqrt{N}}{\sqrt{L}}$  and  $N - 1$  completely decoupled modes. We will start to show how this holds for the Hamiltonian expanded to second order in the light-matter coupling (also compare Eq. (15) of the main text) and later in this section argue why this might also hold for the full Peierls substitution including all order in the LMC (also compare Eq. (2) of the main text). We write the Hamiltonian to second order in the LMC  $g$  for many identical modes as

$$H = \mathcal{T} + \frac{g}{\sqrt{L}} \mathcal{J} \sum_{\lambda} (a_{\lambda}^{\dagger} + a_{\lambda}) - \frac{1}{2} \frac{g^2}{L} \mathcal{T} \left( \sum_{\lambda} (a_{\lambda}^{\dagger} + a_{\lambda}) \right)^2 + \omega \sum_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}. \quad (1)$$

Here  $a_{\lambda}$  annihilates -;  $a_{\lambda}^{\dagger}$  creates a photon in mode  $\lambda$ . All other symbols are as defined in the main text.

To find a form where the modes are decoupled we will represent them in terms of their generalized coordinate and momentum according to

$$\begin{aligned} X_{\lambda} &= \frac{1}{\sqrt{2\omega}} (a_{\lambda}^{\dagger} + a_{\lambda}) \\ P_{\lambda} &= i \frac{\sqrt{\omega}}{\sqrt{2}} (a_{\lambda}^{\dagger} - a_{\lambda}) \end{aligned} \quad (2)$$

with which the Hamiltonian becomes

$$H = \mathcal{T} + \sqrt{2\omega} \frac{g}{\sqrt{L}} \mathcal{J} \sum_{\lambda} X_{\lambda} - \frac{g^2}{L} \omega \mathcal{T} \sum_{\lambda, \kappa} X_{\lambda} X_{\kappa} + \sum_{\lambda} \frac{1}{2} \omega^2 X_{\lambda}^2 + \frac{1}{2} P_{\lambda}^2. \quad (3)$$

This can be written in matrix form as

$$H = \mathcal{T} + \sqrt{2\omega} \frac{g}{\sqrt{L}} \mathcal{J} \sum_{\lambda} X_{\lambda} - \frac{g^2}{L} \omega \mathcal{T} \underline{X}^T \begin{pmatrix} I_e - \frac{\omega L}{2g^2} \mathcal{T}^{-1} & I_e & \dots & I_e \\ I_e & I_e - \frac{\omega L}{2g^2} \mathcal{T}^{-1} & I_e & \dots \\ \dots & \dots & \dots & I_e \\ I_e & \dots & I_e & I_e - \frac{\omega L}{2g^2} \mathcal{T}^{-1} \end{pmatrix} \underline{X} + \frac{1}{2} \underline{P}^T I_{N \times N} \underline{P}. \quad (4)$$

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\* These authors contributed equally

† [dante.kennes@rwth-aachen.de](mailto:dante.kennes@rwth-aachen.de)

Here  $I_e$  is the identity on the electronic part of the Hilbert space. We have introduced  $N$ -dimensional coordinate and momentum vectors as

$$\underline{X} = \begin{pmatrix} X_1 \\ \dots \\ X_N \end{pmatrix} ; \quad \underline{P} = \begin{pmatrix} P_1 \\ \dots \\ P_N \end{pmatrix} \quad (5)$$

and  $I_{N \times N}$  is simply the unity in  $N$  dimensions with  $I_e$  on the diagonal. One eigenvector of the above matrix in Eq. (4) is clearly

$$v^1 = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 \\ \dots \\ 1 \end{pmatrix} \quad (6)$$

with corresponding eigenvalue (that still contains an operator from the electronic subsystem due to the composite nature of the system)

$$\varepsilon^1 = N - \frac{\omega L}{2g^2} \mathcal{T}^{-1}. \quad (7)$$

Each vector  $v = (v_1, \dots, v_N)^T$  from the orthogonal  $N - 1$  dimensional subspace of  $v^1$ , defined through the equation  $\sum_{i=1}^N v_i = 0$ , is an eigenvector with eigenvalue  $\varepsilon = -\frac{\omega L}{2g^2} \mathcal{T}^{-1}$  which is therefore  $N - 1$  times degenerate. Denoting by  $P_+$  and  $X_+$  momentum and coordinate corresponding to the first eigenvector and by  $\tilde{P}_\kappa$ ,  $\tilde{X}_\kappa$ ,  $\kappa = 1, \dots, N - 1$  momenta and coordinates corresponding to the other  $N - 1$  eigenvectors we can write the Hamiltonian with decoupled bosonic modes as

$$H = \mathcal{T} + \sqrt{2\omega}\sqrt{N} \frac{g}{\sqrt{L}} X_+ \mathcal{J} + \frac{1}{2} \left( \omega^2 - 2N \frac{g^2}{L} \omega \mathcal{T} \right) X_+^2 + \frac{1}{2} P_+^2 + \sum_{\kappa} \frac{1}{2} \omega^2 \tilde{X}_\kappa^2 + \frac{1}{2} \tilde{P}_\kappa^2. \quad (8)$$

From this it is clear that the  $X_+$  mode couples to the electrons with effective strength  $\frac{g\sqrt{N}}{\sqrt{L}}$  while all other  $N - 1$  modes don't couple to the electrons or among each other at all.

Next we discuss the case of the full Peierls substitution keeping all orders in the LMC. For this situation the Hamiltonian including many identical modes with zero momentum transfer would read

$$H = \sin \left( \frac{g}{\sqrt{L}} \sum_{\lambda} (a_{\lambda}^{\dagger} + a_{\lambda}) \right) \mathcal{J} + \cos \left( \frac{g}{\sqrt{L}} \sum_{\lambda} (a_{\lambda}^{\dagger} + a_{\lambda}) \right) \mathcal{T} + \omega \sum_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}. \quad (9)$$

We now write this Hamiltonian in terms of the canonical position and momentum operators introduced in Eq. (2)

$$\begin{aligned} H &= \sin \left( \frac{g\sqrt{2\omega}}{\sqrt{L}} \sum_{\lambda} X_{\lambda} \right) \mathcal{J} + \cos \left( \frac{g\sqrt{2\omega}}{\sqrt{L}} \sum_{\lambda} X_{\lambda} \right) \mathcal{T} + \sum_{\lambda} \frac{1}{2} P_{\lambda}^2 + \frac{\omega^2}{2} X_{\lambda}^2 \\ &= \sin \left( \frac{g\sqrt{2\omega}}{\sqrt{L}} \sum_{\lambda} X_{\lambda} \right) \mathcal{J} + \cos \left( \frac{g\sqrt{2\omega}}{\sqrt{L}} \sum_{\lambda} X_{\lambda} \right) \mathcal{T} + \frac{1}{2} \underline{P}^T I_{N \times N} \underline{P} + \frac{\omega^2}{2} \underline{X}^T I_{N \times N} \underline{X} \end{aligned} \quad (10)$$

where in the last step we have again introduced  $N$ -dimensional notation as in Eq. (5). The fact that the harmonic oscillator terms can be written using the  $N$ -dimensional unity  $I_{N \times N}$  stems from our approximation of all modes having equal frequency. Due to this, we can now write the Hamiltonian in terms of any other set of collective modes in particular the one used to write Eq. (8) in which the last term will remain diagonal (ie. in particular not couple different modes) obtaining

$$H = \sin \left( \frac{g\sqrt{2\omega}\sqrt{N}}{\sqrt{L}} X_+ \right) \mathcal{J} + \cos \left( \frac{g\sqrt{2\omega}\sqrt{N}}{\sqrt{L}} X_+ \right) \mathcal{T} + \frac{1}{2} P_+^2 + \frac{\omega^2}{2} X_+^2 + \sum_{\kappa=1}^{N-1} \frac{1}{2} \tilde{P}_\kappa^2 + \frac{\omega^2}{2} \tilde{X}_\kappa^2. \quad (11)$$

Here all operators are defined as in Eq. (8). Thus also in the case of keeping all orders in the LMC we obtain a single mode with effectively enhanced coupling  $\frac{g}{\sqrt{L}} \rightarrow \frac{g\sqrt{N}}{\sqrt{L}}$  and  $N-1$  uncoupled modes.

In Eq. (8) (and also Eq. (11) when expanding again) it seems like the effective frequency of the  $X_+$  mode would scale like  $\sqrt{N}$  for large enough  $N$  which seems counter-intuitive. This is, however, reminiscent of the dipole approximation that is here taken for all modes. When allowing for any small but non-zero momentum transfer, the modes immediately couple to a microscopic quantity instead of all electrons collectively yielding a finite effective frequency.

The here shown mechanism for collective strong coupling is reminiscent of an analogous one considered in the case of vibrational Strong Coupling<sup>1-3</sup> in the case of a cavity coupling to vibrational excitations of a solid or to collective strong coupling of an electro-magnetic resonator coupled to many emitters.<sup>3,4</sup>

## SUPPLEMENTARY NOTE 2: DIAGONALIZATION OF THE HAMILTONIAN IN THE TD LIMIT

In this part we show how to diagonalize the Hamiltonian expanded to second order in the field that gave the only non-vanishing contribution in the TD limit to the GS energy in Eq. (6). It reads

$$H^{2\text{nd}} = \omega_0 \left( a^\dagger a + \frac{1}{2} \right) + \mathcal{T} + \frac{g}{\sqrt{L}} (a^\dagger + a) \mathcal{J} - \frac{g^2}{2L} (a^\dagger + a)^2 \mathcal{T} \quad (S1)$$

and can be diagonalized using a combined squeezing and displacement transformation<sup>5,6</sup>

$$\begin{aligned} H^D &= e^{S^d[\mathcal{T}, \mathcal{J}]} e^{S^{\text{sq}}[\mathcal{T}]} H^{A, A^2} e^{-S^d[\mathcal{T}, \mathcal{J}]} e^{-S^{\text{sq}}[\mathcal{T}]} \\ S^d[\mathcal{T}, \mathcal{J}] &= \frac{g}{\sqrt{L}\omega_0} \left( \frac{\mathcal{W}[\mathcal{T}]}{\omega_0} \right)^{-\frac{3}{2}} (a^\dagger - a) \mathcal{J}, \\ S^{\text{sq}}[\mathcal{T}] &= \frac{1}{4} \ln \left( \frac{\mathcal{W}[\mathcal{T}]}{\omega_0} \right) (a^2 - (a^\dagger)^2). \end{aligned} \quad (S2)$$

The diagonal Hamiltonian  $H^D$  is given in the main text Eq. (7) together with the definition of  $\mathcal{W}[\mathcal{T}]$ . Both displacement and squeezing transformations depend on fermionic operators namely the kinetic energy  $\mathcal{T}$  and the current  $\mathcal{J}$ . Since  $\mathcal{T}$  and  $\mathcal{J}$  are diagonal in  $k$ -space the GS of the whole system is given as (see also Eq. (11) of the main text and below)

$$\begin{aligned} |\Phi_{\text{GS}}\rangle &= |\psi_{\text{GS}}\rangle_f \otimes |0_\beta\rangle \\ &= |\psi_{\text{GS}}\rangle_f \otimes e^{S^d[-t_{\text{GS}}L, j_{\text{GS}}L]} e^{S^{\text{sq}}[-t_{\text{GS}}L]} |0\rangle. \end{aligned} \quad (\text{S3})$$

where  $|\psi_{\text{GS}}\rangle_f$  is the unshifted FS and  $|0_\beta\rangle$  is the vacuum state of the annihilators(creators)  $\beta^{(\dagger)}$  of the coherent squeezed states, defined in the main text Eq. (8).  $|0\rangle$  is the vacuum state of the non squeezed bosonic operators  $a^\dagger$  and  $a$ . Since we found  $j_{\text{GS}} = 0$  due to the vanishing shift of the FS we have  $e^{S^d[-t_{\text{GS}}L, j_{\text{GS}}L]_\beta} = I_b$  where  $I_b$  is the identity on the bosonic part of the Hilbertspace. The photon part of the GS wavefunction is thus given by Eq. (12) of the main part.

### SUPPLEMENTARY NOTE 3: MOMENTUM-RESOLVED SPECTRAL FUNCTION IN THE TD LIMIT

In this part we show how to analytically calculate the spectral function  $A(k, \omega)$  of the electrons in the TD limit. Since we do this at temperature  $T = 0$  the expectation values appearing in the definition of the spectral function (Eq. (16) of the main text) are taken just with respect to the GS. None of the operators in the expectation value creates a macroscopic occupation of the photonic mode. Therefore, the scaling analysis of Eq. (6) of the main text can be applied in this case allowing us to diagonalize the problem by the combined squeezing and displacement transformation Eq. (S2). To evaluate the expectation values we also need the behaviour of the fermionic creation (annihilation) operators under these transformations which read

$$\begin{aligned} e^{S^d} e^{S^{\text{sq}}} c_k e^{-S^{\text{sq}}} e^{-S^d} &= c_k X Y, \\ e^{S^d} e^{S^{\text{sq}}} c_k^\dagger e^{-S^{\text{sq}}} e^{-S^d} &= c_k^\dagger X^\dagger Y^\dagger \end{aligned} \quad (\text{S6})$$

with

$$\begin{aligned} \ln(X) &= -\frac{g\omega_0 \mathcal{W}^{-2}}{\sqrt{L}} v_k (a^\dagger - a) + \mathcal{O}\left(\frac{1}{L^{\frac{3}{2}}}\right), \\ \ln(Y) &= \frac{1}{2} \frac{g^2}{\omega_0 L} \varepsilon_k \left(1 - 2 \frac{g^2}{\omega_0 L} \mathcal{T}\right)^{-1} (a^2 - (a^\dagger)^2) + \mathcal{O}\left(\frac{1}{L^{\frac{3}{2}}}\right). \end{aligned} \quad (\text{S7})$$

Considering the first expectation value from the spectral function, Eq. (16) of the main text, we find

$$\begin{aligned}
\langle c_k(t)c_k^\dagger \rangle &= {}_f \langle \psi_{\text{GS}} | \otimes {}_b \langle \phi_{\text{GS}} | \underbrace{1}_{e^{-S^{\text{sq}}[\mathcal{T}]}e^{-S^{\text{d}}[\mathcal{T},\mathcal{J}]}e^{S^{\text{d}}[\mathcal{T},\mathcal{J}]}e^{S^{\text{sq}}[\mathcal{T}]}} e^{iHt} c_k e^{-iHt} c_k^\dagger \underbrace{1}_{e^{-S^{\text{sq}}[\mathcal{T}]}e^{-S^{\text{d}}[\mathcal{T},\mathcal{J}]}e^{S^{\text{d}}[\mathcal{T},\mathcal{J}]}e^{S^{\text{sq}}[\mathcal{T}]}} | \phi_{\text{GS}} \rangle_b \otimes | \psi_{\text{GS}} \rangle_f \\
&= {}_f \langle \psi_{\text{GS}} | \otimes \langle 0 | e^{iH^{\text{D}}t} c_k X Y e^{-iH^{\text{D}}t} c_k^\dagger X^\dagger Y^\dagger | 0 \rangle \otimes | \psi_{\text{GS}} \rangle_f + \mathcal{O}\left(\frac{1}{L^{\frac{3}{2}}}\right) \\
&= \langle \psi_{\text{GS}} |_f \otimes \langle 0 | c_k(t)_{H^{\text{D}}} X(t)_{H^{\text{D}}} Y(t)_{H^{\text{D}}} c_k^\dagger X^\dagger Y^\dagger | 0 \rangle \otimes | \psi_{\text{GS}} \rangle_f + \mathcal{O}\left(\frac{1}{L^{\frac{3}{2}}}\right).
\end{aligned} \tag{S8}$$

With the subscript  $(\cdot)(t)_{H^{\text{D}}}$  we signify that the time dependence is determined by the diagonal Hamiltonian  $H^{\text{D}}$ , Eq. (7) of the main text.

The operators  $\mathcal{T}$  and  $\mathcal{J}$  appearing in  $X$  and  $Y$  have no time dependence since they commute with  $H^{\text{D}}$  (and in fact also the full  $H$ ). The time dependence of the operators  $X$  and  $Y$  is determined by that of the bosonic operators

$$\begin{aligned}
a(t)_{H^{\text{D}}} &= a e^{-i\mathcal{W}t} \\
a^\dagger(t)_{H^{\text{D}}} &= a^\dagger e^{i\mathcal{W}t}.
\end{aligned} \tag{S9}$$

Evaluating the electronic part of the expectation value will yield  $\mathcal{W} \rightarrow \tilde{\omega}$  restoring a simple time dependence with the dressed cavity frequency  $\tilde{\omega}$ .

Reconsidering the expectation value Eq. (S8) we note that moving the fermionic operators through  $X$  and  $Y$  will only yield higher order corrections such that we can write

$$\langle c_k(t)c_k^\dagger \rangle = e^{\Phi(t)}(1 - n_k) \langle 0 | X_{\psi_{\text{GS}}}(t)_{H_b^{\text{D}}} Y_{\psi_{\text{GS}}}(t)_{H_b^{\text{D}}} X_{\psi_{\text{GS}}}^\dagger Y_{\psi_{\text{GS}}}^\dagger | 0 \rangle \tag{S10}$$

where  $n_k = \langle c_k^\dagger c_k \rangle$ . Here we have evaluated the time dependence of the fermionic annihilators that yields the time dependent phase factor  $e^{\Phi(t)}$ . We find, only keeping the leading order as before

$$c_k(t)_{H^{\text{D}}} = c_k e^{\mathcal{F}(t)} \quad ; \quad \mathcal{F}(t) = -i\varepsilon_k t + i\frac{g^2\varepsilon_k}{L}\omega_0\mathcal{W}^{-1} \left( a^\dagger a + \frac{1}{2} \right) t - i\frac{g^2\omega_0\mathcal{W}^{-2}}{L}v_k^2 t \tag{S11}$$

Evaluating the expectation of this yields

$$\langle e^{\mathcal{F}(t)} \rangle = e^{\Phi(t)} \quad ; \quad \Phi(t) = -i\varepsilon_k t + i\frac{g^2\varepsilon_k}{2L}\frac{\omega_0}{\tilde{\omega}}t - i\Sigma_k t \tag{S12}$$

with

$$\Sigma_k = \frac{g^2\omega_0}{\tilde{\omega}^2 L}v_k^2. \tag{S13}$$

In Eq. (S10) we have already executed the fermionic part of the expectation value performing

$$\begin{aligned}
\frac{\mathcal{T}}{L} &\rightarrow \frac{\langle \psi_{\text{GS}} |_f \mathcal{T} | \psi_{\text{GS}} \rangle_f}{L} = t_{\text{GS}} \\
\frac{\mathcal{J}}{L} &\rightarrow \frac{\langle \psi_{\text{GS}} |_f \mathcal{J} | \psi_{\text{GS}} \rangle_f}{L} = j_{\text{GS}}
\end{aligned} \tag{S14}$$

in the  $X^{(\dagger)}$  and  $Y^{(\dagger)}$  operator writing them as  $X_{\psi_{\text{GS}}}^{(\dagger)}$  and  $Y_{\psi_{\text{GS}}}^{(\dagger)}$ .

Since all operators act on the  $|0\rangle$  state, contributions come only from commutators of the operators in the exponentials. Therefore, all contributions from the  $Y$  operator are at least  $\exp\left(\mathcal{O}\left(\frac{1}{L^{\frac{3}{2}}}\right)\right)^{7,8}$  and will thus be neglected. We are thus left with

$$\langle c_k(t)c_k^\dagger \rangle = e^{\Phi(t)}(1 - n_k) \langle 0| X_{\psi_{\text{GS}}}(t)_{H_b^D} X_{\psi_{\text{GS}}}^\dagger |0\rangle + \mathcal{O}\left(\frac{1}{L^{\frac{3}{2}}}\right). \quad (\text{S15})$$

The evaluation of the remaining expectation value is a standard textbook problem.<sup>9</sup>

Evaluating the other expectation value in the definition of the spectral function (Eq. (16) in the main part) yields the same result, just with a factor  $n_k$  instead of  $1 - n_k$  up front and the final expectation value in Eq. (S15) is complex conjugated as the order of the operators is reversed. This reflects the particle-hole symmetry of the half-filled system, which is inherited from the bare chain.

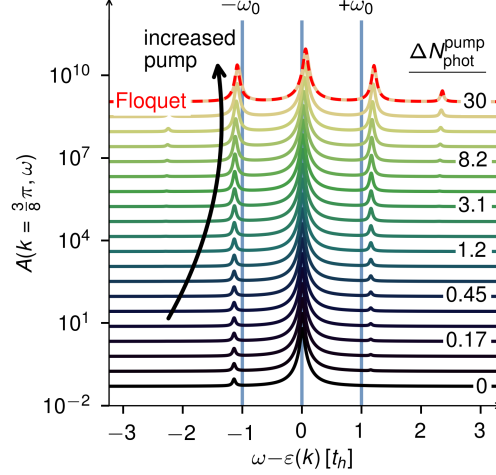
Performing the remaining FT we arrive at the final result reported in Eq. (18) in the main text.

#### **SUPPLEMENTARY NOTE 4: NON-EQUILIBRIUM SPECTRAL FUNCTION FROM COHERENT PUMPING**

In this part we calculate the non-equilibrium spectral function according to Eq. (22) of the main text in analogy to our analysis in the Quantum to Floquet crossover subsection under Results in the main text. However, in contrast to that part, we do not keep  $g^2 \Delta N_{\text{phot}}^{\text{pump}} = \text{const}$  while sending  $\Delta N_{\text{phot}}^{\text{pump}} \rightarrow \infty$  but set  $g = 0.5$ . Hence, we here do not perform the classical limit, since the light-matter hybridization is never lifted, but the limit of strong driving.

The result can be seen in Fig. 1 of this supplement. The side-peaks are at a shifted frequency  $\tilde{\omega}$  which reflects the fact that the effective boson of the system represents a mixture of light and matter degrees of freedom. In contrast to the classical limit, their position stays approximately constant and does not reduce to  $\omega_0$  for stronger pumping. At the same time, the evolution of completely asymmetric side-peaks to fully symmetric ones prevails. The strength of the peaks increases monotonically with stronger pumping while it stayed almost constant previously.

The last line corresponding to the strongest pump is again compared to the non-equilibrium spectral function obtained from a classically driven system according to Eq.(24) of the main text. We set the frequency to  $\tilde{\omega}$  as stated in Eq. (10). The result matches well with that of the strongest drive. For even larger numbers of photons injected into the system one will, however, start to see deviations as the higher, non-harmonic terms in the Hamiltonian become relevant for the dynamics.



Supplementary Figure 1. **Strong pumping limit of the non-equilibrium spectral function.** Non-equilibrium spectral function obtained according to Eq. (22) in analogy to Fig. 3(b) of the main text. The LMC is kept constant at  $g = 0.5$  while the strength of the pump increases from zero to  $\Delta N_{\text{phot}}^{\text{pump}} = 30$  as reported on the right-hand side of the plot. The spectral function corresponding to the strongest pump is overlaid with the non-equilibrium spectral function of the classically driven system (Eq. (24)) at the effective cavity frequency  $\tilde{\omega}$  as stated in Eq. (10). In analogy to Fig. 3(b) of the main text, the structure of the peaks changes from completely asymmetric to symmetric for increased pumping. In contrast to Fig. 3(b), the size of the side-peaks now increases for stronger pumping. Additionally, features that were previously small in the TD limit (see Eq. (18)) now emerge as for example the dynamical localization (shift of central peak) and the shake-off bands (also a second shake-off band is now visible). These features are well reproduced within the classical drive. Parameters, if not specifically mentioned otherwise, are as in Fig. 3(b) but with an increased size of the bosonic Hilbertspace of  $N_{\text{max}}^{\text{boson}} = 130$ .

As expected, features of the electronic spectral function that were previously small in the TD limit (see Eq. (18) of the main text) are enhanced through the driving. The dynamical localization now becomes notable through the shift of the central peak and a second shake-off band appears. These features are also well reproduced by the classical drive in this regime.

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