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Floquet Scattering Theory based on Effective Hamiltonians of Driven Systems

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The design of *time-independent effective Hamiltonians* that describe periodically modulated systems, provides a promising approach to realize new forms of matter. This, so-called, Floquet engineering approach is currently limited to the description of wavepacket dynamics. Here, we utilize the notion of effective Hamiltonians and develop a Floquet engineering scattering formalism that relies on a systematic high-frequency expansion of the scattering matrix. The method unveils the critical role of micromotion. An application to the case of non-reciprocal transport is presented.

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Introduction – The design of periodically driven schemes and their implementation to various physical systems has attracted the attention of the research community during the last decade [1-3]. The interest in this activity, coined *Floquet engineering*, is twofold: from the fundamental side one hopes that these new developments will allow for the realization of novel phenomena and forms of matter which are currently out of reach when using conventional (material development-based) approaches. Examples include systems with dynamical localization [4–9], topologically nontrivial phases [10, 11], quantum phase transitions [12, 13], artificial gauge potentials [3, 14], edge states [15, 16] etc. From the technological side, the hope is that these advances can be utilized towards the development of novel devices that will provide unprecedented control of information carried over by a variety of systems, ranging from optical, microwave, and acoustic to matter waves and quantum electronic framework. This enthusiasm is further backed up by the fact that the properties of a Floquet system are reconfigurable and can be changed on demand by altering the external driving field – a feature that is absent from any "time-independent" system whose physical properties are fixed during the fabrication process.

The cornerstone concept in the Floquet engineering approach is associated with the notion of effective (Floquet) Hamiltonian $H_{\rm F}$. The latter is *time-independent* and allows us to describe the evolution of the original periodically driven system $H_0(t+T) = H_0(t)$ in a stroboscopic manner. In other words, the evolution of the driven system is given by $\hat{U}(t_2, t_1) = \hat{U}_F(t_2) e^{-i(t_2 - t_1)\hat{H}_F} \hat{U}_F^{\dagger}(t_1)$ where $\hat{U}_F(t) = \hat{U}_F(t+T)$ encodes the dynamics taking place within each period T of the drive, the so-called micromotion. The prerequisite for Floquet engineering is that \hat{H}_F can be designed by suitably tailoring the driving protocol [1, 14, 17–19]. Of course, the implicit assumption is that one can theoretically calculate the effective Hamiltonian (as well as the micromotion operator) associated with the specific driving scheme. In general, this is a formidable task. There are, however, experimentally

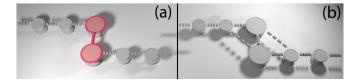


FIG. 1: (a) A schematic of a Floquet two-level system (two coupled resonators- red color) coupled to two semi-infinite leads. The resonance frequency, and the mutual coupling of the (red) resonators, can be periodically modulated in time; (b) The same system can be described effectively as two time-independent resonators for which the on-site potential, their mutual coupling and their coupling to the leads are now altered by the periodic drive. This system, in the scattering framework, is now described by an effective time-independent Hamiltonian \hat{H}_F . Note that up to order $O(1/\omega^2)$ the alteration of the coupling with the leads is solely dictated by the micromotion.

relevant circumstances where \hat{H}_F (and also $\hat{U}_F(t)$) can be computed in the form of an inverse-frequency expansion [14, 17, 19] and takes a simple form that allows for a clear interpretation. In this fast driving regime, in which the driving frequency is larger than any natural energy scale in the problem, the slow degrees of freedom are not coupled resonantly with the drive. Instead, the system typically feels an effective static potential that depends on the amplitude and frequency of the drive and which can be described by \hat{H}_F . Experimental implementation of this scheme includes, dynamical trapping of Paul traps [20] and dynamical localization [5–7], to artificial gauge fields for neutral atoms [21–23], nontrivial topological band structures [24] and quantum phase (superfluid-to-Mott) transitions [12, 13, 25]. It is important to point out that all the existing studies on Floquet engineering are mainly concerned with the so-called wavepacket dynamics scenario (i.e. the spreading of an excitation). It turns out that all these studies highlight the importance of H_F , while the micromotion $U_F(t)$ appears to play a secondary (if at all) role in the description of the dynamics.

Besides all this activity, however, not much has been done for the implementation of the effective (Floquet) Hamiltonian notion within the scattering framework. This is quite surprising since the latter is the appropriate formalism for the analysis of the transport properties of a system. In this paper, we undertake this task and develop a *Floquet engineering scattering theory based* on effective Hamiltonians of periodically driven systems. Specifically we develop a systematic high-frequency expansion of the Floquet scattering matrix, which unveils the important role of micromotion in modifying the coupling of the system to the leads. We demonstrate the efficiency of our scheme, by utilizing it for the design of periodic driving protocols that aim to enhanced (optimized) non-reciprocal transport (NRT).

Theoretical Formalism–We consider a Floquet system described by a finite-dimensional $N_s \times N_s$ time-periodic Hamiltonian $\hat{H}(t) = \hat{H}(t+T)$ ($T \equiv 2\pi/\omega$ is the period of the drive and ω is its frequency),

$$\hat{H}(t) = \hat{H}_0(t) - i\hat{\Gamma}; \quad \hat{\Gamma} = \gamma I_{N_s}, \quad (1)$$

where $\hat{H}_0(t)$ is a $N_s \times N_s$ hermitian matrix, $-i\hat{\Gamma}$ describes the uniform losses in the system and I_N (with an arbitrary subscript N) denotes the $N \times N$ identity matrix. For example, in the context of the coupled mode theory, the Hamiltonian $\hat{H}(t)$ could describe a network of coupled single-mode resonators (sites) with uniform losses γ , whose resonant frequencies and couplings are modulated periodically in time, see Fig. 1a. We turn the system of Eq. (1) to a scattering set-up by attaching to it two static semi-infinite leads $\alpha = L, R$, each of which is supporting plane waves with a dispersion relation E(k).

For periodic driving, the Floquet theorem assures that when an incident wave with frequency $E_0 = E(k_0)$ is approaching the time-periodic modulated target, it will scatter to infinite number of outgoing channels (including evanescent channels) with frequencies $E_n(k_n) = E_0 + n\omega$ where n is an integer. We are interested in the scattering matrix S, which connects only the propagating incoming and outgoing channels. Following the derivation in Ref. [26], we can calculate the flux-normalized $2N_p \times 2N_p$ scattering matrix S where N_p is the number of propagating channels in each lead. We have

$$\mathcal{S} = -I_{2N_p} + \imath W \frac{1}{E_0 + \imath \gamma - H_Q + \Lambda_H + \frac{\imath}{2} W^T W} W^T$$
(2)

where $H_Q = H_Q^0 - [n\omega I_{N_s}]$ is the quasi-energy operator in the extended Floquet-Hilbert space, with the matrix component $(H_Q^0)_{ns,n's'} = \hat{H}_{ss'}^{(n-n')} \equiv \frac{1}{T} \int_0^T dt \left(\hat{H}_0(t)\right)_{ss'} e^{i(n-n')\omega t}$. The subindex $s = 1, \cdots, N_s$ indicates the s-site of the time-periodic system. The notation $[X_n]$ denotes an infinite block diagonal matrix with each diagonal block being a submatrix X_n (the integer n runs from $-\infty$ to $+\infty$). The hermitian operator $\Lambda_H = W_c^T [\Lambda_n I_2] W_c$ describes the channel-coupling induced renormalization for the "Hamiltonian" H_Q in the extended Floquet-Hilbert space. Here the matrix elements Λ_n distinguish between propagating and evanescent channels. Furthermore the operator $(W_c)_{n\alpha,n's} =$ $c_{\alpha}\delta_{nn'}\delta_{\alpha\leftrightarrow s}$ describes the coupling between the channels and the sites of the driven system in the Floquet-Hilbert space, where c_{α} is the bare coupling between the lead α and the sites of the system, and we define $\delta_{\alpha\leftrightarrow s} = 1$ when the lead α is directly coupled with the site s and $\delta_{\alpha \leftrightarrow s} = 0$ otherwise. Finally $(W)_{n_P\alpha,n's} = \sqrt{v_{g,n_P}} c_\alpha \delta_{n_Pn'} \delta_{\alpha\leftrightarrow s}$ describes the coupling of the propagating channels with the driven system in the extended space. The integer n_P labels only the propagating channels and v_{q,n_P} = $\partial E/\partial k|_{k_{n_{P}}}$ represents the group velocity in each of these channels.

We proceed with the high-frequency analysis of the scattering matrix Eq. (2). Our goal is to incorporate the effective Hamiltonian \hat{H}_F in the Floquet scattering framework. Indeed, \hat{H}_F is closely connected with the quasi-energy operator H_Q as [19]

$$U_F^{\dagger} H_Q U_F = \left[\hat{H}_F \right] - \left[n \omega I_{N_s} \right], U_F^{\dagger} U_F = \left[I_{N_s} \right], \qquad (3)$$

where the sub-blocks $\hat{u}_{n-n'} \equiv (U_F)_{n,n'}$ of the unitary matrix U_F are related to the one-point micromotion operator $\hat{U}_F(t)$ as $\hat{u}_n = \frac{1}{T} \int_0^T dt \hat{U}_F(t) e^{in\omega t}$. Therefore, U_F encodes the micromotion generated by $\hat{H}_0(t)$ or equivalently $\hat{H}(t)$ in the uniform-loss case. Note that in general, both the effective Hamiltonian \hat{H}_F and the matrix U_F are not uniquely defined. However, under the canonical van Vleck form of degenerate perturbation theory, they can be uniquely determined order by order with respect to $1/\omega$ in terms of the Fourier components $\hat{H}^{(n)}$ of the $\hat{H}_0(t)$, see Ref. [19] and [27]. We note that the off-diagonal blocks of U_F , i.e. $\hat{u}_{n\neq 0}$, have been found to be $\sim O(1/\omega)$ [19].

In the large driving-frequency limit, the number of the propagating channels in each lead reduce to one, i.e., $N_p = 1$. Using Eqs. (2) and (3), we can write the scattering matrix S in terms of the effective Hamiltonian \hat{H}_F as

$$S = -I_2 + \imath W^F G_s^F W^{F\dagger} \tag{4}$$

where $W^F = WU_F$ and

$$G_s^F = \frac{1}{\left[\left(E_n + i\gamma\right)I_2\right] - \left[\hat{H}_F\right] + U_F^{\dagger}\left(\Lambda_H + \frac{i}{2}W^TW\right)U_F}.$$
(5)

The difficulty of the analysis of the scattering matrix S mainly comes from the presence of the full matrix $U_F^{\dagger} \left(\Lambda_H + \frac{i}{2} W^T W \right) U_F$ in G_s^F . The above matrix can be

formally separated into a block-diagonal part $\begin{bmatrix} \hat{d}_n \end{bmatrix}$ and a block-off-diagonal matrix V, i.e.,

$$U_F^{\dagger} \left(\Lambda_H + \frac{i}{2} W^T W \right) U_F = \left[\hat{d}_n \right] + V \tag{6}$$

where $V_{n_1,n_2} = \hat{d}_{n_1,n_2}$ when $n_1 \neq n_2$ and $\hat{d}_n = \hat{d}_{n,n}$. The above decomposition Eq. (6) to a block-diagonal and a block off-diagonal matrices is inspired by a locator expansion method used in disordered systems [28]. Though, in the current situation, the locator is a matrix. Specifically, taking into account that $V \sim O(1/\omega)$, the matrix G_s^F can be expanded systematically as

$$G_s^F = -\left(g^F + g^F V g^F + \cdots\right),\tag{7}$$

where $g^F = [\hat{g}_n^F]$ and the "locator" is identified as $\hat{g}_n^F = -\left(E_n + i\gamma - \hat{H}_F + \hat{d}_n\right)^{-1}$. Notice that for $n \neq 0$ the locator is of order $g_{n\neq 0}^F \sim O(1/\omega)$.

Our final step involves the expansion of $W^F = WU_F$ (specifically of U_F) in powers of $1/\omega$ and its substitution, together with Eq. (7), into the expression of the *S*-matrix Eq. (4). In this way, a systematic high-frequency expansion for the scattering matrix S can be readily derived.

Next, let us consider a scenario for which $\Lambda_{n\neq0} \sim O(1/\omega)$. This is a typical situation due to the diminishing coupling between the driving system and the evanescent channels $E_{n\neq0}$. Up to order $O(1/\omega^2)$, we can write the scattering matrix S in Eq. (4) as

$$S \approx -I_2 + i\hat{c}\hat{u}_0 \frac{v_{g,0}}{E_0 + i\gamma - \hat{H}_F + \hat{u}_0^{\dagger}\hat{c}^{\dagger} \left(\Lambda_0 + i\frac{v_{g,0}}{2}\right)\hat{c}\hat{u}_0} \hat{u}_0^{\dagger}\hat{c}^{\dagger},$$
(8)

where $(\hat{c})_{\alpha s} = c_{\alpha} \delta_{\alpha \leftrightarrow s}$, $\hat{H}_F = \hat{H}_F^{\dagger} \approx \hat{F}_0 + \frac{1}{\omega} \hat{F}_1 + \frac{1}{\omega^2} \hat{F}_2$ and $\hat{u}_0 \approx I_2 + \frac{1}{\omega^2} \hat{b}_2$. The operators \hat{F}_n appearing above are

$$\hat{F}_0 = \hat{H}^{(0)}, \quad \hat{F}_1 = -\sum_{m=1}^{\infty} \frac{1}{m} \left[\hat{H}^{(m)}, \hat{H}^{(-m)} \right], \quad (9)$$

$$\hat{F}_{2} = \sum_{m \neq 0} \frac{\left[\hat{H}^{(-m)}, \left[\hat{H}^{(0)}, \hat{H}^{(m)}\right]\right]}{2m^{2}} + \sum_{m \neq 0} \sum_{m' \neq 0, m} \frac{\left[\hat{H}^{(-m')}, \left[\hat{H}^{(m'-m)}, \hat{H}^{(m)}\right]\right]}{3mm'}$$

and $\hat{b}_2 = -\frac{1}{2} \sum_{m \neq 0} \frac{1}{m^2} \hat{H}^{(-m)} \hat{H}^{(m)}$ [29]. From Eq. (8) we see clearly that the micromotion via \hat{u}_0 is modifying the coupling of the driven system to the leads, see for example Fig. 1b. Notice that the scattering matrix S in Eq. (8) is independent of the driving phase, i.e., S is invariant when $\hat{H}(t) \rightarrow \hat{H}(t-t_0)$. This property is guaranteed by the structure of both \hat{H}_F and \hat{u}_0 , which involve only the matrix products $\hat{H}^{(m_1)}\hat{H}^{(m_2)}\dots\hat{H}^{(m_p)}$

with $m_1 + m_2 + \cdots + m_p = 0$. Generally, the leading correction of the micromotion to the Floquet scattering problem is $\mathcal{O}(1/\omega^2)$. This is the same order where novel topological properties of \hat{H}_F of the closed system typically manifest themselves. The correct implementation of \hat{H}_F in the scattering framework (where the micromotion is taken into account) is crucial in order to avoid any misinterpretations.

For example, in the case of a tight-binding lead with dispersion relation $E(k) = -2\cos(k)$ (in units of coupling), Eq. (8) applies with $v_{g,0} = 2\sin(k_0)$. In this case $\Lambda_n = \cos(k_n), k_n \in (0, \pi)$ for the propagating channels $E_n \in (-2, 2)$ and $\Lambda_n = e^{ik_n} \sim O(1/\omega), \mathcal{I}m(k_n) > 0$ for the evanescent channels $E_n \notin (-2, 2)$. Therefore we have that $\hat{d}_{n_1,n_2} = \sum_n \hat{u}_{n-n_1}^{\dagger} \hat{c}^{\dagger} e^{ik_n} \hat{c} \hat{u}_{n-n_2}$ (see Eq. (6)). Application: Design of driving schemes for enhanced

Application: Design of driving schemes for enhanced NRT – Let us now implement the above formalism for the Floquet design of driving schemes that can lead to Non-Recirpocal Transport (NRT). We will confine our analysis to the high-frequency limit where Eq. (8) is applicable. The corresponding physical requirement is that the driving amplitudes are small compared with the driving frequency ω . Furthermore, we will consider that the scattering target is having uniform losses of strength γ . In this case, the scattering matrix S is not unitary i.e. $I_2 - S^{\dagger}S = \gamma Z$ where $Z = Z^{\dagger}$ is the absorption matrix. We remark, parenthetically, that one can utilize this framework in order to design driving schemes that lead to a broadband absorption [30].

We proceed with the evaluation of the left/right transmittance difference $\Delta \equiv T_{L \to R} - T_{R \to L}$, where $T_{L \to R} = |t_L|^2$ represents the transmittance from left to right lead for the propagating channel E_0 (and similarly for $T_{R \to L} = |t_R|^2$). We get

$$\Delta = \gamma \operatorname{Tr} \left(Z \begin{pmatrix} t_R & 0\\ 0 & t_L \end{pmatrix} S^* \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix} \right), S = \begin{pmatrix} r_L & t_R\\ t_L & r_R \end{pmatrix}.$$
(10)

Equation (10) applies to any periodically driven system coupled to two propagating channels. We point out that Eq. (10) implies that the transmittance asymmetry and thus NRT will be absent without material loss i.e., $\gamma = 0$. Indeed, this fact is the direct result of a 2×2 unitary scattering matrix. Further substitution of the expression Eq. (8) for the scattering matrix into Eq. (10) will allow us to optimize the driving scheme that will lead to maximum NRT.

Let us consider, for demonstration purposes, the example case of a simple two-mode Floquet system corresponding to $N_s = 2$. We will further assume that the Floquet system is coupled to two tight-binding leads. In this situation the bare coupling matrix takes the form $\hat{c} = \begin{pmatrix} c_L & 0 \\ 0 & c_R \end{pmatrix}$. For simplicity, we assume that $c_L = c_R = -1$ and the static part of $\hat{H}_0(t)$ is $\hat{F}_0 = \begin{pmatrix} 0 & h_0 \\ h_0 & 0 \end{pmatrix}$, $h_0 \in \mathcal{R}$.

Under this simplification, the parametrization $\hat{b}_2 = \hat{b}_2^{\dagger} = \begin{pmatrix} \beta_1 & \beta_r + i\beta_i \\ \beta_r - i\beta_i & \beta_2 \end{pmatrix}$ together with Eqs. (8) and (10) enable us to obtain the transmittance difference Δ up to the order $O(1/\omega^2)$ explicitly

$$\Delta \approx \frac{(32h_0\beta_i\gamma\sin^2 k_0)/\omega^2}{4(\gamma + \sin k_0)^2\cos^2 k_0 + (h_0^2 - \cos^2 k_0 + (\gamma + \sin k_0)^2)}$$
(11)

From Eq. (11) we conclude that in this case, the leading order of NRT in the high-frequency limit is associated with the presence of micromotion and it is $O(1/\omega^2)$. In fact, this estimation can be derived directly from Eq. (8), for a generic (i.e. arbitrary $\hat{F}_0 = \hat{F}_0^{\dagger}$ and c_L, c_R) twomode Floquet system. This result stresses the importance of the micromotion in the scattering framework – its overlook can lead to qualitatively wrong conclusions, as the example case of non-reciprocal transport indicates.

We proceed with the Floquet engineering design of NRT, under the constraint that the driving scheme involves only a first-harmonic i.e.

$$\hat{H}_{0}(t) = \begin{pmatrix} \varepsilon_{L}(t) & h(t) \\ h^{*}(t) & \varepsilon_{R}(t) \end{pmatrix}$$
(12)

where $\varepsilon_{L/R}(t) = 2f_{L/R}\cos(\omega t + \phi_{L/R})$ and $h(t) = h_0 + h_1 \exp(\imath\omega t + \imath\phi_1) + h_2 \exp(-\imath\omega t - \imath\phi_2)$. Without loss of generality, we set $\phi_L = 0$ (we can always choose the driving phase properly to eliminate ϕ_L without affecting NRT). In this respect, our goal is to maximize the transmittance difference Δ by choosing the proper *relative* driving phases, i.e., ϕ_R , ϕ_1 and ϕ_2 when $\phi_L = 0$. Therefore the problem boils down to the study of β_i appearing in Eq. (11). We get

$$\beta_{i} = \frac{1}{2} \Big(-f_{L}h_{1}\sin\phi_{1} + f_{L}h_{2}\sin\phi_{2} \\ -f_{R}h_{1}\sin(\phi_{1} - \phi_{R}) + f_{R}h_{2}\sin(\phi_{2} - \phi_{R}) \Big).$$
(13)

From Eqs. (11,13) we find that in case of real-valued coupling $h(t) \in R$ that involves only a first-harmonic driving associated with the example of Eq. (12), the transmittance asymmetry cannot be stronger than $O(1/\omega^3)$. On the other hand, when the coupling is assumed to take complex values, we have that $\max\{\beta_i\} = \frac{1}{2}(f_Lh_1 + f_Lh_2 + f_Rh_1 + f_Rh_2)$ occurs when $\phi_R = 0$, $\phi_2 = -\phi_1 = \pi/2$, thus resulting in an optimized NRT.

In Fig. 2a, we present the numerical (lines) results for the left $(T_{L\to R})$ and right $(T_{R\to L})$ transmittance versus the frequency of an incident wave for the Floquet system of Eq. (12). In our simulations we have used high values of the driving frequency $\omega = 6$ and the optimized values of the relative driving phases which we have find to be $\phi_L = \phi_R = 0$ and $\phi_2 = -\phi_1 = \pi/2$. At the same figure we also present the theoretical (symbols) results

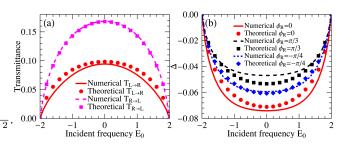


FIG. 2: The analysis of transport properties of the specific two-mode Floquet system defined in Eq. (12). (a) Numerical and theoretical calculation of $T_{L \to R}$ $(T_{R \to L})$ for the transmittances from the left (right) to right (left) lead versus the incident frequency E_0 in the case of the optimized phase when $\phi_L = \phi_R = 0$ and $\phi_2 = -\phi_1 = \pi/2$. Theoretical calculation refers to the application of Eq. (8) while the numerical rigorous results come from Eq. (2) and the convergence was tested by increasing the Floquet lattice. (b) The transmittance difference Δ versus the incident frequency E_0 for various different relative driving phases $\phi_R = 0, \pi/3$ and $-\pi/4$ when $\phi_L = 0$ and $\phi_2 = -\phi_1 = \pi/2$. Theoretical results come from the explicit formula Eq. (11) with β_i given in Eq. (13). Clearly the optimized phase $\phi_R = 0$ presents a relatively large magnitude of the transmittance difference $|\Delta|$. The other common parameters for the calculation of both (a) and (b) are: the bare coupling between the leads and the Floquet system $c_L = c_R = -1$, the static coupling between the two modes $h_0 = -1$, the driving amplitudes $f_L = f_R = h_1 = h_2 = 1$ and the uniform loss strength $\gamma = 1$ and the driving frequency $\omega = 6.$

for $T_{L\to R}$ and $T_{R\to L}$ which are based on Eq. (8). Finally in Fig. 2b we show the theoretical (symbols) and numerical (lines) transmittance difference Δ for various values of the relative driving phases ϕ_R . The maximum magnitude of the transmittance difference is observed for $\phi_R = 0$ as predicted by our theoretical analysis.

Conclusions – We have developed a scattering Floquet engineering approach which is applicable in the high driving-frequency limit. The method utilizes the notion of the effective (Floquet) Hamiltonian which have been recently developed in the framework of wavepacket dynamics of Floquet systems. The approach highlights the importance of micromotion in the scattering framework and allows us to design driving schemes with predefined transport characteristics. We have demonstrated the validity of our scheme by applying it to the case of nonreciprocal transport associated with a two-site periodically modulated target with uniform losses and a firstharmonic time-periodic modulation. We furthermore find that the transmittance asymmetry is proportional to $O(1/\omega^2)$ for any two-site Floquet-system with uniform loss. It will be interesting to utilize the scattering Floquet engineering approach in order to identify periodically modulated scattering geometries for which the nonreciprocity will be of order $O(1/\omega)$. A promising direction along this lines is the investigation of modulated targets with spatio-temporal symmetries (like parity-time

symmetry) [30, 31].

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