

Floquet physics

Periodic driving, formalism, and spectroscopy

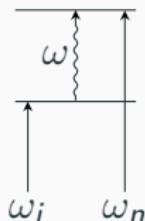
Jinyuan Wu

December 12, 2023

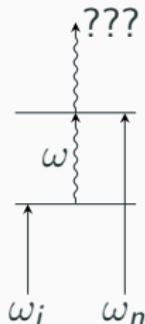
Introduction

Time-dependent perturbation theory, $\omega_{\text{eg}} + \omega$

\Rightarrow Fermi golden rule (finite wave packet or not)



What happens when we consider high order perturbations?



Inherently non-equilibrium The state of photons is a coherent state: $|\Psi\rangle$ far from any eigenstate!

Overview

- Floquet quasienergies and quasi-stationary states
- Relation with time-dependent perturbation theory and rotating wave approximation (RWA)?
- Floquet correction to ARPES

The Floquet formalism

Quasi-stationary states and quasienergies

Periodically driven Hamiltonian: quasi-eigensystem

Floquet theory $H(t) = H(t + T) \Rightarrow$ for every $|\psi(t)\rangle$,

$$|\psi(t)\rangle = \sum_n c_n \underbrace{|\psi_n(t)\rangle}_{\text{quasi-stationary basis}}, \quad |\psi_n(t)\rangle = e^{-i\varepsilon_n t/\hbar} \underbrace{|\Phi_n(t)\rangle}_{\text{period is } T},$$

- Time evolution of arbitrary states $\Leftrightarrow \{|\psi_n(t)\rangle\}$
- $\{\psi_n(t)\}$: **quasi-stationary states**
- $\{\varepsilon_n\}$: **quasienergies** (c.f. crystal momentum)

Our task How to find $\{\psi_n(t)\}$ and $\{\varepsilon_n\}$?

$$|\Phi_n(t)\rangle = \underbrace{\sum_m e^{-i m \omega t}}_{\text{discrete Fourier series}} |\phi_n^{(m)}\rangle, \quad \omega = 2\pi/T.$$

Floquet effective Hamiltonian

Our task A Hamiltonian for $\{\phi_n^{(m)}\}$ and $\{\varepsilon_n\}$?

$$\begin{aligned} & \underbrace{H(t)}_{=: \sum_m e^{-i m \omega t} H^{(m)}} | \psi_n(t) \rangle = i \hbar \partial_t | \psi_n(t) \rangle = \varepsilon_n + i \hbar \partial_t | \Phi_n(t) \rangle \\ \Rightarrow & \sum_{m'} H^{(m-m')} | \phi_n^{(m')} \rangle = (\varepsilon_n + m \hbar \omega) | \phi_n^{(m)} \rangle \end{aligned}$$

Floquet effective Hamiltonian

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$$\Rightarrow \boxed{\varepsilon_n |\phi_n^{(m)}\rangle = \sum_{m'} (H^{(m-m')} - m \hbar \omega \delta_{mm'}) |\phi_n^{(m')}\rangle}.$$

Floquet effective Hamiltonian Indeed we have a Hamiltonian!!

Floquet effective Hamiltonian

$\varepsilon_n, (\dots, |\phi_n^{(-1)}\rangle, |\phi_n^{(0)}\rangle, |\phi_n^{(1)}\rangle, \dots)$ are obtained by diagonalizing

$$m' = -2 \quad m' = -1 \quad m' = 0 \quad m' = 1$$

$$\begin{array}{c} \\ \\ \\ \end{array} \left(\begin{array}{cccc} & & \vdots & \vdots \\ H^{(0)} + 2\hbar\omega & H^{(-1)} & H^{(-2)} & H^{(-3)} \\ \dots & H^{(1)} & H^{(0)} + \hbar\omega & H^{(-1)} & H^{(-2)} & \dots \\ \dots & H^{(2)} & H^{(1)} & H^{(0)} & H^{(-1)} & \dots \\ \dots & H^{(3)} & H^{(2)} & H^{(1)} & H^{(0)} - \hbar\omega & \\ & \vdots & \vdots & & & \end{array} \right) \begin{array}{c} \\ \\ \\ \end{array}$$

- Each “element” is a matrix on \mathcal{H}
- $H^{(0)}$: H without driving; $H^{(m)}$: driving with frequency $m\omega$
- H^{Floquet} is on the extended Hilbert space

$$\mathcal{H} \otimes \{m = \dots, -1, 0, 1, \dots\}$$

Floquet Brillouin zone

Redundancy in H^{Floquet} The number of independent quasienergies is not really multiplied by Floquet subspaces.

$$e^{-i(\varepsilon_n - m\hbar\omega)t} \underbrace{e^{i m \hbar \omega t} |\Phi_n(t)\rangle}_{\text{still periodic!}}$$

So only *one* energy Brillouin zone is needed.

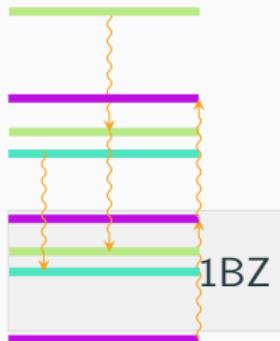
The number of independent quasi-stationary states = $\dim \mathcal{H}$

But all $\phi_n^{(m)}$ are all needed to decide $|\psi_n(t)\rangle$.

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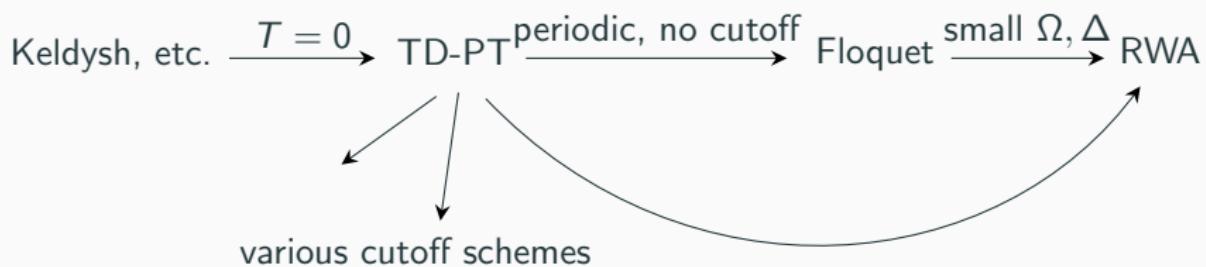
Floquet formalism in eyes of other formalisms

“full” Floquet theory, perturbation theory, and RWA

Floquet formalism in hierarchy of approximations

Other ways to describe periodic driving

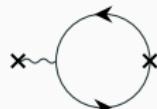
- Time-dependent perturbation theory (TD-PT)
- Rotating wave approximation (RWA)



Floquet formalism v.s. TD-PT

Response from time-dependent perturbation theory = response from $T = 0$ Feynman diagrams.

Example: first-order PT = Lindhard response function

$$\langle \mu^{(1)} \rangle = \mu_{\text{eg}} \underbrace{\Omega}_{\text{Rabi freq.}} \left(\frac{\Omega}{\omega_{\text{eg}} - \omega} e^{-i\omega t} + \frac{\Omega}{\omega_{\text{eg}} + \omega} e^{i\omega t} + \text{h.c.} \right) = \text{Diagram}$$


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And when we sum over all of them...

$$\uparrow = \uparrow + \begin{array}{c} \uparrow \\ \diagdown \quad \diagup \\ \text{---} \end{array} + \begin{array}{c} \uparrow \\ \diagdown \quad \diagup \\ \text{---} \\ \diagdown \quad \diagup \\ \text{---} \end{array} + \dots$$

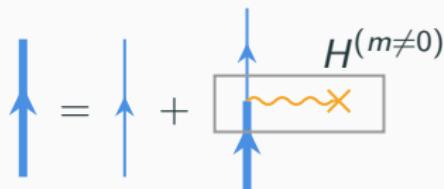
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H^{Floquet} is the non-equilibrium self-energy



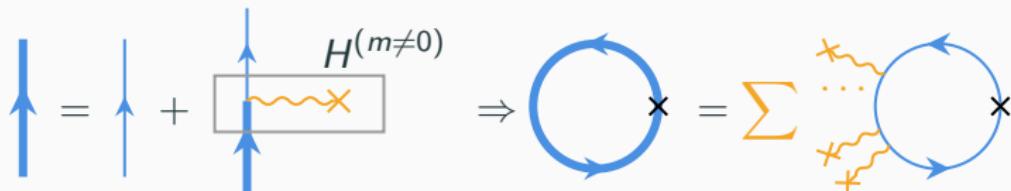
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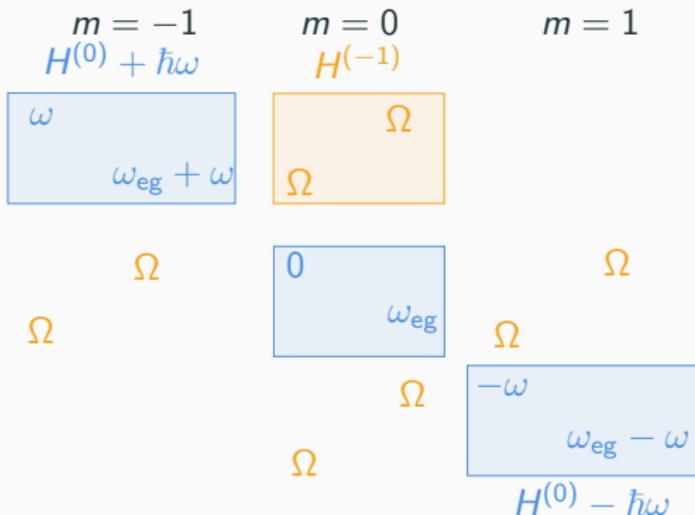
$$\langle \mu^{(1)} \rangle = \mu_{\text{eg}} \underbrace{\frac{\Omega}{\omega_{\text{eg}} - \omega}}_{\text{Rabi freq.}} \left(\frac{\Omega}{\omega_{\text{eg}} - \omega} e^{-i\omega t} + \frac{\Omega}{\omega_{\text{eg}} + \omega} e^{i\omega t} + \text{h.c.} \right) = \times \circlearrowleft \times$$

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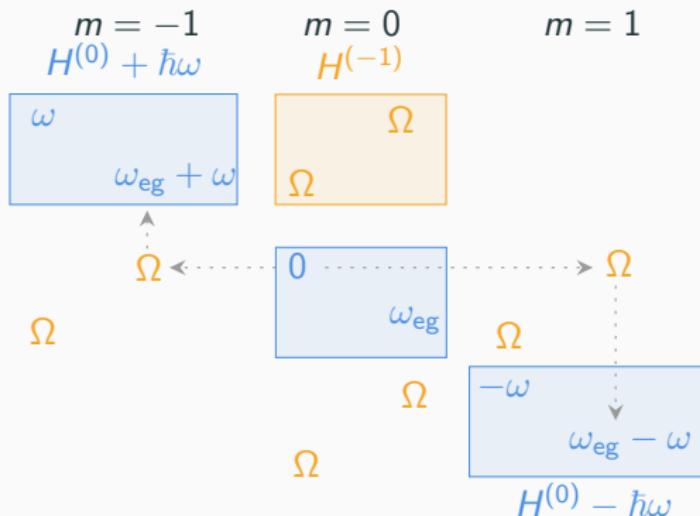
In the full H^{Floquet} , automatically all PT terms are considered!

Floquet formalism v.s. RWA



From Floquet to RWA

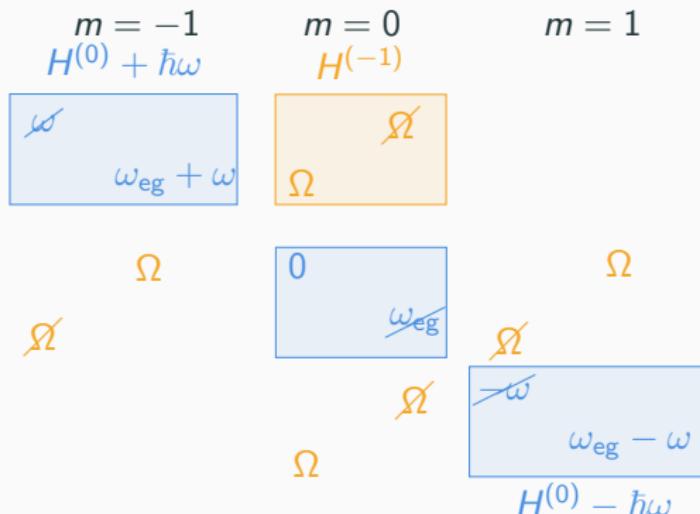
Floquet formalism v.s. RWA



From Floquet to RWA

- Small coupling: only first-order transitions from $|g\rangle$ matters

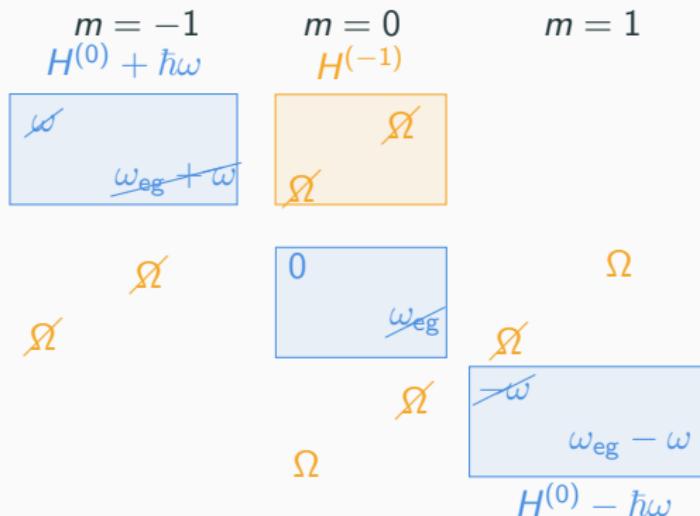
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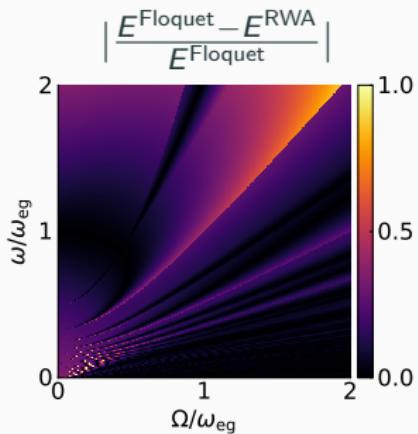


From Floquet to RWA

- Small coupling: only first-order transitions from $|g\rangle$ matters
- Near resonance: only the $m = 1$ $\omega_{\text{eg}} - \omega$ state matters

Floquet formalism v.s. RWA

$$H^{\text{RWA}} = \begin{pmatrix} 0 & \Omega \\ \Omega & \omega_{\text{eg}} - \omega \end{pmatrix}.$$



From Floquet to RWA

- Small coupling: only first-order transitions from $|g\rangle$ matters
- Near resonance: only the $m = 1$ $\omega_{\text{eg}} - \omega$ state matters

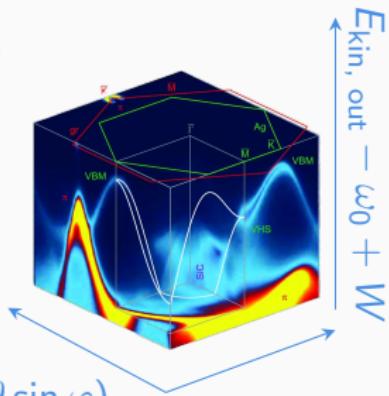
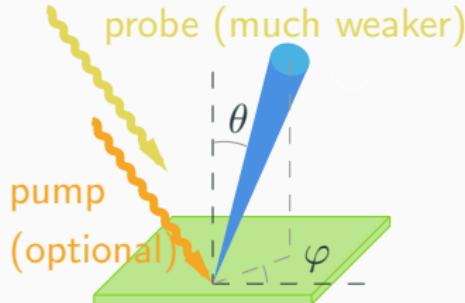
Indeed when $\Omega/\omega_{\text{eg}} \lesssim 0.5$, $\omega/\omega_{\text{eg}} \sim 1$, RWA works the best!

ARPES of Floquet systems

Are Floquet states “real” ?

Angle-resolved photoemission spectroscopy (ARPES)

ARPES sheds *probe* beam to material (possibly *pumped* by another beam) and detects output electrons' (\mathbf{k}, E)^a



^aFigure from Rosenzweig et al. 2022.

$$I_{\text{Chan et al. 2023}}(\mathbf{k}, \omega) \propto \underbrace{\int dt_1 \int dt_2 e^{i\omega(t_2-t_1)} |M_{\text{probe}}^{\text{dipole}}|^2 G_{\mathbf{k}}^{\text{pumped}, <}(t_2, t_1)}_{\text{generalized Fermi golden rule for probing}}$$

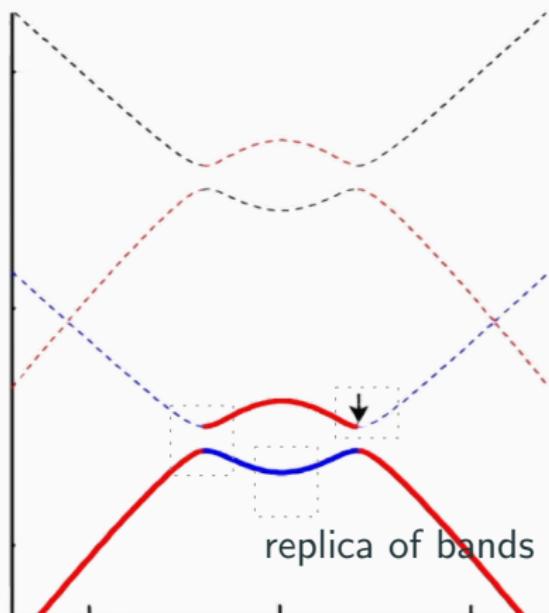
$$\Rightarrow I_{\text{Floquet}}(\mathbf{k}, \omega) \sim \sum_{n,m} |\phi_{n\mathbf{k}}^{(m)}|^2 \delta(\omega - \varepsilon_{n\mathbf{k}}).$$

ARPES for Floquet-driven electron bands

Three effects of Floquet correction to ARPES spectra

In the figure:^a

- Band replica:
 $H^{(0)} + m\hbar\omega$



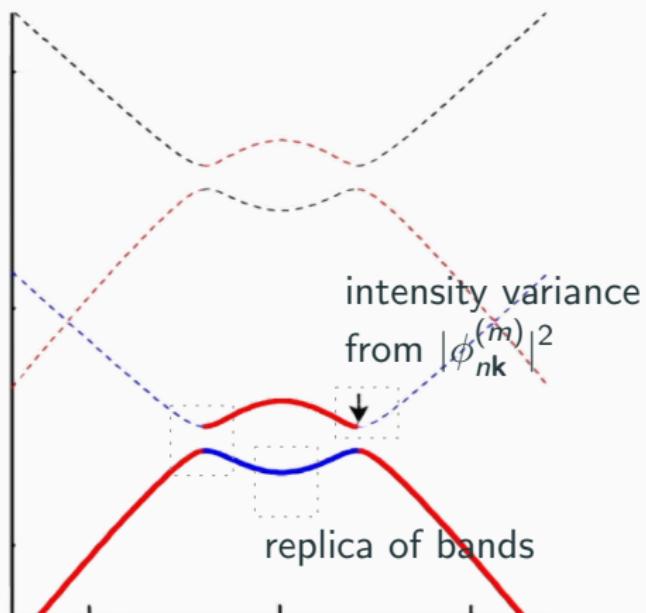
^aFigure from Zhou et al.
2023

ARPES for Floquet-driven electron bands

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- Band replica:
 $H^{(0)} + m\hbar\omega$
- Intensity peak:
 $|\phi_n^{(m)}|^2$



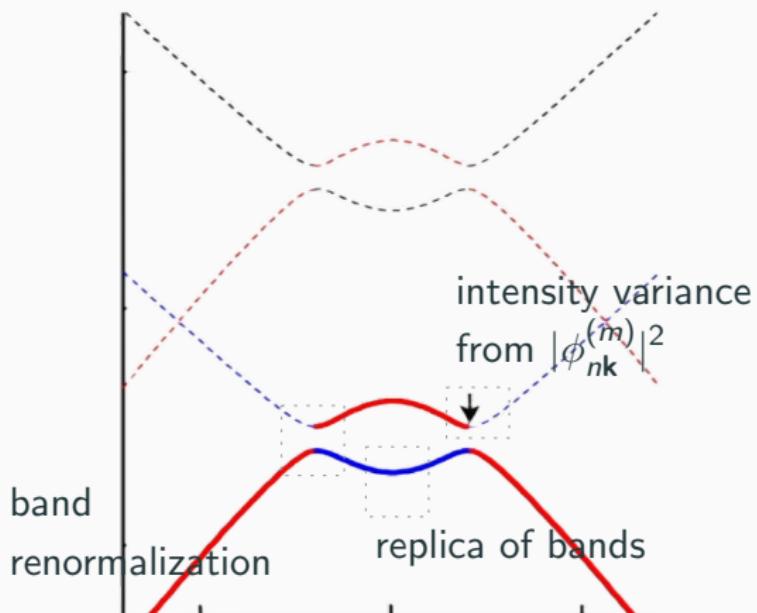
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ARPES for Floquet-driven electron bands

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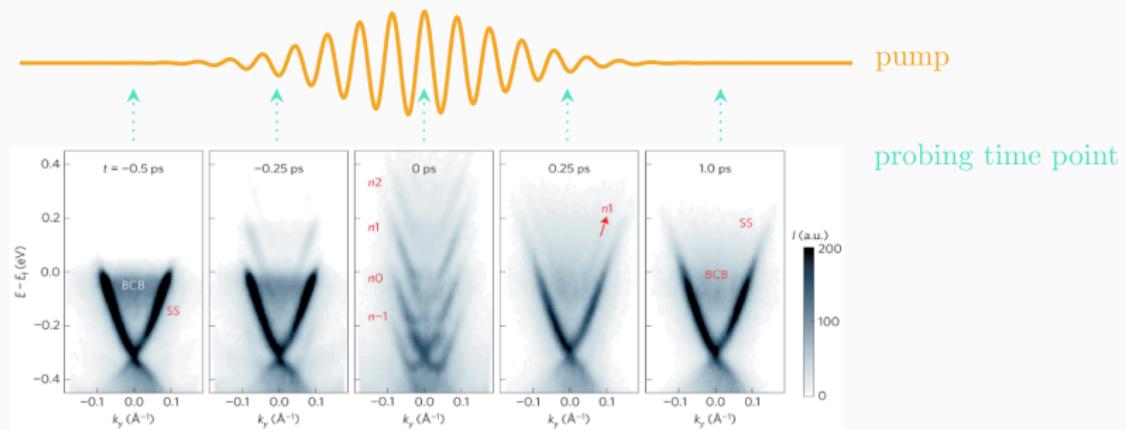
- Band replica:
 $H^{(0)} + m\hbar\omega$
- Intensity peak:
 $|{\phi}_n^{(m)}|^2$
- Band renormalization:
 $H^{(m \neq 0)}$



^aFigure from Zhou et al.
2023

ARPES for Floquet-driven electron bands

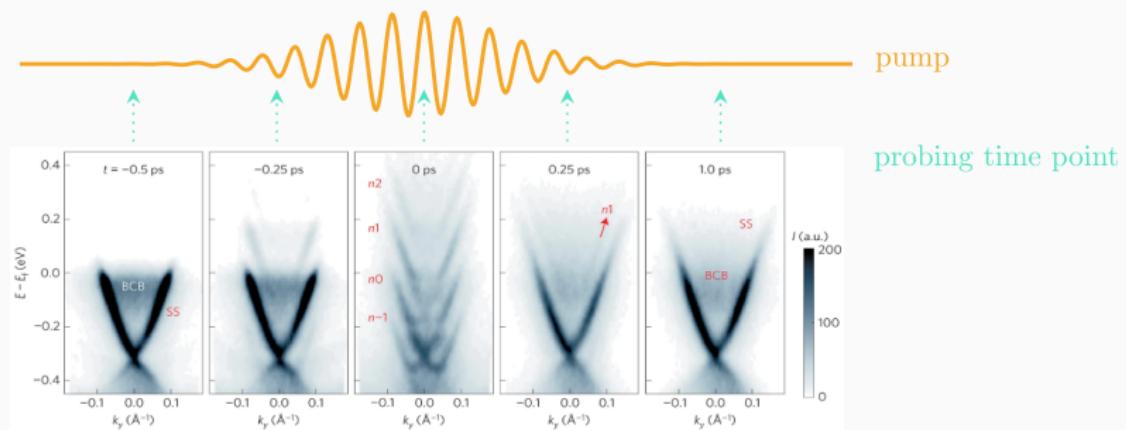
Probe at different stages of pump in topological insulator
(Mahmood et al. 2016)



Probe before the start of pump nothing happens to ARPES spectrum

ARPES for Floquet-driven electron bands

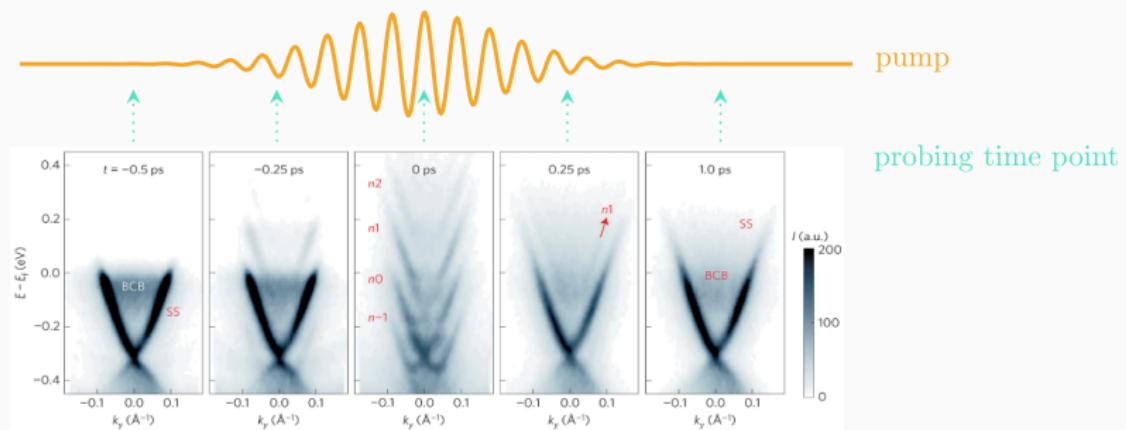
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Probe at the start of pump mild Floquet features

ARPES for Floquet-driven electron bands

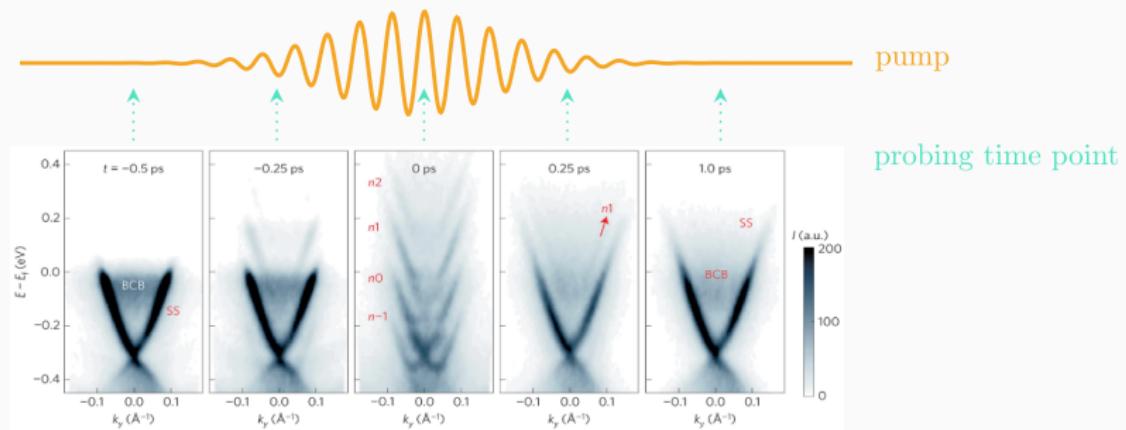
Probe at different stages of pump in topological insulator
(Mahmood et al. 2016)



Probe at the middle of pump Floquet

ARPES for Floquet-driven electron bands

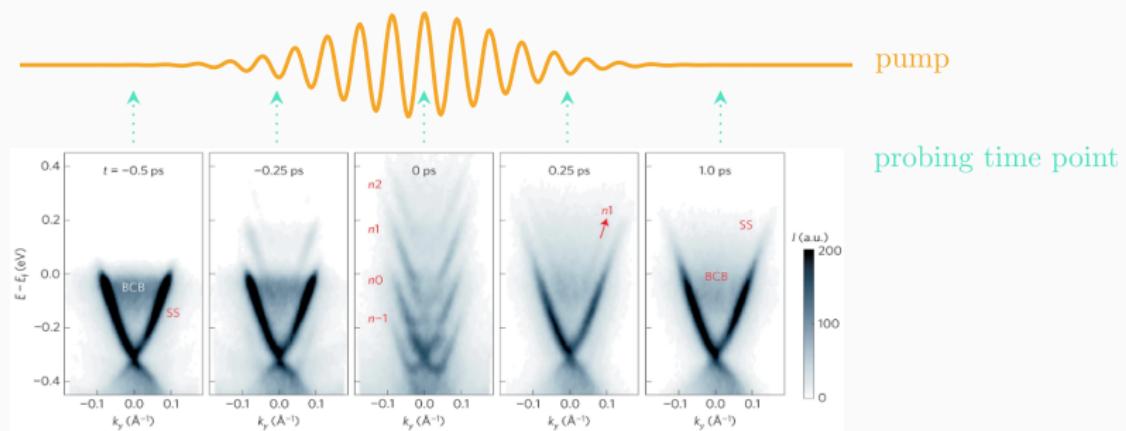
Probe at different stages of pump in topological insulator
(Mahmood et al. 2016)



Probe at the tail of pump mild Floquet features, plus signatures from usually unoccupied states

ARPES for Floquet-driven electron bands

Probe at different stages of pump in topological insulator
(Mahmood et al. 2016)

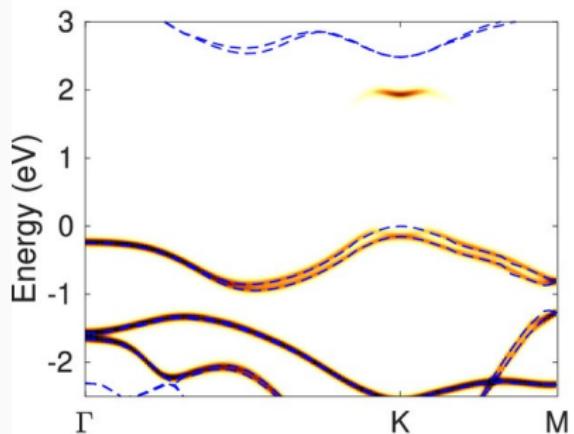


Probe after pump signatures from usually unoccupied states

Self-driven Floquet effect

Even after pump ends we may still see Floquet effects . . .

Floquet by exciton excited by pump – self-driven Floquet effects (Chan et al. 2023)



Dotted line: band structure without pumping

Discussion

- Floquet quasienergies and quasi-stationary states
- They are “resummation” of external field’s perturbation
- They can be seen!

References

-  Chan, Y.-H. et al. (2023). "Giant self-driven exciton-Floquet signatures in time-resolved photoemission spectroscopy of MoS₂ from time-dependent *GW* approach". In: *Proceedings of the National Academy of Sciences* 120.32, e2301957120.
-  Mahmood, Fahad et al. (2016). "Selective scattering between Floquet–Bloch and Volkov states in a topological insulator". In: *Nature Physics* 12.4, pp. 306–310.

References ii

-  Rosenzweig, Philipp et al. (2022). "Surface charge-transfer doping a quantum-confined silver monolayer beneath epitaxial graphene". In: *Physical Review B* 105.23, p. 235428.
-  Zhou, Shaohua et al. (2023). "Pseudospin-selective Floquet band engineering in black phosphorus". In: *Nature* 614.7946, pp. 75–80.