Moiré Polaritonic Fourier Engineering

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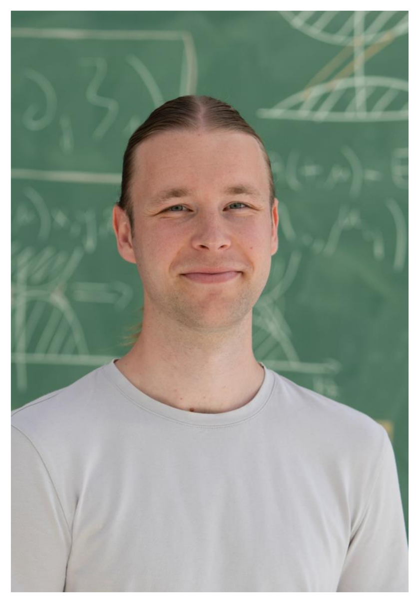

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Analytical model for dispersion calculation

Periodic dimensionless conductivity : $\alpha(\mathbf{r}) = \sum_{m,n} \alpha_{m,n} e^{i\mathbf{r}\cdot(m\mathbf{g_1}+n\mathbf{g_2})}$

- A lattice is created by the periodic variation of the conductivity.
- Different periodic variations of the conductivity can be combined to obtain a commensurate moiré lattice in a single lattice.

Bloch (plane wave) expansion : $\mathbf{E}(\mathbf{r}) = \sum_{m,n} t_{m,n} \begin{pmatrix} E_{x,(m,n)} \\ E_{y,(m,n)} \\ E_{z,(m,n)} \end{pmatrix} e^{i\mathbf{r}\cdot(\mathbf{k_t}+m\mathbf{g_1}+n\mathbf{g_2})}$

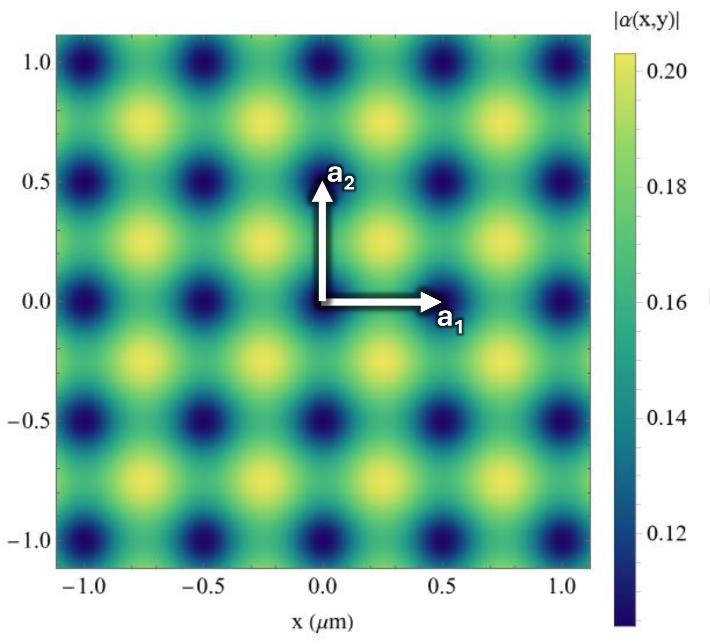
- When an electric field is applied, the lattice becomes a polaritonic crystal. The electric field of those polaritons can be expanded into Bloch waves.

Boundary conditions of Maxwell's equations : $\sum_M D_{NM}\, t_M = 2IY_0\delta_{N,0}$, $D_{NM} = 2\left[\delta_{N,M}Y_N + \alpha_{N-M}W_{N,M}\right]$

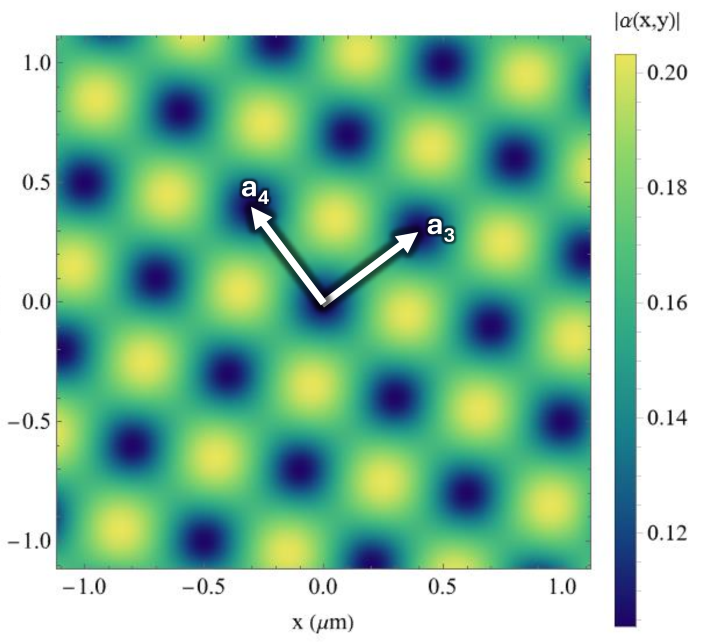
with $M = \{m,n\}$, $N = \{m',n'\}$, $Y_N = \frac{k_0}{\sqrt{k_0^2-(\mathbf{k_t}+m'\mathbf{g_1}+n'\mathbf{g_2})^2}}$ and $W_{N,M} = \frac{\mathbf{k_{tN}}\cdot\mathbf{k_{tM}}}{\|\mathbf{k_{tN}}\|\|\mathbf{k_{tM}}\|}$.

- k_0 is the momentum of the source and I the source amplitude.
- $\mathbf{k_t}$ is the momentum of the polaritons in the (x,y) plane and $\mathbf{k_{tM}} = \mathbf{k_t} + m\mathbf{g_1} + n\mathbf{g_2}$.
- By solving the boundary conditions of Maxwell's equations, we obtain a system of equations (encoded in matrix D) that allow us to compute the band structure of the polaritonic Fourier crystal.

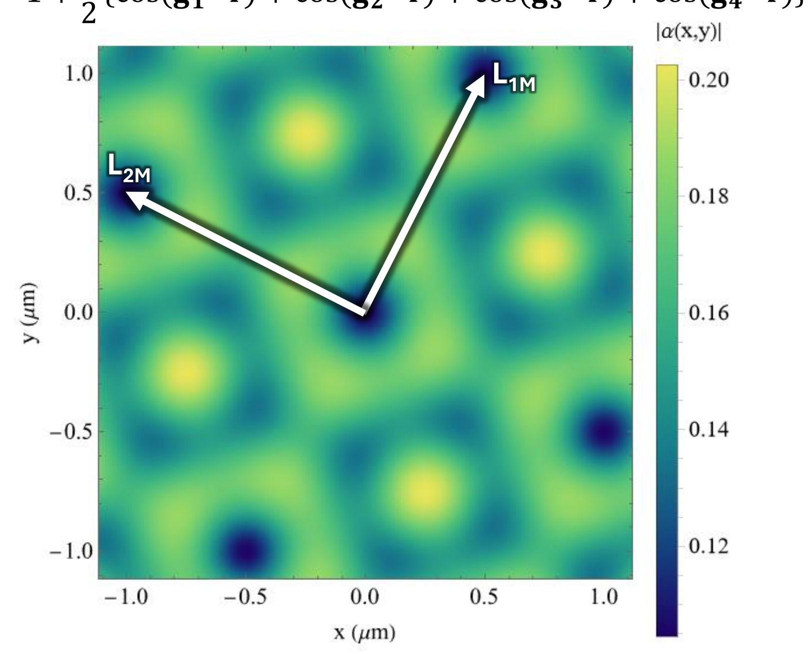
$z(\mathbf{r}) = 1 + \{\cos(\mathbf{g_1}\cdot\mathbf{r}) + \cos(\mathbf{g_2}\cdot\mathbf{r})\}$



$z(\mathbf{r}) = 1 + \{\cos(\mathbf{g_3}\cdot\mathbf{r}) + \cos(\mathbf{g_4}\cdot\mathbf{r})\}$



$z(\mathbf{r}) = 1 + \frac{1}{2}\{\cos(\mathbf{g_1}\cdot\mathbf{r}) + \cos(\mathbf{g_2}\cdot\mathbf{r}) + \cos(\mathbf{g_3}\cdot\mathbf{r}) + \cos(\mathbf{g_4}\cdot\mathbf{r})\}$

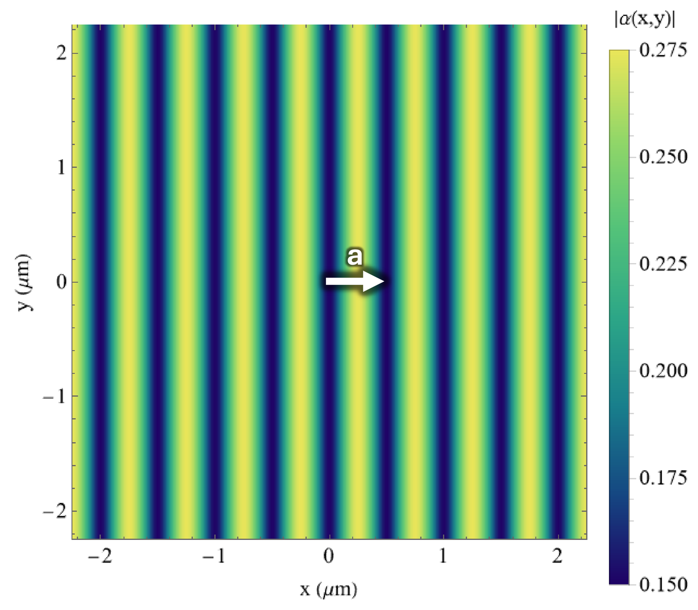


- The diagonal terms of the D matrix are related to the dispersion of the polaritons while the off diagonal terms are related to the lattice Fourier harmonics. Those last are responsible for the interactions in the band structure.
- We set the source amplitude to $I = 0$ to study the eigenmodes of the system : $\sum_M D_{NM}\, t_M = 0 \leftrightarrow |D| = 0 \rightarrow \mathrm{Log}\left(\frac{1}{|D|}\right)$
- A commensurate moiré lattice is a periodic large-scale interference pattern.
- Polaritons are light coupling to a dipole induced in matter.
- $z(\mathbf{r})$ is the function used to shape the conductivity.

1D

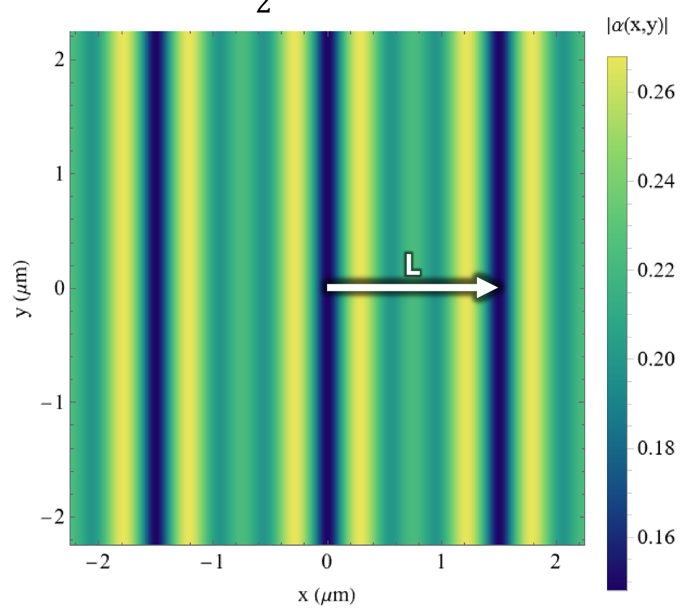
Primitive lattice

$z(x) = 1 + \cos(g_1 x)$



Moiré superlattice

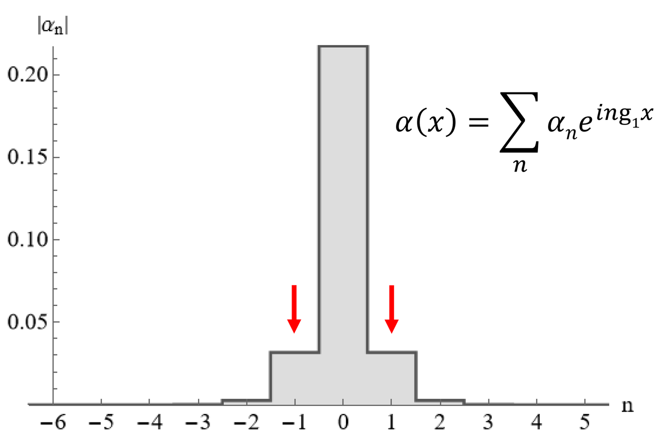
$z(x) = 1 + \frac{1}{2}\{\cos(g_1 x) + \cos(g_2 x)\}$

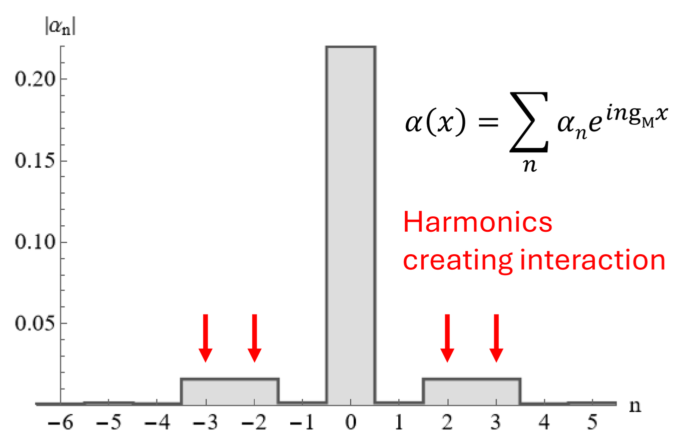


- Two primitive 1D lattices with different periodic variations of the conductivity, are combined to form a 1D moiré superlattice (in a single lattice).
- Commensurate configurations (like here) require $\frac{b}{a} \in \mathbb{Q}$.
- The moiré period is bigger than the period of the primitive lattices, then the moiré reciprocal lattice vector is smaller.

Lattice periods :
a=500 nm, b=750 nm, L=1,5 μm.
Reciprocal lattice vectors :
$g_1 = 2\pi/a$, $g_2 = 2\pi/b$,
$g_M = 2\pi/L = g_1/3 = g_2/2$.

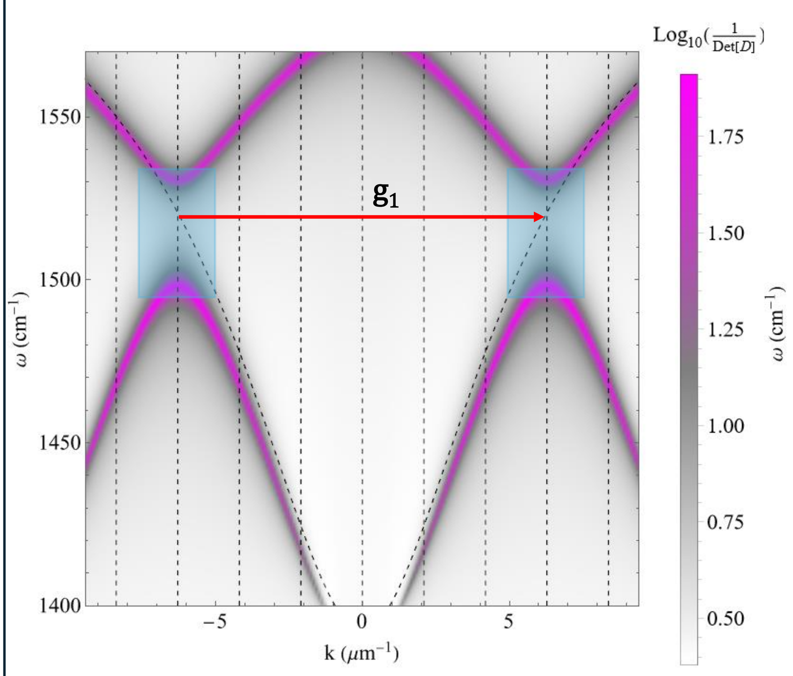
Fourier spectrum

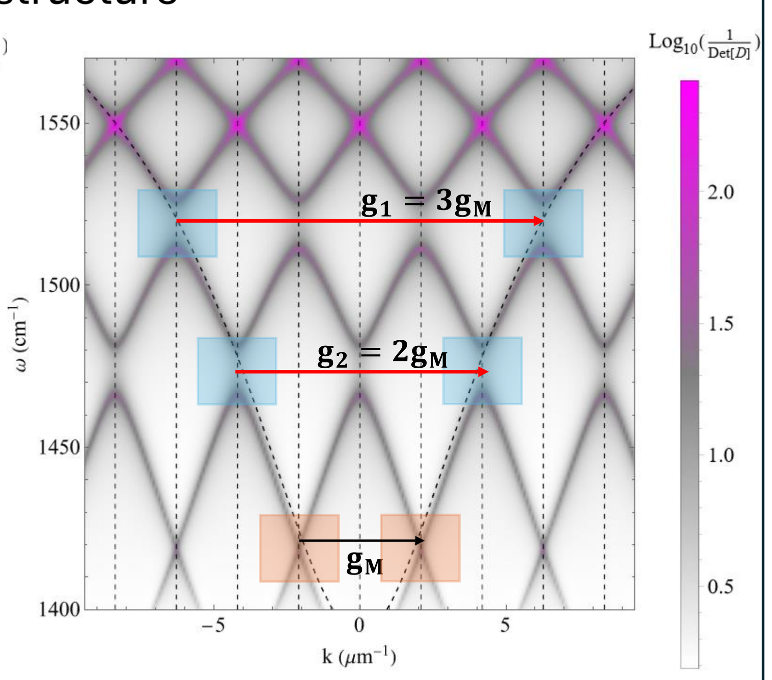




- In the moiré case, the reciprocal vectors allowing the Bragg scattering are related to the harmonics of the Fourier spectrum (not to the moiré reciprocal lattice vector).
- We can engineer the band structure of the polaritonic crystal by selecting harmonics forming commensurate moiré patterns.

Band structure





- The thickness of the dispersion band is due to losses of the polaritonic crystal.

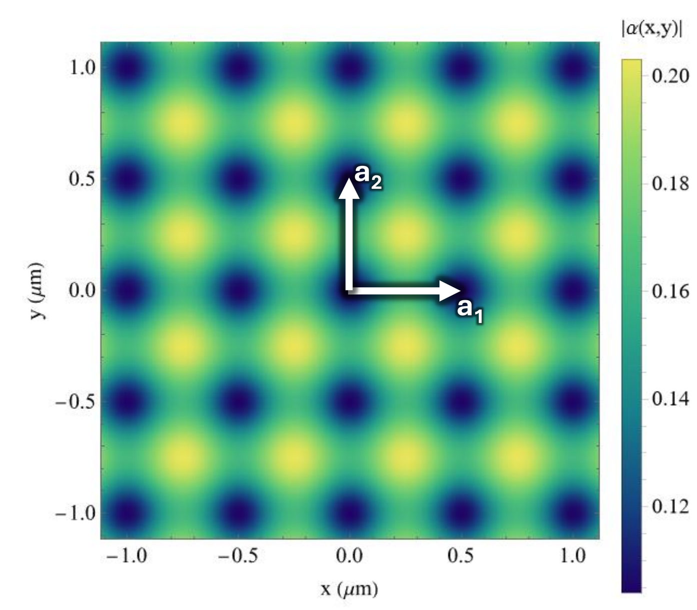
Fourier interaction analysis

- Primitive lattice : the band interaction arises from Bragg scattering between Bloch modes whose wavevectors differ by a reciprocal lattice vector.
- Moiré superlattice : the reciprocal vectors allowing the Bragg scattering (here $\mathbf{g_1} = 3\mathbf{g_M}$ and $\mathbf{g_2} = 2\mathbf{g_M}$) are related to the harmonics of the Fourier spectrum (here ±2 and ±3). Then the interaction is repeated in the momentum space thanks to the folding of the 1st Brillouin zone (BZ).
- The gap induced by the interaction is proportional to the conductivity terms $\alpha_{N-M\neq N}$.

2D square

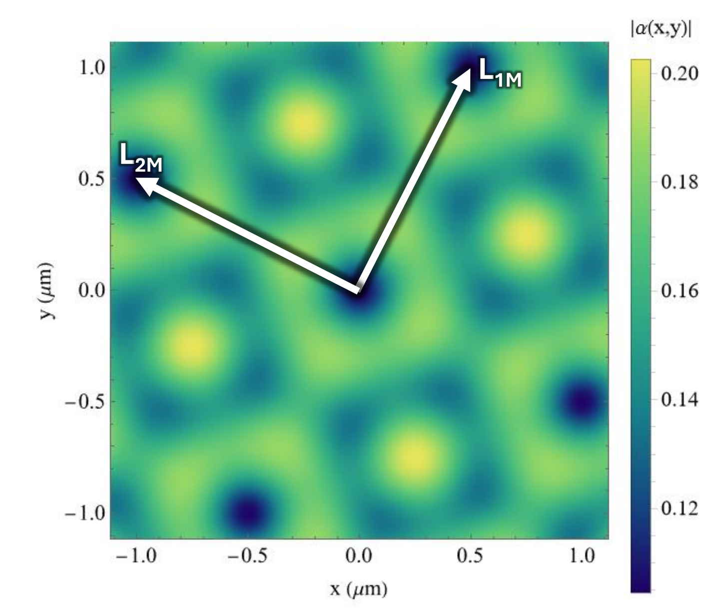
Primitive square lattice

$z(\mathbf{r}) = 1 + \{\cos(\mathbf{g_1}\cdot\mathbf{r}) + \cos(\mathbf{g_2}\cdot\mathbf{r})\}$



Moiré square superlattice

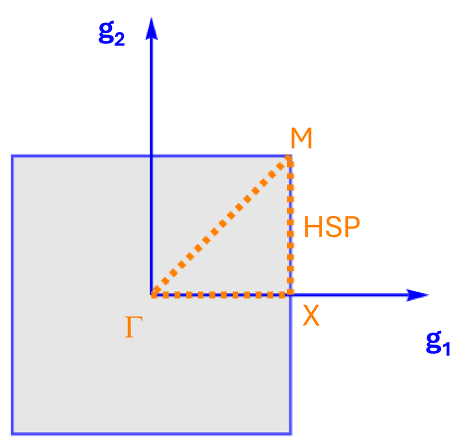
$z(\mathbf{r}) = 1 + \frac{1}{2}\{\cos(\mathbf{g_1}\cdot\mathbf{r}) + \cos(\mathbf{g_2}\cdot\mathbf{r}) + \cos(\mathbf{g_3}\cdot\mathbf{r}) + \cos(\mathbf{g_4}\cdot\mathbf{r})\}$

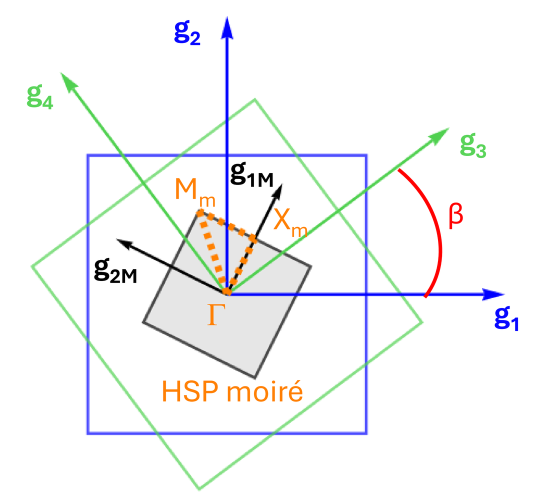


- Two primitive 2D lattices, twisted with respect to each other, are combined to form a 2D moiré superlattice (in a single lattice).
- Commensurate configurations (like here) require : $m_c\mathbf{g_1} + n_c\mathbf{g_2} = n_c\mathbf{g_3} + m_c\mathbf{g_4}$ with m_c and n_c integers, $\mathbf{g_1}$ and $\mathbf{g_2}$ are reciprocal primitive lattice vectors, $\mathbf{g_3}$ and $\mathbf{g_4}$ are reciprocal primitive lattice vectors twisted with respect to $\mathbf{g_1}$ and $\mathbf{g_2}$ with angle β.

Lattice spacing : a=500 nm
$\|\mathbf{g_i}\| = 2\pi/a$ with $i = \{1,2,3,4\}$
$m_c = 1, n_c = 2$, β=36,87°
$\|\mathbf{L_{iM}}\| = 1{,}12$ μm with $i = \{1,2\}$

1st Brillouin zone

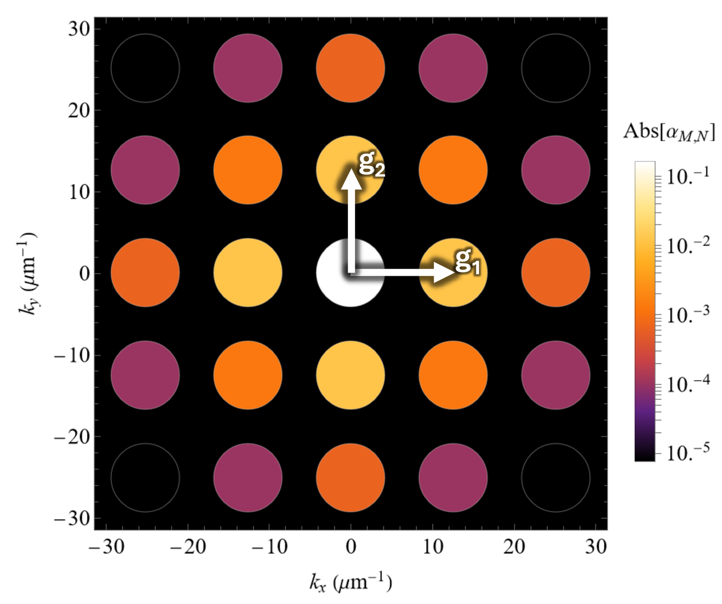




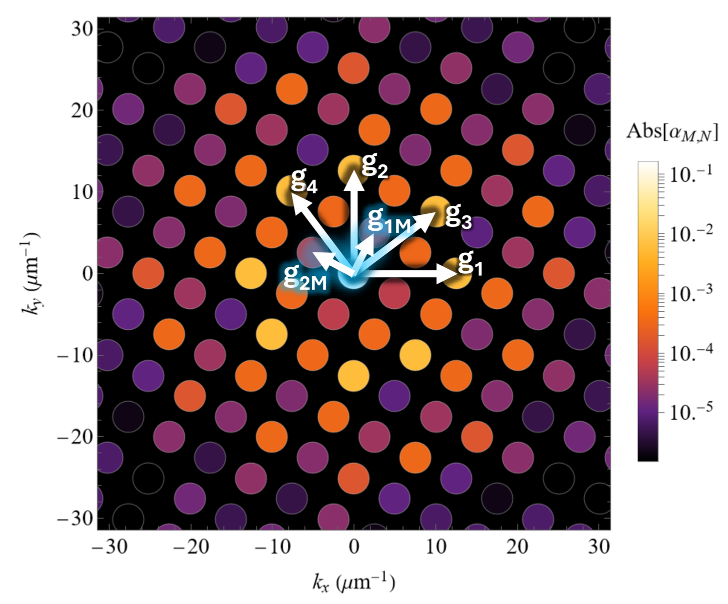
- The high symmetry path (HSP) of the primitive square lattice is different than the one of the moiré square superlattice and depends on the twist angle.
- The moiré 1st BZ is often called mini BZ.
- The reciprocal lattice vectors of a moiré commensurate square superlattice are :

$$\mathbf{g_{1M,S}} = \frac{m_c}{m_c^2+n_c^2}\mathbf{g_1} + \frac{n_c}{m_c^2+n_c^2}\mathbf{g_2},$$
$$\mathbf{g_{2M,S}} = \frac{-n_c}{m_c^2+n_c^2}\mathbf{g_1} + \frac{m_c}{m_c^2+n_c^2}\mathbf{g_2}.$$

Fourier spectrum

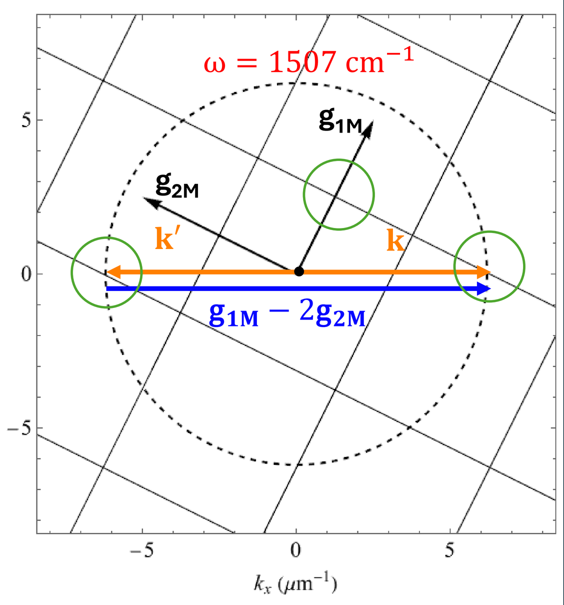


$\alpha(\omega,x,y) = \sum_{M,N} \alpha_{M,N} e^{i\mathbf{r}(M\mathbf{g_1}+N\mathbf{g_2})}$



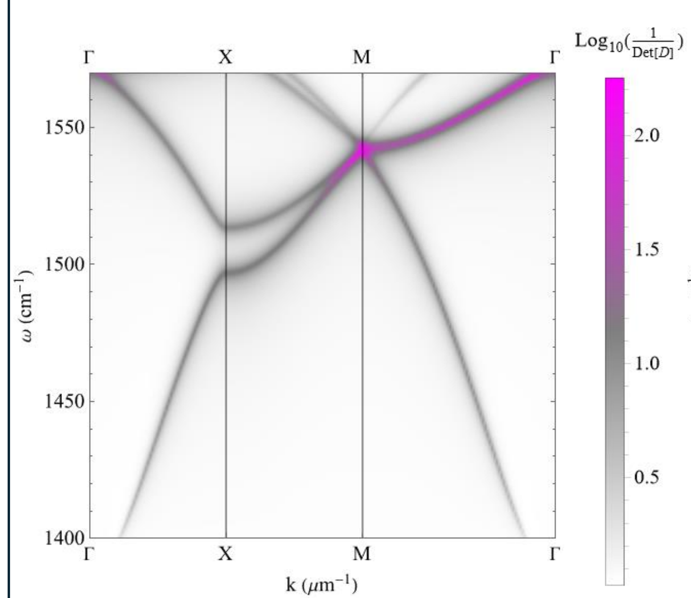
$\alpha(\omega,x,y) = \sum_{M,N} \alpha_{M,N} e^{i\mathbf{r}(M\mathbf{g_{1M}}+N\mathbf{g_{2M}})}$

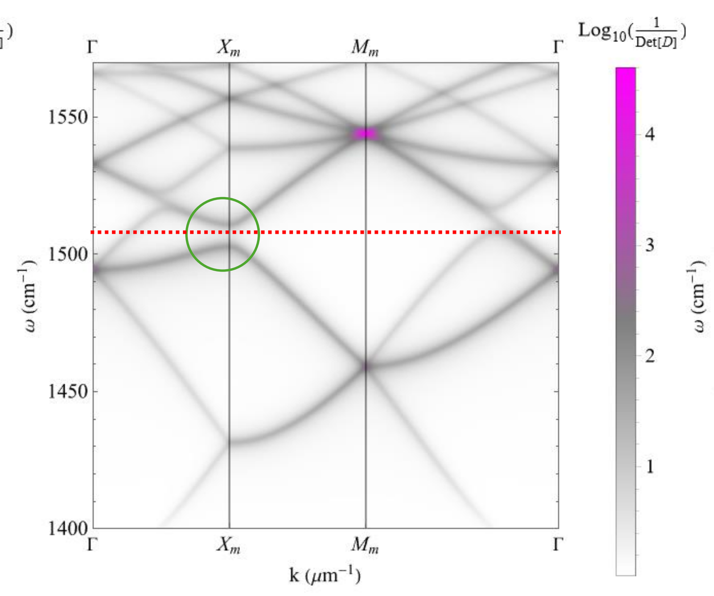
Fourier interaction analysis

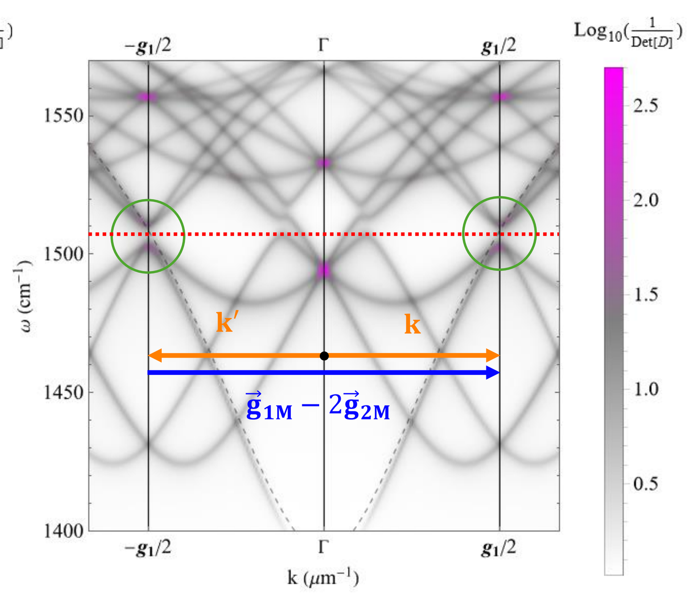


- The Bragg scattering induced by the primitive reciprocal lattice vectors is replicated with the mini BZ.

Band structure







- The 2 left band structures correspond to the primitive and moiré lattices in their respective HSP.
- The right band structure is plotted along the direction of the primitive reciprocal lattice vector $\mathbf{g_1}$ but for the moiré square super lattice.
- Together, those band structure plots explain how engineering the harmonics using a moiré square lattice creates interactions in the band structure.

Main references

[1] Álvarez-Pérez, G. *et al.* Analytical approximations for the dispersion of electromagnetic modes in slabs of biaxial crystals. *Phys. Rev. B* 100, 235408 (2019).
[2] Capote-Robayna, *et al.* Twisted Polaritonic Crystals in Thin van der Waals Slabs. *Laser & Photonics Reviews* 16, 2200428 (2022).
[3] Menabde, S. G. *et al.* Polaritonic Fourier crystal. *Nat Commun* 16, 2530 (2025).

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