Fourier modal method for Moiré lattices

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In recent years twisted bi-layers of 2D materials became very popular in the field due to the possibility to totally change their electronic properties by simple rotation. At the same time, in the wide field of photonic crystals, this idea still remains almost untouched, and only some particular problems were considered. One of the reasons is the computational difficulty of the accurate consideration of Moiré superlattices that appear due to the superimposition of misaligned lattices. Indeed, the unit cell of the complex lattice is typically much larger than the original crystals and requires much more computational resources for the computations. Here, we propose a careful adaptation of the Fourier modal method in the form of the scattering matrices for the description of twisted 1D gratings' stacks. Our approach allows us to consider sublattices in close vicinity to each other and account for their interaction via the near-field. In the developed numerical scheme, we utilize the fact that each sublattice is only 1D-periodic and therefore simpler than the resulting 2D superlattice, as well as the fact that even a small gap between the lattices filters out high Fourier harmonics due to their evanescent origin. This accelerates the computations from 1 up to 3 and more orders of magnitude for typical structures depending on the number of harmonics. This paves the way for rigorous study of almost any photonic crystals of the proposed geometry and demonstration of specific Moiré-associated effects.

I. INTRODUCTION

The Moiré effect, known for centuries, is a result of superimposing of similar but misaligned lattices. Probably, everyone met Moiré fringes as an occasional effect (recognizable patterns on silk clothes and curtains), as a side-effect (prominent grids on photos of LCD screens and imposition of the computational grid on the true picture on the map graphs), but the most important are their practical applications. For example, the Moiré pattern underlies the widely-known Vernier scale, which is implemented in micrometers and other measuring devices. Also, Moiré effect is successfully applied in strain analysis [1–3], optical alignment [4–7], medicine [8], biosensors [9–11], detection of document counterfeiting [12–15] and in many other spheres [16, 17]. Nevertheless, the original principle of the complex superlattice design by the superimposition of identical or similar sublattices is still widely applied to observe the associated phenomena. In the last few years, there has been a breakthrough in the field of twisting 2D materials. It has been demonstrated the possibility to observe superconductivity [18–20], ferromagnetism [21–24], and other impressive effects [25–28] just by the appropriate choice of the rotation angle between two layers. The obvious success attracted attention to the Moiré lattices and even led to the rise of the separate field of twistronics.

In this paper, we consider Moiré patterns in the context of nanophotonic metasurfaces. All kinds of photonic crystals and metasurfaces were studied intensively for the last several decades, and their optical properties are known in much detail. In recent years there was a growth of attention to stacks of metasurfaces [29–38] due to the new opportunities that they provide for the control and manipulation of light. Simultaneously, much fewer studies considered the interaction of crystals that do not have a mutual lattice either because of the periods discrepancy or even misalignment of crystallographic axes. The rise of twistronics attracted the deserved attention to this field and gave a significant boost. As a result, currently, there is a number of studies available that demonstrate various effects in photonic Moiré metasurfaces. Twisted stacks have been used to demonstrate topological transitions of the guided modes [39–45], light localization in Moiré supercells [46, 47], tunable metasurfaces [48], and chirality enhancement [49–50]. Also, it has been shown that in the near-field radiative heat transfer between parallel planar metasurfaces [51–59], the heat flux can be controlled by twisting one of the corrugated plates relative to the other [55, 57, 59]. Some of the studies utilize laser interference lithography (LIL) to obtain stacks of large-area lattices [49] and single-layer, gradient Moiré-metasurfaces [56, 57]. Nevertheless, the general understanding of the optical Moiré physics and potential capabilities are still to be understood in the nearest future.

The available calculation approaches for predicting properties of such structures do not provide the full picture as well. In recent studies, it has been proposed either to apply effective medium approximation [60] or to build a transfer/scattering matrix approach for the main (0th) diffraction channel [49, 61–67]. Such ap-
appropriate twisting angles. The accurate study of these
the radiation from the circularly polarized emitter) for
circularly polarized thermal emission (as well as to route
slab with inclusions of graphite is able to generate cir-
monic stack allows controlling the shape of the plasmon
twisted stacks. The most difficult for computations plas-
applications on examples of both plasmonic and dielectric
To demonstrate the proposed approach performance, we
acceleration from 1 up to 3 and more orders
compare its computation speed with the standard FMM

density and thin metasurfaces, whereas the main diffrac-
tion order approximation requires the large distance be-
tween the sublattices to prevent their interaction via the
evanescent waves forming the near field. In this way, none
of the approaches allows considering the hybridization of
typical quasiguided modes of the twisted photonic struc-
tures – a backbone for plenty of physical systems. Univer-
universal computational methods such as finite element method
(FEM), finite difference time domain one (FDTD), or
Fourier modal method (FMM) [68], also known as Rigor-
ous coupled-wave analysis method (RCWA) [69], are not
efficient in the application for such structures as well.
From one side, the unit cell of the Moiré superlattice is
larger (and often much larger) than the unit cells of the
original gratings, which significantly complicates the real-
space-based calculations (FEM, FDTD). From the other
side, a large unit cell corresponds to the small Bragg
vector in the reciprocal space and, in turn, a large num-
ber of Fourier harmonics have to be accounted for to
reach the convergence of reciprocal-space-based FMM.
Remarkably, the most bright twistronic effects are ob-
served for identical materials rotated on very small angles
of [18, 20–22, 26], which corresponds to extremely large
periods of the resulting superlattice. This configuration,
together with non-twisted sublattices of very close peri-
ods, are the most hard-to-compute structures. In this
way, there is a great need for a fast and universal com-
putational method specialized for considering stacks of
twisted metasurfaces.

In this paper, we present the adaptation of the Fourier
modal method in the form of scattering matrices [68] for
the consideration of twisted stacks of 1D-periodic meta-
surfaces. Scattering matrices of each sublattice are calcu-
lated efficiently, accounting for their 1D-periodic origin,
which makes the procedure lean and efficient. To calcu-
late the scattering matrix of the whole stack, we addition-
ally propose to ignore high-k1 evanescent waves that de-
cay such fast in the gap-layer between sublattices that do
not affect the coupling between them at all. Both proce-
dures strongly boost the calculations without noticeable
loss of accuracy and pave the way to study any optical
properties of the twisted stacks in a reasonable time.
To demonstrate the proposed approach performance, we
compare its computation speed with the standard FMM
and show the acceleration from 1 up to 3 and more orders
of magnitude. Finally, we demonstrate the possible ap-
plications on examples of both plasmonic and dielectric
twisted stacks. The most difficult for computations plas-
monic stack allows controlling the shape of the plasmon
dispersion just by a relative rotation of the sublayers.
We also show that the chiral diamond photonic crystal
slab with inclusions of graphite is able to generate cir-
cularly polarized thermal emission (as well as to route
the radiation from the circularly polarized emitter) for
appropriate twisting angles. The accurate study of these
and many other effects become possible with the help of the
new approach.

II. CALCULATIONS

Here, we are going to consider twisted stacks of 1D-
periodic gratings that form 2D-periodic Moiré pattern as
shown in Fig. 1. The upper and lower sublattices might be
different, have different periods and arbitrary rotation
angles as depicted in Fig. 1

Figure 1. Schematic of the twisted stack consisting of two
arbitrary 1D-periodic lattices twisted around a common axis.

Each separate 1D lattice has a corresponding 1D recip-
rocal lattice (Fig. 2 a-b), which is formed by the Bragg
vectors \( \mathbf{G}^1 \) and \( \mathbf{G}^2 \) that might be imparted by the lat-
tices to the in-plane wavevector of the incident wave \( \mathbf{k}_1 \).
The optical properties of the upper and lower sublattices
can be described in terms of the scattering matrices that
connect the amplitudes of incoming and outgoing waves.
Nevertheless, the relative rotation and different periods
of the lattices result in misalignment and mismatch of
their reciprocal lattices (see Fig. 2 a-b). This means that
each diffraction harmonic of the light passed through one
of the lattices generates a new family of harmonics after
the diffraction on the second one. Therefore, the struc-
ture consisting of upper and lower sublattices is essen-
tially two-dimensional, and its scattering matrix should
connect all the corresponding harmonics (see Fig. 2 c).

The straightforward approach to calculate spectra of
such stacks is just to consider each 1D-periodic sublayer
as it is a 2D-periodic metasurface (see the second column
in Fig. 2 a-b). For the desired convergence, 2D structures
typically require to take into account much more harmon-
ics than 1D ones. Given that the calculation time scales
cubically with the number of harmonics [68], this makes
2D calculations relatively slow and resource-consuming.
The straightforward approach becomes especially ineffi-
cient for plasmonic lattices, for which even 1D sublattices
require a huge number of harmonics to resolve the high-
gradient fields. Brute-force calculation of such structures
is challenging even in a single dimension and almost un-
achievable in 2D. Moreover, for Moiré lattices, this issue
might be even more critical than for typical 2D crystals.
As it was already mentioned, the Moiré pattern composed
Figure 2. Sketches of the upper (a), lower (b) sublattices and their stack (c) in real and reciprocal spaces. The first column (a,b) schematically shows the structure of the rotated 1D-periodic sublattices and their reciprocal lattices with respect to coordinate axes and wavevector of the incident light $k_\parallel$. The second column (a,b) formally considers the same sublattices as structures with mutual 2D-periodicity. Each sublattice binds harmonics either of common row or column. The last column (c) shows the superimposing of 1D-sublattices resulting in a formation of the true 2D-periodic structure, which substantially connects all the harmonics.

of the sublayers with close vectors of reciprocal lattices $|G^1 - G^2| \ll k$ (where $k$ is the typical wavevector of light in ambient media) has a large number of opened diffraction channels. Thus, in this case, an achievement of the full convergence for some structures could be especially challenging, which will be shortly discussed on a practical example below.

Nevertheless, we do not consider 2D photonic crystals of the general form, but focus our attention on a rather narrow class of the structures. Utilization of the distinctive features of this class makes it possible to simplify and boost corresponding calculations.

A. Scattering matrix of 1D lattice

We start with the consideration of the first (upper) 1D sublattice. It is important to note that the derivations will be based on the assumption that the lattice is sandwiched between the two homogeneous layers (see Fig. 3). Such environment makes it possible to consider the eigenmodes of the boundary layers as plane linearly-polarized waves, which simplifies the derivations. Although the proposed configuration does not describe the arbitrary structure, we can implement it without losing generality. Indeed, the virtual zero-thickness homogeneous layer can always be inserted, for example, between two back-to-back gratings.
Let us separate out the layer bounded by horizontal dashed lines (see Fig. 2(a), Fig. 3) that includes upper sublattice in specially aligned with it $x’ - y’$ coordinate system. Looking ahead, the similar layer for the lower sublattice should be chosen standing back-to-back with the first one, i.e. the gap interlayer is virtually divided in an arbitrary ratio between the layers. Incident light determines the in-plane components of the main harmonic wavevector $\mathbf{k}_\parallel = k_x \hat{x} + k_y \hat{y} = k_{x'} \hat{x'} + k_{y'} \hat{y'}$, where $\hat{x}$, $\hat{y}$, $\hat{x'}$ and $\hat{y'}$ are unit vectors defining the direction of the corresponding axes. Interaction of light with lattice hypervectors:

Corresponding wavevectors that might be arranged in a standard FMM realisations. This matrix is a function of properties of the considered layer and can be found by standard FMM realisations. This matrix is a function of $k_{x'}$ and $k_{y'}$ projections:

where $G_{x'}^1, G_{y'}^1$ are projections of the Bragg vector on denoted axes and the number of harmonics that are taken into account is $N_y = 2N + 1$. The finite number of these harmonics makes it possible to build the scattering matrix that connects the amplitudes of incoming $[d_{+}^r, \hat{u}_{+}^r]^T$ and outgoing $[d_{-}^r, \hat{u}_{-}^r]^T$ waves on the boundaries of the considered layer (horizontal dashed lines in Fig. 3). Since the consideration is held in the primed basis, we consider the matrix $S_1(\omega, \mathbf{k}_\parallel) = S_1(\omega, [k_{x'}, k_{y'}]^T)$ as a function of $k_{x'}$ and $k_{y'}$ projections:

where $\hat{u}_{+}^r$ and $d_{+}^r$ are hypervectors of amplitudes correspond to the upward and downward propagating waves, $\pm$ signs indicate the section that has a larger and smaller $z$-coordinate correspondingly. Each of the hypervectors $\hat{u}_{+}^r, \hat{d}_{+}^r$ describes $2N_y$ modes of different polarizations, whereas scattering matrix $S_1^r$ has $4N_y \times 4N_y$ size respectively. If the boundaries of the considered layer are located inside a homogeneous environment (the case which we consider here), then according to our definition, amplitudes correspond to $x’ -$ and $y’-polarized plane waves:

where the amplitudes are sorted in accordance with hypervectors $[\hat{K}_{x'}^1, \hat{K}_{y'}^1]$ in such a way that the field of upward and downgoing waves on the boundaries of the unit cells. Arrows illustrate the incoming and outgoing harmonics that are connected via the scattering matrix.

$E_{\pm, x}(r_{\parallel}) = \sum_{n=0}^{N_y} \left[ u_{\pm, x_n}^{r} \hat{u}_{\pm, y_n}^{r} + d_{\pm, x_n}^{r} \hat{d}_{\pm, y_n}^{r} \right] e^{\pm k_{1,n}^r r_{\parallel}}$, (4)

where index $n$ indicates $n$-th component of the hypervectors, $\mathbf{k}_\parallel = k_{1,n}^x \hat{x} + k_{1,n}^y \hat{y}$ and $r_{\parallel} = x \hat{x} + y \hat{y}$.

**B. Scattering matrix of the rotated sublattice**

Scattering matrix $S_1$, fully describes the optical properties of the considered layer and can be found by standard FMM realisations. This matrix is a function of frequency $\omega$ and in-plane component of the wavevector $\mathbf{k}_\parallel$, but also depends on the structure’s parameters. The scattering matrix’s transformation with the rotation of the lattice can be easily found and does not require some additional computations. To demonstrate this, we consider the first lattice rotated by an angle $\alpha$ and find the connection of scattering matrix in $x – y$ coordinate system $S_1(\omega, \mathbf{k}_\parallel) = S_1(\omega, [k_x, k_y]^T)$ with matrix $S_1'(\omega, \mathbf{k}_\parallel) = S_1(\omega, [k_{x'}, k_{y'}]^T)$ defined in $x’ – y'$ basis (see Fig. 2(a)). The latter one has already been considered:

$S_1'(\omega, [k_{x'}, k_{y'}]^T) = S_1(\omega, [k_{x}, k_{y}]^T)$

(5)
Hypervectors that are connected by the scattering matrix might be easily expressed in the original $x-y$ coordinate system:

$$
\begin{bmatrix}
d_{+x} \\
d_{+y} \\
u_{-x} \\
u_{-y}
\end{bmatrix}
= \mathbb{R}_\alpha
\begin{bmatrix}
d_{+x'} \\
d_{+y'} \\
u_{-x'} \\
u_{-y'}
\end{bmatrix},
$$

$$
\begin{bmatrix}
d_{-x} \\
d_{-y} \\
u_{+x} \\
u_{+y}
\end{bmatrix}
= \mathbb{R}_\alpha
\begin{bmatrix}
d_{-x'} \\
d_{-y'} \\
u_{+x'} \\
u_{+y'}
\end{bmatrix},
$$

$$
\mathbb{R}_\alpha =
\begin{bmatrix}
\cos(\alpha)\hat{I} - \sin(\alpha)\hat{J} & 0 & 0 \\
\sin(\alpha)\hat{I} \cos(\alpha)\hat{J} & 0 & 0 \\
0 & 0 & \cos(\alpha)\hat{I} - \sin(\alpha)\hat{J}
\end{bmatrix},
$$

(6)

where $\mathbb{R}_\alpha$ is the rotation matrix for the hypervectors, $\hat{I}$ is $N_y \times N_g$ identity matrix and $0$ is $N_y \times N_y$ zero matrix. Due to the fact that both scattering matrices describe the same mapping in different bases, we can easily obtain the final expression for the scattering matrix in the original coordinates:

$$
\mathbb{S}_1(\omega, [k_x, k_y]^T) = \mathbb{R}_\alpha\mathbb{S}_1'(\omega, \hat{R}_{-\alpha} [k_x, k_y]^T)\mathbb{R}_{-\alpha},
$$

(7)

where

$$
\begin{bmatrix} k_x' \\ k_y' \end{bmatrix} = \hat{R}_{-\alpha} \begin{bmatrix} k_x \\ k_y \end{bmatrix},
$$

$$
\hat{R}_{-\alpha} = \begin{bmatrix} \cos(\alpha) - \sin(\alpha) \\ \sin(\alpha) \cos(\alpha) \end{bmatrix}.
$$

(8)

We should remember that the in-plane components of the wavevectors of the diffraction harmonics, $\mathbb{K}^{1,n}_I = K^{1,n}_x x + K^{1,n}_y y = K^{1,n}_x x' + K^{1,n}_y y'$, are transformed accordingly:

$$
\begin{bmatrix} K^{1,n}_x \mathbb{K}^{1,n}_I \end{bmatrix} = \begin{bmatrix} k_x' \\ k_y' \end{bmatrix} + n \begin{bmatrix} G^1_x \\ G^1_y \end{bmatrix} = \hat{R}_{-\alpha} \begin{bmatrix} K^{1,n}_x \mathbb{K}^{1,n}_I \end{bmatrix} = \hat{R}_{-\alpha} \begin{bmatrix} k_x' \\ k_y' \end{bmatrix} + n\hat{R}_{-\alpha} \begin{bmatrix} G^1 \\ 0 \end{bmatrix},
$$

(9)

where $G^1$ is the absolute value of the Bragg vector of the first lattice ($G^1 = G^1_x = \sqrt{G^1_x^2 + G^1_y^2}$).

The same procedure holds for the second lattice, which is rotated on an angle $\beta$ and is aligned with the double-primed axes:

$$
\mathbb{S}_2(\omega, [k_x, k_y]^T) = \mathbb{R}_\beta \mathbb{S}_2'(\omega, \hat{R}_{-\beta} [k_x, k_y]^T)\mathbb{R}_{-\beta}.
$$

(10)

The corresponding basis is the following:

$$
\begin{bmatrix} K^{2,m}_x \mathbb{K}^{2,m}_I \end{bmatrix} = \begin{bmatrix} k_x' \\ k_y' \end{bmatrix} + m \begin{bmatrix} G^2_x \\ G^2_y \end{bmatrix} = \hat{R}_{\beta} \begin{bmatrix} k_x' \\ k_y' \end{bmatrix} + m\hat{R}_{\beta} \begin{bmatrix} G^2 \\ 0 \end{bmatrix},
$$

(11)

where $\hat{R}_{\beta}$ is the rotation matrix for the second lattice.

The number of harmonics for this case is denoted $M_y = 2M + 1$.

C. Scattering matrix of the stack in mutual basis

We have obtained the scattering matrices of the rotated 1D metasurfaces, but our final goal is to construct the scattering matrices derived in a mutual basis, which requires us to attribute them formally as 2D crystals. The mutual, reciprocal lattice for both sublattices might be found as a direct sum of their own 1D reciprocal lattices. In practical calculations, we take into account only a finite number of harmonics, and the easiest approach is also to take the direct sum of finite sublattices as shown in Fig. 2 (a-b), second column. Such an approach is not the only one, but it is highly convenient for practical implementation.

The wavevectors of the 2D superlattice harmonics might be arranged in a single hypervector in different orders. The straightforward approach is to place wavevectors of the 2D lattice "row" after "row" or "column" after "column." In other words, harmonics of the mutual basis can be constructed as a concatenation of sets of harmonics of 1D lattices for different wavevectors of the main harmonic.

For the consideration of the first (upper) lattice, it is convenient to arrange the wavevectors in the order, which we indicate by the letter $A$ (see the second column of Fig. 2 (a-b)):

$$
\begin{bmatrix}
A \tilde{K}^{2D}_x \\
A \tilde{K}^{2D}_y
\end{bmatrix} =
\begin{bmatrix}
\tilde{K}^{1}_x(k_{||} - MG^2) & \tilde{K}^{1}_y(k_{||} - MG^2) \\
\tilde{K}^{1}_x(k_{||} + (-M + 1)G^2) & \tilde{K}^{1}_y(k_{||} + (-M + 1)G^2) \\
\vdots & \vdots \\
\tilde{K}^{1}_x(k_{||} + MG^2) & \tilde{K}^{1}_y(k_{||} + MG^2)
\end{bmatrix}
$$

$$
\begin{bmatrix}
\tilde{K}^{2}_x(k_{||} - M^2G^2) & \tilde{K}^{2}_y(k_{||} - M^2G^2) \\
\tilde{K}^{2}_x(k_{||} + (-M^2 + 1)G^2) & \tilde{K}^{2}_y(k_{||} + (-M^2 + 1)G^2) \\
\vdots & \vdots \\
\tilde{K}^{2}_x(k_{||} + M^2G^2) & \tilde{K}^{2}_y(k_{||} + M^2G^2)
\end{bmatrix}
$$

(12)

where the expression $\tilde{K}^{1}_{x/y}(q)$ indicates the corresponding hypervector is calculated for the wavevector of the main harmonic equal to $q$.

With such a choice of the basis, each block of the scattering matrix of the first lattice (considered as 2D one) splits into sub-blocks that describe the internal coupling of each "row"'s harmonics. Since the lattice is fundamentally one-dimensional, all the inter-"row" connections are equal to zero, which makes sparse the scattering matrix $A\mathbb{S}_1$ of the first lattice formally considered as 2D crystal. To demonstrate this, we first represent the scattering matrices in the form, where each block is responsible for either reflection or transmission of $x$- or $y$- polarized incident light to the $x$- or $y$- polarized channels:
\[ A^S_1(\omega, k_\|) = \begin{pmatrix} A^S_{11} & A^S_{12} & A^S_{13} & A^S_{14} \\ A^S_{21} & A^S_{22} & A^S_{23} & A^S_{24} \\ A^S_{31} & A^S_{32} & A^S_{33} & A^S_{34} \\ A^S_{41} & A^S_{42} & A^S_{43} & A^S_{44} \end{pmatrix}, \]

\[ S_1(\omega, k_\|) = \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{pmatrix}, \]

where blocks \( A^S_1 \) have \( N_g M_g \times N_g M_g \) size, whereas blocks \( S_1 \) are \( N_g \times N_g \) size correspondingly. In turn, the blocks are obviously connected as follows:

\[ \begin{pmatrix} A^S_{ij}(\omega, k_\|) \\ S_1(\omega, k_\|) \end{pmatrix} = \begin{pmatrix} 0 & \ldots & 0 \\ 0 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & S_1(\omega, k_\|) \end{pmatrix}. \]

Next, we need to build the scattering matrix of the second lattice \( A^S_2 \) in the same basis \( A \). However, it is hard to do it once and therefore, we first consider the scattering matrix of the second lattice in its natural basis denoted \( B \) (see the "chains" in the second column of Fig. 2 b):

\[ B^S_2(\omega, k_\|) = \begin{pmatrix} 0 & \ldots & 0 \\ 0 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & S_2(\omega, k_\|) \end{pmatrix}. \]

where the harmonics are sorted as follows:

\[ \begin{bmatrix} B K^2D \ K^2D \end{bmatrix} = \begin{bmatrix} K_2^x(\omega, k_\| + N G^1) \\ \vdots \\ K_2^y(\omega, k_\| + N G^1) \end{bmatrix}. \]

The block-wise computation of the matrices must be faster than a straightforward approach. Indeed, the calculation time of each scattering matrix scales cubically with the number of harmonics. Therefore, the naive consideration of each sublayer as 2D crystal takes \( \tau_{\text{naive}} \propto N_g^3 M_g \), whereas our block-wise calculation approach for the first and second lattices scales as \( \tau_1 \propto N_g^3 M_g \) and \( \tau_2 \propto N_g M_g^3 \), which is much faster in practice, especially for the large number of harmonics.

The knowledge of \( A^S_1(\omega, k_\|) \) and \( B^S_2(\omega, k_\|) \) matrices is still not enough to obtain the stack scattering matrix. To do that, we need to consider matrices of both sublayers in a mutual basis. In our case, bases \( A \) and \( B \) differ only by the order of their elements and, therefore, one of them can be reduced to another by simple rearrangement. The transition matrix that connects them can be easily derived.

Indeed, when we consider the basis \( A \), then the \((n,m)\) harmonic (see Fig. 2 a) has the index number \( p_A = (m+M)N_g+n+N+1 \). The same harmonic in the basis \( B \) (see Fig. 2 b) has the index number \( p_B = (n+N)M_g+m+M+1 \). In this terms the matrices in \( A \) and \( B \) representations are connected in a very simple way:

\[ A^S_{ij}(\omega, k_\|) = B^S_{ij}(\omega, k_\|), \]

where indexes \( ij \) indicate one of sixteen blocks (see Eqn. 13) and the indices \( p_{A/B} \) run inside each of the blocks.

In practice, there are several possible ways to implement the described permutation. The most obvious is just to iterate over all the indices in a loop to find the scattering matrix components. Nevertheless, more effective approach is to build once the mappings \( p_A = T_{AB}(p_B) \) and \( p_B = T_{BA}(p_A) \) between the representations in advance and apply it on demand. \( T_{AB} \) and \( T_{BA} \) are primitive functions tabulated according to the described rule. In this way, we need just to apply the permutation operation, which is available in most packages for numerical computations.

\[ \begin{pmatrix} A^S_{ij}(\omega, k_\|) \end{pmatrix} = B^S_{ij}(\omega, k_\|). \]

The resulting matrix \( A^S_2 \) is still sparse but is no longer block-diagonal, which results in the "mixing" of blocks related to the upper and lower sublattices and arise of specific Moiré-induced physical effects.

Once we get scattering matrices of both sublayers in a mutual basis \( A \) (or any other one) the total scattering matrix of the whole stack might be found \( A^S = A^S_1 \otimes A^S_2 \) via the well-known formulas \([70]\) (from here on we omit index \( A \) implying that all the matrices are derived in the same basis):

\[ S_{dd} = S_{dd}^{(1)} (\ldots)^{-1} S_{dd}^{(1)}, \]

\[ S_{uu} = S_{uu}^{(1)} + S_{uu}^{(2)} (\ldots)^{-1} S_{uu}^{(1)}, \]

\[ S_{sd} = S_{sd}^{(1)} + S_{sd}^{(2)} (\ldots)^{-1} S_{sd}^{(1)}, \]

\[ S_{ud} = S_{ud}^{(1)} + S_{ud}^{(2)} (\ldots)^{-1} S_{ud}^{(1)}, \]
where the matrices are considered in terms of large
$2N_gM_g \times 2N_gM_g$ blocks:

$$S(\omega, k_\parallel) = \begin{pmatrix} S_{dd} & S_{du} \\ S_{ud} & S_{uu} \end{pmatrix}, \quad (23)$$

$$S_1(\omega, k_\parallel) = \begin{pmatrix} S_{dd} & S_{du} \\ S_{ud} & S_{1u} \end{pmatrix}, \quad (24)$$

$$S_2(\omega, k_\parallel) = \begin{pmatrix} S_{dd} & S_{du} \\ S_{ud} & S_{2u} \end{pmatrix}. \quad (25)$$

Each of the formulas contains the inversion of the
sparse matrices for which, according to our knowledge,
there are no effective specialized algorithms. In this way,
since the time of the matrix inversion scales cubically
with its size, the total computation time for the stack
scattering matrix has the same cubic asymptotic $\tau \propto
N_g^3M_g^3$ as the naive approach. Nevertheless, even the
least calculation of each sublattice matrix, as we will show
below, accelerates the whole procedure multiple times.

III. FILTRATION OF HARMONICS

In most practical cases, calculation of the Moiré stack
scattering matrix might be additionally boosted as well.
If there is a thin but finite homogeneous gap-layer of
thickness $H$ (see Fig. 1) in-between twisted metasurfaces,
then additional physical-based simplification can be im-
plemented. Indeed, high-$k_\parallel$ evanescent waves (requiring
a large number of harmonics in the calculation to be ac-
counted for) might be needed to accurately describe the
optical properties of separate upper or lower lattice. Nev-
evertheless, these harmonics decay in the gap in such a fast
way that they do not make almost any contribution in
their interaction. Therefore, it is easy to formulate the
criterion of taking harmonic into account for the calcu-
lation of matrices combination:

$$e^{-\text{Im}(\sqrt{\omega^2/c^2-(k_\parallel+\kappa G^3+mG^2)^2}H)} > \Theta, \quad (26)$$

where $\varepsilon_{\text{gl}}$ is the permittivity of the gap-layer and $\Theta$ is the
cut-off level, which determines the tolerance of the fully
converged results and should be in the range of $10^{-2} -
10^{-10}$ for most of the structures. The fulfillment of this
condition results in throwing away a significant number of
corresponding rows and columns from the matrices
$S_1$ and $S_2$ and subsequent drastic increase of Eqns. 19
22 calculation speed. Moreover, the number of remain-
ning harmonics saturates rapidly, making the computation
time of matrices combination almost constant as well. In
this case, the asymptotic time-scaling will be determined
by the sublattices $S_1$ and $S_2$ since sublattices might efficiently
"mix" all the harmonics. Therefore, the number of har-
nonics $N_gM_g$ used for $S_1$ and $S_2$ calculation should be in
general significantly larger than the number, which fulfil
the condition 26.

In the case of zero or extremely small $H$, the filter-
ing technique is not applicable and does not increase the
calculation efficiency. However, this case corresponds to
tightly bound lattices that form a true 2D crystal, and it is reasonable that the simplification based on the con-
cept of complex independent structures connected via the
limited number of channels is irrelevant.

A. Further development

Computational approaches presented in the previous
sections provide a fast and efficient calculation of twisted
Moiré stacks spectra, which will be demonstrated below.
Nevertheless, the computations can be further improved,
which might be vital in most complicated cases.

The most obvious improvement is associated with the
filtration of harmonics. In most practical cases we keep
rather limited number of low-$k_\parallel$ harmonics that lie in
a circle defined by the cut-off level in Eqn. 26. With-
out loss of generality, if one consider the upper lattice
then it becomes obvious that most of the "chains" of the
harmonics (second column of Fig. 2 (a)) are out of
any relation to the low-$k_\parallel$ of our interest. Therefore cor-
responding blocks of the scattering matrices can be ex-
cluded, which additionally improves the time calculation
asymptotic $\tau \propto \max(N_g^3/M_g^3)$. Such approach requires
a little bit more complicated procedure for the choice of the
mutual basis and harmonics of individual lattices,
which should account for the cut-off level. Nevertheless,
this procedure is straightforward and might be easily re-
alised in the spirit of the technique presented in the study.
Potential interest for efficient calculations might be at-
ttracted by the choice of other alternative 2D harmonics
sets that are not direct sums of any other 1D harmonics
sets.

One more opportunity to improve the computations
for the weakly-coupled metasurfaces lies in a simplified
accounting for their interaction. Indeed, it such cases it is
most likely possible to develop some sort of perturbation
theory. Apparently, it will be associated with the sub-
stitution of expressions with inversion of matrices with
series expansion (see Eqns. 1922). Potentially, the use
of only sparse matrix multiplication, which is a fast op-
eration, might significantly boost the calculations. Never-
theless, this approach requires separate detailed consid-
eration and rigorous study of its potential applicability.

Yet another acceleration can be applied for the hard-to-compute Moiré superlattices of large Moiré-periods. As it was already discussed, similar sublattices superimposition results in a formation of very dense reciprocal lattice, and according to the described procedure, one needs to calculate the blocks of the matrices that connect very closely-located chains of harmonics. Therefore, corresponding scattering matrices might be found not directly, but from the interpolation of precalculated matrices on a mesh in reciprocal space. Such approach, not only strongly reduces the number of repeated calculations, but also helps to choose the optimal for the problem set of harmonics (not necessarily direct-sum-generated).

**IV. PERFORMANCE**

In the previous sections, we have proposed an effective computational approach and estimated its asymptotic time consumption. Nevertheless, it is important to observe the acceleration in practice. To do that, we have chosen one of the most hard-to-compute structures - the stack of two 1D plasmonic lattices in silica ($\varepsilon_{\text{SiO}_2} = 1.46^2$). Fig. 4 (a) indicates the dimensions of perpendicular golden lattices that are identical to each other. The optical properties of gold are described by Johnson&Christy optical constants [71].

As an illustration, we consider the normal incidence of x-polarized 1200-nm light on the structure. Fig. 4 (b) and (c) show the dependence of the absorption and the calculation time, respectively, on the number of accounted Fourier harmonics correspondingly (we take $N_g = M_g$ for all the computations). Green lines and markers are responsible for the application of the standard Fourier-modal method (enhanced by Li’s factorization rules [72, 73]) to a 2D grating (straightforward approach) and act as reference values. One can see from Fig. 4 (c) that in logarithmic axes, single-processor calculation time almost immediately goes to a straight line of almost constant slope $\approx 2.5$, which is slightly smaller than the theoretical asymptotic limit of 3. The last computed point corresponding to $47^2 = 2209$ Fourier harmonics takes approximately 600 seconds. Nevertheless, due to the peculiarities of the metal properties, the absorption value is still far from convergence even for such a large number of harmonics as 2209 (see Fig. 4).

The application of the techniques proposed in this paper allows us to accelerate the calculations significantly. For the zero cut-off level (yellow lines and markers in Fig. 4 (b-c)) there is no filtration of high-$k$$_{∥}$ harmonics at all, which results in the same asymptotic time scaling (panel (c)) and the identical absorption (panel (b)), which matches the standard FMM up to machine precision. Nevertheless, the optimal approach for calculating the sublayers scattering matrices makes the computations approximately one order of magnitude faster, which

![Figure 4.](image-url)
is clearly seen from the gap between the parallel green and yellow lines (panel (c)). It is just because the number of the most asymptotically expensive mathematical operations is reduced approximately tenfold. This gives the possibility to account for a much larger number of harmonics at the same time.

Nevertheless, even more promising results are demonstrated by the approximate method that filters out high Fourier harmonics on the stage of calculating the combination of sublayers scattering matrices. Even such a small cut-off level as $\Theta = 10^{-10}$ results in a total change of the computation time dependence (red line in panel (c)). Indeed, while the number of harmonics is relatively small, none of them is ignored (Fig. 4(c), red and yellow lines coincide), but as soon as their number overcomes the threshold of approximately 670 harmonics, time to compute scattering matrices combination stops growing. This results in a bend of the graph line and flattening of its asymptotic. As it was shown before, theoretical estimation gives the quadratic scaling of the computation time $\tau \propto (N_g M_g)^2$ (for $N_g = M_g$), but in practice, we see the power of approximately $\approx 1.7$. In this way, the harmonics filtration results in an additional strong acceleration of the computations, and, moreover, this acceleration becomes the greater, the more harmonics are taken into account. It is also important that although the filtration-based approach is approximate, the computed absorption values match perfectly with the previous results, and no significant deviation is seen (see Fig. 4(b)). Therefore, the level of the filtration-specified precision does not prevent obtaining almost the full convergence potentially.

A relatively high cut-off level of $\Theta = 10^{-5}$ (blue lines and markers) shifts the threshold of line-bending to a much smaller number of harmonics so that it is no longer distinguishable (panel (c)). As it is seen from the graphs, this gives us a significant acceleration for the middle number of harmonics (300-3000), which can be most practical in calculations for many structures. At the same time, the coincidence with the previous, accurate calculations is perfect, which proves the remaining high level of precision (panel (b)).

The optimal choice of the number of harmonics and the cut-off level significantly depends on the materials and geometry of the structure, physical effects observed in the considered frequency range, and obviously on the desired precision.

V. EXAMPLES

The high speed and precision of computations makes it much easier to compute spectra of Moiré metasurfaces. In particular, here we explore the potential applications of the computational approach on the examples of the already discussed plasmonic lattices (twisted on different angles) and membrane diamond photonic crystal slab.

### A. Plasmonic crystal

Plasmonic crystals and as well as inclusions of plasmonic nanoparticles in photonic crystal slabs are well known for their ability to localize light at the nanoscale and form hybrid high-Q collective resonances [23, 33, 74]. Without a doubt, they can become the basis for a variety of Moiré superlattices as well.

The natural way to study the optical properties of the twisted plasmonic gratings is to consider isofrequency dispersion curves. In order to do that, we employ auxiliary high-index optical prism ($\varepsilon_{\text{prism}} = 16$) at a small distance from the structure (see schemes in Fig. 5) and use it for excitation of the guided modes. The absorption maps for $p$–polarized 1200 nm light, which excite surface plasmons in the plasmonic structures, are shown in Fig. 5. Panels (a) and (b) demonstrate that solitary lattices (constituents of the up-following stacks) support plasmons propagating along the golden sheets. Indeed, the longitudinally polarized surface waves that propagate along the structure almost do not feel the vertical walls of nanostrips and behave similarly to plasmons in an infinite metal slab. At the same time, the plasmonic modes polarized perpendicularly to the strips faces strong depolarization due to subwavelength dimensions of the latter one. For this reason such modes are naturally associated with localized resonances that are observed for smaller wavelengths. The fact that at the considered wavelength plasmon waves can propagate in one direction and cannot in the other one leads to concavity of its dispersion. An effective anisotropic medium can not accurately describe these plasmons due to the proximity of the first Brillouin zone boundaries (green dashed lines) to dispersion curves. Nevertheless, dispersion curves demonstrate typical hyperbolic-like behavior [91], which is widely spread in various nanophotonic applications [39]. It is worth noting that the modes of the structure located 100 nm from the prism (panel (a)) are obviously excited stronger than the ones of the 165 nm-disposed structure (panel (b)) due to decay of evanescent waves in SiO$_2$ layer.

Hybridization of upper- and lower-lattice plasmons in a stack is able to change their dispersion significantly. Interestingly, even interaction of perpendicularly crossed lattices leads to a formation of the closed square-like dispersion curve (see Fig. 5(c)). This effect is very similar to a topological transition in twisted graphene metasurfaces [39] and probably also can be implemented for so-called field canalization [39, 92]. Nevertheless, similar to the solitary lattices (panels a-b) $x$-propagating plasmons are less pronounced than $y$-propagating ones, which is explained just by an asymmetric prism-assisted excitation.

Relative rotation of the lattices is a powerful tool to shape the dispersion in a desired way. The 60° angle between nanoribbons makes the first Brillouin zone (Wigner–Seitz cell) a regular hexagon (see Fig. 5(d)), whereas the structure remains $C_2$-symmetric. Two pairs of its boundaries shown by green dashed lines originate
Figure 5. Absorption maps of p-polarised 1200 nm-wavelength light in four sketched SiO$_2$-embedded plasmonic lattices illuminated through the prism ($x$-$y$ projections show the bottom-up view, which is in accordance with other figures). Panels (a-b) demonstrate the hyperbolic-like behavior of plasmons in solitary lattices placed at different distances from the prism. Panels (c-d) show the modes hybridization in stacks of (c) perpendicularly- and (d) 60°-angle-crossed identical plasmonic lattices. Green dashed lines indicate the boundaries of the 1D lattices Brillouin zones, whereas the cyan lines are Moiré-pattern-associated boundaries.

from the reciprocal lattices of separate 1D sublattices, whereas the cyan pair corresponds to a specific Moiré-inspired effect associated with both sublattices. The interaction of lattices is most pronounced, where the resonances of individual lattices intersect (superimposition of panels (a) and (b)). Indeed, we observe strong anti-crossing of the surface plasmons near the "cyan" boundary of the Brillouin zone. Nevertheless, in this example, hybridization is mostly due to the interaction through the main harmonic. The lattice effect associated with a vicinity of the Brillouin zone boundary and corresponding interaction with Bragg-vector-coupled harmonics is very weak and does not significantly affect the behavior of the structure. The shape of the newly-formed dispersion curve is obviously determined by the original plasmons but strongly differs form them at the same time. Most importantly, dispersion becomes convex, which totally changes the behavior of the plasmon wavepackage propagation.

B. Dielectric crystal

As an example of dielectric Moiré structure, we explore optical properties of diamond photonic crystal slabs (see insets in Fig. 6) in the mid-infrared frequency range ($\lambda = 10\mu m$). These structures are diamond membranes in which identical periodic series of grooves are cut from both sides. The bottom of the grooves is covered by a thin, several-dozen-nanometer layer of graphite, which is naturally formed during the direct laser writing $^{[93]}$. The grooves are twisted on an angle $\alpha$ with respect to each other (the lower one is aligned with $y$ axis, $\beta = 0$), whereas the upper is rotated by the angle, $\alpha < 0$); the exact dimensions of the structures are indicated in Fig. 6. Diamond and graphite permittivities at 10$\mu$m wavelength are $\varepsilon_d = 5.6581 + 0.0004i$ and $\varepsilon_g = 9.99 + 35.55i$ correspondingly $^{[93]}$.

The considered structures do not have any mirror symmetry in the general case, which makes them chiral and
Figure 6. Absorption (a) and emission (b) of 10μm-light from the twisted diamond photonic crystal slab with graphite inclusions (insets). Panel (a) shows the absorption of the right- and left-handed circularly-polarized light as well as the degree of circular polarisation in absorption as a function of the rotation angle. Panel (b) demonstrates the angle-dependence of the upwards and downwards emission in the normal directions for the circularly polarised $\sigma^\pm$ dipoles. The bottom figure shows the routing efficiencies $\eta^- = -\eta^+$, which almost reach the ultimate unitary value.

perspective for manipulating circularly polarized light. In this way, we illuminate the structure by normally incident light of complementary circular polarizations and observe the absorption, which occurs predominantly (but not completely) in graphite. As one can see from Fig. 6 (a), absorption strongly depends on the angle $\alpha$ - there are lots of resonances that are excited for different angles. We see that the degree of circular polarisation, $\text{DCP} = (A_{RCP} - A_{LCP})/(A_{RCP} + A_{LCP})$, for the absorption reaches the high level of approximately 73% for approximately 57° angle of rotation (see the lower graph in Fig. 6 (a)). Even higher levels can be achieved with a thinner layer of graphite, but the finite physically meaningful thickness "blurs" the pure effect and limits its maximal value. According to the Lorentz reciprocity principle, the shown effect means that the thermal emission of a 10μm-wavelength, which can be observed from the Moiré structure, will be strongly circularly polarized in the normal direction. In this way, we can consider this structure as a passive source of circularly polarized thermal emission, which might be potentially implemented in the radiative heat transfer problems [45, 57, 59].

As for the angular dependence, it is clear that relatively large angles such as 50-90° correspond to typical 2D lattices, which have comparable to each other periods in two direction. Periods of the structure, as well as its optical properties, slowly change with an angle variation in this range, and therefore the resonances are wide in terms of the angular width. Nevertheless, as we discussed hereinafter, one of the structure periods tends to infinity with an angle going to zero. This results in a large number of sharp resonances and Rayleigh anomalies that interchange each other in the range of 15 – 50°. At the same time, the efficiency of the high harmonics excitation rapidly falls with angle decrease, and as a result, the amplitude of the dense modulation in Fig. 6 (a) becomes negligible for 0 – 15°. It is important to emphasize once again that small angles of rotation potentially require taking into account a huge number of harmonics at least to cover open diffraction channels. Nevertheless, in practice, we observe that up to a high level of precision, the convergence is achieved even when not all the opened channels are accounted for, which indirectly proves the weak contribution of the ignored harmonics to the properties of the whole structure. This effect paves the way to the potential studies of even large Moiré-period superlattices.

We consider the chiral structure, which has not only z-axis possessing a 2-fold rotation, but also two other axes of the same kind lying in the x – y plane. Overall, the structure has $D_2$ point group symmetry, making it perspective for the routing of the radiation from the circularly polarized dipole emitter [91]. Indeed, let us consider a point dipole that is located in the structure according to the inset of Fig. 6 (b) - in the middle of each of the graphite strips (in terms of x – y plane projection) and in the center of the slab (in terms of the z coordinate). We denote the dipoles of complementary circular polarisations $\mathbf{P}^\pm = [1, \pm i, 0]^T$ as $\sigma^\pm$ correspondingly. In this way, due to the symmetry of the structure, the intensity of light emitted upwards at a normal angle by $\sigma^+$ dipole $I_u^{+}$ is equal to the intensity of the $\sigma^-$
dipole downwards emission $I_{d}^{-} = I_{u}^{+}$. The same relation is valid for the complementary quantities $I_{u}^{-} = I_{d}^{+}$. This peculiarity simplifies the route of $\sigma^{\pm}$ dipoles emission to opposite directions. In case we manage to nullify the downwards emission of $\sigma^{-}$ dipole $I_{d}^{-} = 0$ that would automatically make the upwards emission of $\sigma^{+}$ dipole zero as well $I_{u}^{+} = 0$, which means that each dipole will radiate in its own direction. Such routing effect in $D_{3d}$ symmetric structure was already studied in detail in our previous paper [94].

It is convenient to evaluate the emission directivity numerically via the efficiencies $\eta^{\pm} = \frac{I_{d}^{-} - I_{u}^{+}}{I_{d}^{-} + I_{u}^{+}}$, which are connected with each other as well $\eta^{+} = -\eta^{-}$. The accurate choice of the geometric parameters allowed us to achieve almost perfect routing (more than 99.5% efficiency) for approximately 68° angle of rotation (Fig. 6(b)). It is clear from the upper graph in Fig. 6(b) that the most strong effect corresponds to the nullification of the emission in one of the directions due to the Fano lineshape of the resonance (blue line). In principle, the structure might be optimized to demonstrate this effect for narrow small-angle resonances that are observed in emission as well.

CONCLUSION

In this paper, we have proposed a modification of the Fourier modal method for consideration of twisted 1D lattices that form Moiré patterns. We have demonstrated the possibility of speeding up the computations from 1 to 3 and more orders depending on the number of harmonics without a noticeable decrease in the accuracy. Such an approach paves the way for rigorous study of modes hybridization in twisted photonic crystals slabs and the potential design of optical devices based on them. As an example, we have demonstrated the tuning of plasmonic modes dispersion and in a stack of plasmonic lattices. Also, the utilization of the diamond photonic crystal slab for circularly polarized thermal emission in the mid-infrared range and the emission routing from the circularly-polarized dipole source have been shown.

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