Equivalence of reflection paths of light and Feynman paths in stacked metasurfaces

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We show the existence of virtual polarization states during the interaction of modes in metasurface stacks. In support of our findings we experimentally realize a metasurface stack, consisting of an isotropic layer of nano-patches and an anisotropic layer of nano-wires. Utilizing an analogy to the interaction of electrons at junctions in mesoscopic electron transport via Feynman paths, we present a semi-analytical description of the modal interaction inside this stack. We then derive a series of all possible reflection paths light can take inside the metasurface stack.

I. INTRODUCTION

The concept of metasurfaces has permeated many aspects of technological advancement in photonics ⁴⁻⁷. Commonly, metasurfaces comprise artificial two-dimensional arrangements of sub-wavelength structures or particles ⁸⁻⁹. They promise arbitrary control of light ¹⁰⁻¹² and the creation of precisely engineered photon states ¹³⁻¹⁴. Recent examples of metasurface applications, ranging from hyperspectral imaging ¹⁷⁻¹⁸ to holography ¹⁹⁻²¹, lensing ²²⁻²⁴ and quantum photonics ²⁵⁻²⁸, substantiated that promise.

Many studies suggest it to be beneficial to combine different metasurfaces in multi-layered stacks ³¹⁻³⁴. A recent example enabled multi-wavelength meta-lensing by combining geometrically independent dielectric metasurfaces ²². Another work proposed cascading multiple layers of graphene with dielectric spacer layers to create a broadband optical absorber ²⁹. When light propagates through a stack, metasurfaces interact through inter-layer coupling. Adjacent metasurfaces couple either dominantly in the near-field ²² ³² or in the far-field ³¹ ³³ ³⁶. The coupling of near-fields depends on the structures of the metasurface and their local wavelength dependent resonances ³³ ³⁴ ²⁹. Far-field coupling, on the other hand, does not depend on any local resonance of the metasurfaces. Here, the only interaction mechanism between the metasurfaces is of a Fabry-Perot type ³¹ ³³ ³⁶ ³⁷. Due to the resonant characteristic of this mechanism it modifies the far-field coupling of the modes to adjacent metasurfaces ³³ ³⁶. Hence, we call this type of coupling modal coupling. Both numerical ³⁴ and semi-analytic ³⁶ simulations of far-field coupled metasurfaces reveal this phenomenon as part of the overall stack response. However, the actual interaction process during propagation through a stack is irretrievable from the overall response and, thus, remains hidden.

We aim to derive an interaction picture of stacked metasurfaces by expanding the modal interaction into a series of interfering reflected modes. In particular, we explore the interaction of modes inside a stack consisting of both an isotropic layer of gold nano-patches and an anisotropic layer of gold nano-wires. We analyze how isotropic and anisotropic modes contribute to the interaction and how they influence the total response. Finally, we reveal the existence of virtual polarization states during the modal interaction of the stack.

This work was motivated by the concept of electron scattering paths in mesoscopic solid state physics ³⁸⁻³⁹. Here, we attempt to compare and partially transfer this concept to the physics of nano-optics in the specific case of metasurface stacks.

The study of conduction in mesoscopic systems uses descriptive concepts equivalent to the aforementioned modal coupling in metasurface stacks ³⁰⁻³². Specifically, the process of electron scattering at junctions in mesoscopic structures can be considered analogously to the scattering of light at nano-structures ³²⁻³⁴. Scattering processes can be described by a set of connected ports in or out of which particles or waves can be transmitted or reflected ³⁰ ³⁵. In the case of mesoscopic electron transport this is the interaction of electrons from different leads at a given junction. Whether an electron is transmitted or reflected into a specific port or not is given by a probability ³⁰ ³⁶ ³⁷. Thus, for each combination of ports and whether the interaction results in transmission or reflection there exists a certain combined probability. When a scattering process is complete the final path an electron took can be described as a sum of all its possible paths, weighted by their probability for a given initial port ³⁹. Therefore, these paths give a picture of the interaction during the scattering process. In electron scattering theory they represent what is sometimes called the ‘Feynman paths’ of the system ³⁸⁻³⁹.

Similar to the scattering of electrons at junctions the interaction of light with metasurfaces can be formulated as a scattering problem and described by a set of connected ports ⁴⁵. Using scattering matrices (S-
matrices) these ports describe the transmitted and reflected modes in different diffraction orders and polarization states. Additionally, the scattering ports encode whether a mode propagates from front to back of a metasurface or vice versa. Here, we focus on the interaction in modally coupled stacks and establish our model based on the fundamental mode approximation (FMA) in optics of stratified media such an expansion is generally known as a Bremmer series. It leads to the optical WKB (Wentzel, Kramers, Brillouin) approximation of the Helmholtz equation for one-dimensionally inhomogeneous media. For the much more involved case of stacked metasurfaces we separate the response of the stack into a leading order term (i.e. the WKB term) and a series of consecutive interferometric terms. For two adjacent layers and front to back propagation this takes the form of

\[ S_{\text{Stack}} = S_N \cdots S_i \cdots S_1. \] (1)

In this notation light propagates along the z-axis from metasurface 1 to N. Each occurrence of the star product gives an overlap of the transmission functions of adjacent metasurfaces and includes all contributions of reflections between them. Mathematically, these contributions are represented by a reflection kernel of the form

\[ (\mathbb{I} - \tilde{R}_i^b \tilde{R}^d_{i+1})^{-1}, \] (2)

marking \(2 \times 2\) matrices with a hat and defining the two-dimensional identity as \(\mathbb{I}\). Here, \(\tilde{R}_i^b\) is the Jones-matrix for reflection of layer \(i\) when propagating back to front, as referred to by superscript \(b\), and \(\tilde{R}^d_{i+1}\) of layer \(i+1\) when propagating from front to back, as referred to by superscript \(d\). The reflection kernels contain exactly the Fabry-Perot type interactions of modally coupled metasurfaces. For a detailed picture of this interaction process it is therefore necessary to decompose it into its individual reflection paths.

III. REFLECTION PATHS IN STACKED METASURFACES

A. Geometric expansion of stacked S-matrices

In the following we will introduce the mathematical approach we employ to find individual reflection paths during the modal interaction between metasurfaces.

We can expand the reflection kernel of the star product of two S-matrices (\(N = 2\)) into a geometric matrix series, such that

\[ \left( \mathbb{I} - \tilde{R}_i^b \tilde{R}^d_{i+1} \right)^{-1} = \mathbb{I} + \sum_{\alpha=1}^{\infty} \left( \tilde{R}_i^b \tilde{R}^d_{i+1} \right)^\alpha. \] (3)

Then, each block matrix \(\tilde{S}^{ij}\) of a stacked S-matrix can be written as a matrix series

\[ \tilde{S}^{ij} = \tilde{S}_0^{ij} + \tilde{S}_1^{ij} + \tilde{S}_2^{ij} + \ldots, \] (4)

where \(i, j \in \{1, 2\}\) are the S-matrix’s block indices.

In optics of stratified media such an expansion is generally known as a Bremmer series. It leads to the optical WKB (Wentzel, Kramers, Brillouin) approximation of the Helmholtz equation for one-dimensionally inhomogeneous media. For the much more involved case of stacked metasurfaces we separate the response of the stack into a leading order term (i.e. the WKB term) and a series of consecutive interferometric terms. For two adjacent layers and front to back propagation this takes the form of

\[ \tilde{T}^f = \tilde{T}_1^f \tilde{T}_2^f + \tilde{T}_1^f \left( \sum_{\alpha=1}^{\infty} \left( \tilde{R}_1^b \tilde{R}_2^d \right)^\alpha \right) \tilde{T}_1^f \] (5)

for transmission and

\[ \tilde{R}^f = \tilde{R}_1^f + \tilde{T}_1^f \tilde{R}_2^d \tilde{T}_1^f + \tilde{T}_1^f \tilde{R}_2^d \left( \sum_{\alpha=1}^{\infty} \left( \tilde{R}_1^b \tilde{R}_2^d \right)^\alpha \right) \tilde{T}_1^f. \] (6)

for reflection. The infinite power series of reflection matrices contains all possible paths light can take between layers after consecutive reflections. For coherent excitation these paths will interfere, including the leading transmissive term. However, separating the pure transmission from inter-layer reflections allows us to analyze how these reflection paths influence the final result.

For more than two layers, we need to expand this concept to an arbitrary number of layers. Using the associativity of the star product eqs. \(\tilde{S}^{ij}\) and \(\tilde{S}_0^{ij}\) can be generalized to \(N\) layers by applying each new layer to all the previous ones combined. For this, we introduce the multi-index \(M_k \defeq 1, \ldots, (N - k)\), denoting
all modal contributions from the 1st to the \((N - k)\)th layer. A transmission or reflection matrix equipped with \(M_k\) includes all paths and recurring reflections up to the \((N - k)\)th layer, excluding those from following layers, \(N - k + 1, N - k + 2, \ldots\) and so forth. Imagining the propagation through a stack iteratively this is equivalent to successively connecting the scattering ports of each following layer to the input and output ports of all previous layers combined. Obeying the correct propagation directions (forward and backward) we thereby cascade all possible paths through a stack until the final output port to its substrate.

Then, the transmission through an \(N\)-layer stack can be written as

\[
\tilde{T}^{\text{f}}_{N,k} = \tilde{T}^{\text{f}}_{N-k} \prod_{p=1}^{N-k-1}\left(\mathbb{I} + \sum_{\alpha=1}^{\infty} \left(\tilde{R}^{\text{b}}_{M_p} \tilde{T}^{\text{f}}_{n_p-1}\right)^{\alpha}\right) \tilde{T}^{\text{f}}_{n_p}, \tag{7}
\]

using the compact index notation \(n_p \equiv N - k - p\). The occurring reflection matrices can be found recursively. Given the meaning of the multi-index \(M_k\) we also have to obey the order of products in eq. \((7)\). In the context of forward propagation, each backward reflection matrix \(\tilde{R}^{\text{b}}_{M_p}\) has its own frame of reference within the layer system of the stack. This allows us to comprehend where certain bundles of reflection paths originate from, both mathematically and physically.

Generally, a recursive multi-index reflection matrix is determined as follows,

\[
\tilde{R}^{\text{f}}_{M_k} = \tilde{R}^{\text{f}}_{M_{k+1}} + \tilde{T}^{\text{b}}_{M_{k+1}} \tilde{R}^{\text{f}}_{N-k-1} M_{k+1} + \tilde{T}^{\text{b}}_{M_{k+1}} \tilde{R}^{\text{f}}_{N-k-1} M_{k+1}
\]

Changing from forward to backward direction simply results in interchanging the superscripts \(f\) and \(b\) as well as reversing the index order. If \(M_k = 1\), only the first layer matrices are applied. The case \(k = 0\) gives the transmission or reflection of the complete system. Note that the order of indices results from applying the matrices right to left.

\[\text{B. Interpreting reflection path coefficients}\]

To gain insight on each single reflection path we can subtract series that are truncated at different orders \(\Psi\). For brevity, we choose an arbitrary, scalar transmission coefficient \(T\) of a stack described by eq. \((7)\). Introducing the subscript notation \(\{\Psi\}\) for a series up to order \(\Psi\), we define

\[
T_{\{\Psi\}} \overset{\text{def}}{=} \sum_{\alpha=0}^{\Psi} T_{\alpha}. \tag{9}
\]

With this, the \(\Psi\)th order contribution is given by

\[
T_{\Psi} = T_{\{\Psi\}} - T_{\{\Psi-1\}}. \tag{10}
\]

\[\text{IV. REFLECTION PATHS OF A PATCH-WIRE METASURFACE STACK}\]

\[\text{A. Design and fabrication}\]

Having established a theoretical framework we now have to ascertain how reflection paths of certain order contribute to an actual physical system.

In order to explore the effect of reflection paths in a real sample we designed and fabricated a metasurface stack consisting of two metasurfaces separated by a glass sample.
The upper or front facing metasurface is comprised of a 2D-array of gold nano-patches with period $\Lambda_p = 200 \text{ nm}$, average diameter $d_p = 70 \text{ nm}$, and height $h_p = 55 \text{ nm}$. The lower metasurface comprises a 2D-array of gold nano-wires with period $\Lambda_w = 300 \text{ nm}$, average lateral dimensions $d_w = 108 \text{ nm}$ and $l_w = 176 \text{ nm}$, and height $h_w = 45 \text{ nm}$. Both metasurfaces were embedded in a glass matrix. Fig. 1(a) shows a scanning electron beam (SEM) image of the sample.

Our fabrication technique employed structuring of a two layer resist via electron beam lithography, gold evaporation, and chemical lift-off. To obtain reference fields of each metasurface layer in the stack, we fabricated each on two separate fields: the stack itself (fig. 1(a)) and a single layer of the respective metasurface (figs. 1(b), (c)), resulting in a total of three samples. After fabricating the first metasurface with this technique, we added a spacer layer using spin-on glass (Futurrex IC1-200) and etched it to the desired thickness of $h_{sp} = 450 \text{ nm}$. We then fabricated the upper layer metasurface using the same approach as for the lower one. Finally, we added a fused silica cladding layer of thickness $h_c = 585 \text{ nm}$ by chemical vapor deposition.

### B. Semi-analytic modeling

We specifically chose patches and wires for their different symmetry, i.e. $C_4$ and $C_2$, respectively. This gave us the opportunity to analyze the effect of each reflection path on the anisotropic response of the stack, being itself anisotropic with an overall $C_2$ symmetry. Furthermore, the periods of the arrays have a ratio of $\Lambda_w/\Lambda_p = 3/2$, creating a super-period of the stacked unit cells, as shown in fig. 1(d). Modelling such super-periodic systems usually demands rigorous simulations with high computational effort. In our case, however, the spacer thickness of $h_{sp} = 450 \text{ nm}$ permits applying the FMA, enabling a more efficient semi-analytic approach.

We developed a model of the stack utilizing the semi-analytic-stacking algorithm (SASA) presented in [33, 36], which separates the problem into an analytic and a numeric part using S-matrices as described above. Berkhout and Koenderink recently published a comparable approach using transfer matrices. Since we deal with S-matrices and aim to analyze the properties of each scattering channel, SASA is the more suitable choice.

First, using the Fourier modal method (FMM) [45, 56], we computed the two metasurfaces’ S-matrices ($S_p$ for the patches and $S_w$ for the wires) separately for wavelengths ranging from 470 nm to 1200 nm, while assuming symmetric embedding. We specifically chose patches and wires for their different propagation characteristics.

Ellipsometric measurements of the materials produced by our fabrication processes supplied refractive index data [57]. Next, all homogeneous dielectric layers, i.e. the spacer, $S_{sp}$, and the cladding covering the stack, $S_c$, were calculated analytically as propagators of phases [36]. Furthermore, we applied Fresnel equations for the interface S-matrix $S_i$ at the top of the stack, representing the glass-air interface of the cladding [33]. In terms of S-matrices the stack is then given by the cascaded star product

$$S_{stack} = S_w \ast S_{sp} \ast S_p \ast S_c \ast S_i. \quad (12)$$

The glass wafer at the base of the sample can be considered as a glass half-space with respect to the stack and needs no representation by an S-matrix.

### C. Experimental validation

To ensure the validity of our SASA model we compared it against experimental results. Using a custom-built in-house characterization setup [58, 59], we performed interferometric measurements of both the single layer fields and the full stack, simultaneously measuring transmittance and phase in x- and y-polarization. The left column of plots shows transmittance and the right column phase. From top to bottom the plots show the results for the single layer control fields of the upper and lower metasurface, and of the full stack at the bottom. Dashed lines refer to SASA results and solid lines to the measurement. Blue and green differentiate between x- and y-polarization, respectively. Note that only x-polarization is plotted for the patch-metasurface as it is isotropic.
very good agreement between the SASA model and the measurement, both for transmittance and phase.

The isotropic patch-metasurface of the upper layer exhibits a single resonance at approximately 580 nm. On the other hand, the $C_2$ symmetric wire-metasurface of the lower layer shows two distinct resonances for different polarization at approximately 600 nm and 800 nm. The isotropic resonance overlaps with polarization sensitive resonances in the stacked configuration. For $x$-polarization this results in a broader and more prominent resonance at 600 nm. However, in $y$-polarization the transmittance now shows two resonances. The phase is mainly determined by the collective heights of spacer and cladding. Phase jumps at the resonance positions of the single layers combine in the stack.

D. Reflection path extraction

Having a valid model of the patch-wire stack we now move on to the extraction and analysis of its reflection paths. For brevity, we focus on forward transmission, i.e. propagation from top to bottom of the stack. The S-matrices of the homogeneous layers $S_{sp}$ and $S_{c}$ are diagonal matrices with exponential propagation phase terms of the form $e^{i \alpha k_0 h_n}$. Here, $n$ is the refractive index of the homogeneous medium, $h$ its thickness, and $k_0$ the vacuum wavenumber. With this we can write the geometric expansion of the patch-wire stack up to order $\Psi$ as

$$T_{M_0}^f = T_{w}^f \left( \mathbb{I} + \sum_{\alpha=1}^{\Psi} \left( R_{M_1}^b R_{w}^b \right)^\alpha \right) P_{sp} T_{p}^f \times \left( \mathbb{I} + \sum_{\beta=1}^{\Psi} \left( P_{c} R_{w}^b R_{p} \right)^\beta \right) P_{c} T_{t}^f, \quad (13)$$

where $P_{sp}$ and $P_{c}$ denote the propagation coefficients of spacer and cladding, respectively. Reflection and transmission at the glass-air interface of the cladding are given by the Jones matrices $\hat{R}_{t}^w$ and $\hat{T}_{t}^w$ of the interface S-matrix $S_t$ [36].

This can be interpreted as follows. The transmission matrices $\hat{T}_{t}^w$ are the input and output ports of the stack. Reading eq. (13) from right to left, the first parenthesis gives all interactions between the patch-metasurfaces and the top interface of the stack. The second parenthesis includes all interactions between the wire-metasurface and the patch-metasurface. The summations contribute all recurring reflections between those layers. In this context, the multi-index reflection matrix $\hat{R}_{M_1}^w$ bundles all recurring reflections between the top and the spacer of the stack in backward direction.

With the notation from eqs. [9] and [10] as well as using eq. (10) to calculate the reflection matrices in (13), we can formulate the explicit expressions of the physical reflection paths in eq. (13). In $x$-polarization the transmission coefficients of zeroth order and the first three paths contained at first order ($\Psi = 1$) read as

$$T_0 = T_w^x P_{sp} T_p P_c T_t, \quad (14)$$

$$T_1^{(1)} = T_w^x P_{sp} T_p T_c R_c P_c^3 T_t \quad (15)$$

$$T_1^{(2)} = T_w^x R_w^x P_{sp} P_{c}^2 T_p P_c T_t \quad (16)$$

$$T_1^{(3)} = T_w^x R_w^x P_{sp} T_p^3 T_c P_c^3 T_t, \quad (17)$$

where we omitted the superscripts f and b for the sake of readability. Above, eqs. (15) through (17) show the
coefficients of the paths emerging at first order, such that
\[ T_{11} = T_0 + (T_{11}^{(1)} + T_{11}^{(2)} + T_{11}^{(3)} + \ldots). \]
The graphical representation of these coefficients in fig. 3 shows the
paths in the context of the fabricated stack. Whereas
the leading transmissive term \( T_0 \) expresses propagation
straight through the stack, the first order paths include
different combinations of recurring reflections.

The leading transmissive term \( T_0 \) is composed of the
single layer transmission coefficients, with \( P_c \) and \( P_ap \)
imposing an additional phase shift. Both the isotropic
patch-metasurface and the anisotropic wire-metasurface
contribute equally to the combined transmission coefficient.
At higher orders each reflection path shows
different compositions of the isotropic and anisotropic
contributions. Therefore, they add different degrees of
anisotropy to the interferometric part of the stack’s
transmission.

Inputting the SASA results into eqs. (10) and (13)
we computed both the truncated series \( T_{\Psi} \) and the
coefficients \( T_{\Psi} \) of the patch-wire stack numerically. To
see how the series converges we truncated this time at
second order (\( \Psi = 2 \)). Fig. 4 shows amplitude and
phase of both sets of coefficients, \( \{T_{00}, T_{11}, T_{22}\} \) and
\( \{T_0, T_1, T_2\} \), both for x- and y-polarized light. Looking
at the set of truncated coefficients \( T_{\Psi} \) (figs. 4 (a), (b))
we see that the series already approximates the amplit-
uide of the full result well at 1st order. The phase, how-
ever, seems to be insensitive to the expansion. But this
is no surprise since the phase is mainly determined by
the propagation lengths in the stack and its resonances.
Any extra phase vanishes due to interference. In con-
trast, the set of coefficients contributing to each order
\( T_{\Psi} \) (figs. 4 (c), (d)) shows the accumulated phase of the
taken paths, albeit without interference. Here, we see
that the metasurfaces’ resonances manifest themselves
in the amplitude of the 1st order contribution.

E. Virtual polarization states

The discussion above showed how and to what degree
different orders of reflection paths contribute to the overall
stack response. Now, we can pose the question: what
other physical insights can we deduce from the properties
of reflection paths? Indeed, with an anisotropic stack at
hand we can gauge the degree of anisotropy at different
expansion orders.

By calculating the ellipticity of the sets of coefficients
from fig. 4 we can compare the stack’s overall anisotropic
response to that of each expansion order. From the
results shown in fig. 4 (a) we can conclude that for x-
polarization the stack’s response is mostly linearly polar-
ized with a slight deviation around the resonance wave-
length at 600 nm. In y-polarization (fig. 4 (b)) elliptical
polarization is produced around the stronger resonance
at 800 nm. As before, the geometric series converges al-
ready at 1st order.

The ellipticity of the individual reflection paths shows
more complex behavior (figs. 4 (c), (d)). For instance, at
first order in x-polarization a circular polarization state
emerges at a wavelength of 1000 nm (fig. 4 (c)). We term
such states virtual polarization states since they interfere
with other paths and produce only low amplitudes. This
demonstrates that the reflection paths of the patch-wire
stack are anisotropic to varying degree. Even though it is
small, they have a distinguishable influence on the stacks
overall anisotropic response.

V. CONCLUSIONS

In conclusion, we revealed the existence of virtual po-
larization states of a metasurface stack by analyzing the
reflection paths of its internal modal interactions. Our
approach was motivated by the treatment of electron
scattering in mesoscopic electron transport using a mul-
tiport formalism. This concept is mathematically equiv-
alent to the scattering matrix formalism we employed.
Based on this conceptual overlap we could adopt the
analogy of Feynman paths and electron scattering paths
to the scattering problem in stacked metasurfaces.

In this work we applied a geometric expansion to the
S-matrix of an anisotropic patch-wire metasurface stack
under the necessary condition of the FMA. We demon-
strated that its transmission could be separated into a
leading transmissive term and a series of interferometric terms, representing the reflection paths of the stack. By truncating the series and analyzing its constituent coefficients, we revealed the properties of paths of different order as well as their influence on the overall response.

The knowledge of reflection paths could prove useful in understanding the interaction of more complex stacks with multiple diffraction channels. Furthermore, we believe that the concept of Feynman paths could help in developing semi-analytic models of near-field interactions of complex nano-structures which can be challenging to comprehend, even numerically.

Finally, we would like to emphasize the benefit of adopting concepts from different fields of physics and identifying their similarities in order to gain more insight on certain physical phenomena.

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