Abstract — A generic semi-analytical approach is proposed for the self-consistent analysis of combinatorial frequency generation in stacks of binary nonlinear layers illuminated by a pair of pump waves. It is shown that the quasi-periodic stacks can be treated as the defected periodic structures with the defect located at the specific positions determined by a particular layer sequence. The developed technique combining the Harmonic Balance and Transfer Matrix Methods is illustrated by the cases of periodic and quasi-periodic (Fibonacci and Thue-Morse type) stacks of nonlinear dielectric layers.

1. G. D’Aguanno et al, Photonic band edge effects in finite structures and applications to c(2) interactions, Phys Rev E 64, 016609, 2001.

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Modified Transfer Matrix Method for the Problems of Nonlinear Scattering by Periodic and Quasi-Periodic Layered Structures

Oksana Shramkova & Alex Schuchinsky
Queen’s University Belfast, UK
Outline

- Introduction
- Problem statement & assumptions
- Solution framework
- Periodic and quasi-periodic (Fibonacci and Thue-Morse) stacks
- Primitive cells and defects in Fibonacci and Thue-Morse stacks
- Simulation examples
- Concluding remarks

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Periodic Stack

$q$ unit cells with alternating $A$ and $B$

\[ L_q = q(d_A + d_B) \]

Electric displacement in nonlinear anisotropic dielectric layers:

\[
D_{n}^{A,B} = \varepsilon_0 \left( \varepsilon_{nm}^{A,B} + \chi_{nmk}^{A,B} E_{k}^{A,B} \right) E_{m}^{A,B}
\]

\[
\hat{\varepsilon}^{A,B} = \left( \varepsilon_{xx}^{A,B}, \varepsilon_{xx}^{A,B}, \varepsilon_{zz}^{A,B} \right)
\]

\[
\hat{\chi}^{A,B} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \chi_{xxz} & 0 \\
0 & 0 & 0 & \chi_{xxz} & 0 & 0 & 0 \\
\chi_{zxx} & \chi_{zxx} & \chi_{zzz} & 0 & 0 & 0 & 0
\end{pmatrix}
\]
Quasi-Periodic Stacks

Fibonacci stack of order $q$

$S_q = \{S_{q-1} \cup S_{q-2}\}$, $S_1 = \{A\}$, $S_2 = \{AB\}$

$S_{q} = \{A\}$, $S_{2} = \{AB\}$

$L_{q} = L_{q-1} + L_{q-2}$

$L_1 = d_A$, $L_2 = d = d_A + d_B$

Thue-Morse stack of order $q$

$Q_q = \{Q_{q-1} \cup Q'_{q-1}\}$ & $Q'_{q} = \{Q'_{q-1} \cup Q_{q-1}\}$

$Q_0 = \{A\}$, $Q'_0 = \{B\}$

$L_{q} = 2L_{q-1}$

$L_1 = d = d_A + d_B$
Two TM plane waves of frequencies $\omega_1$ and $\omega_2$ are incident on the stacks at angles $\Theta_{i1}$ and $\Theta_{i2}$

Nonlinearity is assumed weak and the three-wave mixing process is dominant

The problem is linearized by harmonic balance method to obtain combinatorial frequency fields

In the non-depleting wave approximation the fields are determined recursively at each frequency

- Pump waves: only reflected and refracted fields
- Combinatorial frequencies: excited & scattered fields
Linearized Problem

In the three-wave mixing process, fields $H_y(\omega)$ of TM waves satisfy Helmholtz equation in each layer $A$ and $B$ at pump $\omega_{1,2}$ and combinatorial $\omega_3=\omega_1+\omega_2$ frequencies:

$$
\left( \frac{\partial^2}{\varepsilon_{xx} \partial z^2} + k_p^2 - \frac{k_{xp}^2}{\varepsilon_{zz}} \right) H_y(\omega_p) = \begin{cases} 
0, & p = 1, 2 \\
8\pi k_3 \left[ \frac{\partial}{\partial x} \left( \frac{\chi_{xxx}}{\varepsilon_{zz}} E_x(\omega_1) E_x(\omega_2) + \frac{\chi_{zzz}}{\varepsilon_{zz}} E_z(\omega_1) E_z(\omega_2) \right) - \\
\frac{\chi_{xxz}}{2\varepsilon_{xx}} \frac{\partial}{\partial z} \left( E_x(\omega_1) E_z(\omega_2) + E_x(\omega_2) E_z(\omega_1) \right) \right], & p = 3
\end{cases}
$$

where

$$
k_p = \omega_p / c, \quad k_{x1,x2} = k_{1,2} \sqrt{\varepsilon_a} \sin \Theta_{i1,i2}$$

$$
k_{x3} = k_{x1} + k_{x2} = k_3 \sqrt{\varepsilon_a} \sin \Theta_3$$
Solution of the Linearized Problem

In a layer of type $j=A, B$ in $n^{th}$ primitive cell:

- At pump wave frequencies $\omega_{1,2}$
  \[ H_{yj}^{(n)}(\omega_p) = \left[ B_{pj}^{n+} e^{ik_{zj}^{(p)} z} + B_{pj}^{n-} e^{-ik_{zj}^{(p)} z} \right] e^{-i\omega_p t + ik_{zp} x}, \quad p = 1, 2 \]

- At combinatorial frequency $\omega_3$
  \[ H_{yj}^{(n)}(\omega_3) = \left( B_{3 j}^{n+} e^{ik_{zj}^{(3)} z} + B_{3 j}^{n-} e^{-ik_{zj}^{(3)} z} + D_{1j}^{n+} e^{ik_{zj}^{+} z} + D_{2j}^{n+} e^{-ik_{zj}^{+} z} + D_{1j}^{n-} e^{ik_{zj}^{-} z} + D_{2j}^{n-} e^{-ik_{zj}^{-} z} \right) e^{-i\omega_3 t + ik_{z3} x}, \]

where

\[ B_{pj}^{n\pm} = B_j^{n\pm}(\omega_p), \quad k_{zj}^\pm = k_{zj}^{(1)} \pm k_{zj}^{(2)}, \quad k_{zj}^{(p)} = \sqrt{\varepsilon_{xj} \left( k_p^2 - k_{zp}^2 / \varepsilon_{zzj} \right)}, \quad p = 1, 2, 3 \]

\[ D_{1j}^{n+} = \alpha_j \beta_j \frac{B_{1j}^{n+} B_{2j}^{n+}}{(k_{zLj}^+)^2 - (k_{zLj}^{(3)})^2}, \quad D_{2j}^{n+} = \alpha_j \beta_j \frac{B_{1j}^{n-} B_{2j}^{n-}}{(k_{zLj}^+)^2 - (k_{zLj}^{(3)})^2} \]

\[ D_{1j}^{n-} = \alpha_j \gamma_j \frac{B_{1j}^{n+} B_{2j}^{n-}}{(k_{zLj}^-)^2 - (k_{zLj}^{(3)})^2}, \quad D_{2j}^{n-} = \alpha_j \gamma_j \frac{B_{1j}^{n-} B_{2j}^{n-}}{(k_{zLj}^-)^2 - (k_{zLj}^{(3)})^2} \]
Amplitude Coefficients $B_{j}^{n\pm}(\omega_{p})$

The problem has been reduced to evaluating amplitudes of waves refracted into a layer of type $j = A, B$ in an $n^{th}$ primitive cell of the stack.

$$B_{j}^{n\pm}(\omega_{p}) = \left( \eta_{j11}^{(n-1)}(\omega_{p}) \pm \frac{k_{p}}{k_{zLj}} \varepsilon_{xxj} \eta_{j21}^{(n-1)}(\omega_{p}) \right) \left[ 1 + R(\omega_{p}) \right] +$$

$$+ \frac{k_{zLj}}{k_{p} \varepsilon_{a}} \left( \eta_{j12}^{(n-1)}(\omega_{p}) \pm \frac{k_{p}}{k_{zLj}} \varepsilon_{xxj} \eta_{j22}^{(n-1)}(\omega_{p}) \right) \left[ 1 - R(\omega_{p}) \right]$$

where $R(\omega_{p})$ - the reflection coefficient of the stack;

$\eta_{j}^{(n-1)}(\omega_{p})$ - the transfer matrices of a subset of $(n - 1)$ primitive cells preceding the layer of type $j$ in the $n^{th}$ primitive cell.
Emission Coefficients

Amplitudes of the combinatorial frequency emission in the reverse ($F_r$) and forward ($F_t$) directions

$$F_r = \left(\frac{k_3 \varepsilon_a}{k_{za}^{(3)}} \tilde{\eta}_{N_q} (\omega_3)_{2,1} + \tilde{\eta}_{N_q} (\omega_3)_{2,2}\right) \lambda_1 - \left(\frac{k_3 \varepsilon_a}{k_{za}^{(3)}} \tilde{\eta}_{N_q} (\omega_3)_{1,1} + \tilde{\eta}_{N_q} (\omega_3)_{1,2}\right) \lambda_2,$$

$$F_t = -\left(\lambda_1 + \lambda_2 \frac{k_3 \varepsilon_a}{k_{za}^{(3)}}\right),$$

where $\tilde{\eta}_{N_q} (\omega_3)$ - a transfer matrix of the whole stack containing $N_q$ primitive cells

$$\lambda_{1,2} = \sum_{n=1}^{N_q} f \left(\tilde{\eta}_j^{(n)} (\omega_3), D_{1j}^{n\pm}, D_{2j}^{n\pm}\right)$$
The transfer matrices of the stack and any its subset depend on
- Stack configuration and layer sequence
- Transfer matrices of the constituent layers

The transfer matrices are to be calculated at each frequency: both pump waves and mixing products

The transfer matrices at frequency $\omega_3$ are used in the expression of $F_{r,t}$ and $B_j^{n\pm}(\omega_3)$
Regular Periodic Stacks

- Transfer matrices for
  - Stack of $n$ unit cell:  \[ \hat{\eta}_A^{(n)} = \hat{\eta}_n = \left[ \hat{m}_{LA}(\omega_3) \hat{m}_{LB}(\omega_3) \right]^n \]
  - 1st layer in $n$ unit cell stack:  \[ \hat{\eta}_B^{(n)} = \hat{\eta}_{n-1} \hat{m}_{LA}(\omega_3) \]
  - Layers $A$ and $B$:  \[ \hat{m}_{LA}(\omega_3) \text{ and } \hat{m}_{LB}(\omega_3) \]

- Transfer matrices $\hat{\eta}_j^{(n)}$ have closed form relating $\hat{\eta}_1$ with Bloch phase in periodic stacks
- There is no advantage of using the closed form here – fields must be calculated inside each layer
- The recursive relation for  \[ \hat{\eta}_n = \hat{\eta}_{n-1} \left[ \hat{m}_{LA}(\omega_3) \hat{m}_{LB}(\omega_3) \right] \]
Quasi-Periodic Stacks

Transfer matrices for Fibonacci & Thue-Morse stacks are defined by the recursive relations

**Fibonacci stacks of order** \( q \geq 2 \)

\[ S_q = \{ S_{q-1} \cup S_{q-2} \}, \quad S_1 = \{ A \}, \quad S_2 = \{ AB \} \]

**Transfer matrix**

\[ \hat{M}_q (\omega_p) = \hat{M}_{q-1} (\omega_p) \hat{M}_{q-2} (\omega_p) \]

where

\[ \hat{M}_0 (\omega_p) = \hat{m}_{LB} (d_B, \omega_p), \quad \hat{M}_1 (\omega_p) = \hat{m}_{LA} (d_A, \omega_p); \]

**Examples:**

\[ S_5 = \{ AB AAB AB A A \} \]
\[ S_6 = \{ AB AAB AB AAB AAB \} \]

**Thue-Morse stacks of order** \( q \geq 1 \)

\[ Q_q = \{ Q_{q-1} \cup Q'_{q-1} \} \quad & \quad Q'_q = \{ Q'_{q-1} \cup Q_{q-1} \} \]

\[ Q_0 = \{ A \}, \quad Q'_0 = \{ B \} \]

**Transfer matrices**

\[ \hat{M}_q (\omega_p) = \hat{M}_{q-1} (\omega_p) \hat{M}'_{q-1} (\omega_p) \]

\[ \hat{M}'_q (\omega_p) = \hat{M}'_{q-1} (\omega_p) \hat{M}_q (\omega_p) \]

\[ \hat{M}_0 (\omega_p) = \hat{m}_{LA} (d_A, \omega_p), \quad \hat{M}'_0 (\omega_p) = \hat{m}_{LB} (d_B, \omega_p) \]

**Examples:**

\[ Q_3 = \{ AB BA BA AB \} \]
\[ Q_4 = \{ AB BA BA AB \} \]

Defective cells
Fibonacci & Thue-Morse stacks can be treated like periodic stacks with defects

**Fibonacci stacks**

\[ S_5 = \{ AB \ A'B \ AB \ A \} \]
\[ S_6 = \{ AB \ A'B \ AB \ A'B \ A'B \} \]

- Two types of primitive cells:
  - regular \{AB\}
  - “defective” \{A'B\}
- Layer A' in “defective” cells is a doublet \(A' = AA\) with \(d'_A = 2d_A\)
- Both “regular and “defective” cells have the layers in the same order

**Thue-Morse stacks**

\[ Q_3 = \{ AB \ BA \ BA \ AB \} \]
\[ Q_4 = \{ AB \ BA \ BA \ AB \ BA \ AB \ BA \ AB \ BA \} \]

- Two types of primitive cells:
  - regular \{AB\}
  - “defective” \{BA\}
- Layers A and B in “defective” cells are interchanged
- Both “regular and “defective” cells have the same thickness \(d = d_A + d_B\)

Positions of “defective” cells in the stacks are to be determined
Primitive Cells in Thue-Morse Stacks

- The number of primitive cells in a stack of order $q$:
  \[ N_q = 2^{q-1} \]

- The positions of the regular and defective cells are determined by their serial number $n$ using the following recurrence relation at $n \geq 3$
  \[
  t_n = \begin{cases} 
  1 - t_{n-1}, & n \text{ odd} \\
  t\left(\frac{n-1}{2} + 1\right), & n \text{ even}
  \end{cases}
  \]
  where $t_n = 0$ for the regular cell $\{AB\}$
  $t_n = 1$ for defective cells $\{BA\}$
  $t_1 = 0$, $t_2 = 1$
Primitive Cells in Fibonacci Stacks

The number of primitive cells in a stack of order $q$:

$$N_q = \begin{cases} 
\frac{\Phi_{q+1} - \Gamma_q}{2}, & q \text{ even} \\
\frac{\Phi_{q+1} - \Gamma_q - 1}{2}, & q \text{ odd}
\end{cases}$$

where $\Phi_q = \Phi_{q-1} + \Phi_{q-2}$ is Fibonacci number, $\Phi_1 = \Phi_2 = 1$

The number of “defective” cells $\Gamma_q$: $\Gamma_q = 0$ at $q \leq 3$ and at $q \geq 4$

$$\Gamma_q = \begin{cases} 
\left(\frac{3 + \sqrt{5}}{2}\right)^{q-1} - \left(\frac{3 - \sqrt{5}}{2}\right)^{q-1}, & q \text{ even} \\
\sqrt{5}^q, & q \text{ odd}
\end{cases}$$
“Defective” Cells in Fibonacci Stacks

Positions of additional $A$ layers in Fibonacci stack of order $q$ are defined by a row-matrix $\widehat{P}_q$ of length $\Phi_{q+1}$ with 1’s in the columns for the first $A$ layer of the doublets:

$$S_6 = \{AB \ AAB \ AB \ AAB \ AAB\}$$

$$\widehat{P}_6 = [00 \ 100 \ 00 \ 100 \ 100]$$

$\widehat{P}_q$ is defined by the recurrence relations:

$$\widehat{P}_q = \widehat{P}_{q-1} + \widehat{P}_{q-2} \widehat{\Phi}(\Phi_q) + \begin{cases} \widehat{u}(\Phi_q), & q - \text{even} \\ 0, & q - \text{odd} \end{cases}$$

where $\widehat{u}(\Phi_q) = \{\delta_{i,\Phi_q}\}$ is a row-matrix with 1’s in $\Phi_q$ column only; $\widehat{\Phi}(\Phi_q) = \{\delta_{i+\Phi_q,j}\}$ is a square Toeplitz matrix with 1’s only at the secondary diagonal offset for $\Phi_q$ from the main diagonal.
Stack Reflectance: QPS vs Periodic

Periodic \( q=16 \)

- Periodic \( q=16 \) (32 layers, \( d_B=13\mu m \))
- Fibonacci \( S_8 \) (34 layers, \( d_B=12\mu m \))
- Thue-Morse \( Q_5 \) (32 layers, \( d_B=13\mu m \))

- \( \Theta_i = 30^\circ \) (dashed lines)
- \( \Theta_i = 45^\circ \) (solid lines)

\[ d_A = d_B \left(1 + \sqrt{5}\right)/2 \]
$\omega_3$ Emission: QPS vs Periodic

Fibonacci $S_8$ (34 layers, $d_B=12\mu m$)

Thue-Morse $Q_5$ (32 layers, $d_B=13\mu m$)

Periodic $q=16$ (32 layers, $d_B=13\mu m$)

$\Theta_{i1} = 30^\circ$, $\Theta_{i2} = 45^\circ$; $d_A = d_B \left(1 + \sqrt{5}\right)/2$

$|F_r|$ - solid lines

$|F_t|$ - dashed lines

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Effect of Loss

**Fibonacci** $S_8$: 34 layers, $d_B=12\mu m$

**Thue-Morse** $Q_5$: 32 layers, $d_B=13\mu m$

$\tan \delta = 0.01$

$\Theta_{i1} = 30^\circ$, $\Theta_{i2} = 45^\circ$;
Concluding Remarks

- The semi-analytical approach to modelling combinatorial frequency generation by periodic and quasi-periodic multilayers has been developed.
- The technique provides a unified framework for the analysis of periodic and quasi-periodic stacks.
- It is shown that Fibonacci and Thue-Morse stacks can be treated like periodic structures with defects.
- The developed theory is illustrated by simulations and provides an insight in the mechanisms of three-wave frequency mixing in the binary stacks.