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Beyond the Parity and Bloch Theorem: Local Symmetry as a Systematic Path-way to the Breaking of Discrete Symmetries

P. Schmelcher

Center for Optical Quantum Technologies
University of Hamburg
Germany

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Workshop and Guest Program

in collaboration with

- C. Morfonios (University of Hamburg)
- F.K. Diakonos (University of Athens)
- P.A. Kalozoumis (Univ. Athens and Hamburg)

Outline

1. Introduction and Motivation
2. Invariant Non-Local Currents
3. Generalized Parity and Bloch Theorems
4. Locally Symmetric Potentials
5. Summary - Theoretical Foundations of Local Symmetries
6. Application to Photonic Multilayers

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1. Introduction and Motivation

Symmetries

- represent a cornerstone and fundamental principle in physics
- are ubiquitous in nature
- apply to many different disciplines of physics
- allow to make predictions for a system without solving the underlying equations of motion !
  - quantum mechanics: group and representation theory
  - $\Rightarrow$ multiplets, degeneracies, selection rules and structure (redundancy)

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Global Symmetries we are used to

- rotation O(3): atoms, quantum dots,....
- molecular point group symmetries: inversion, reflection, finite rotation (C_{2v}, $C_{\infty h}$, ...)
- discrete translational symmetry: periodic crystals
- gauge symmetries $U(1)$, $SU(3) \times SU(2) \times U(1)$

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Introduction: Symmetries and Invariants

Symmetries: Emergence of conservation laws (invariants) that simplify mathematical description

Classical particles and fields: Noether theorem (invariant currents), continuity and boundary effects

Quantum mechanics: Commutation relations, not restricted to continuous transforms, good quantum numbers

Yes or No access to symmetry: Global !

What about remnants ? $\Rightarrow$ Local !

In general: no systematic way to describe the breaking of symmetry !

Field theory: Spontaneous symmetry breaking (Higgs mechanism, global)

Introduction

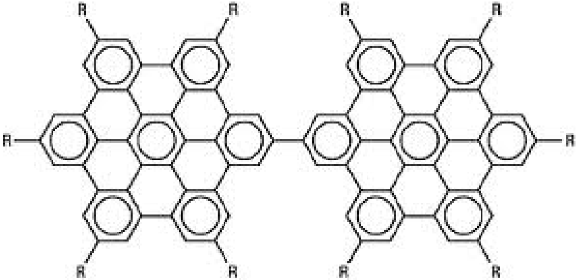
But what about more complex ’less pure and simply structured’ systems

Nature: From global to local symmetry !

In most cases a local symmetry, spatially varying, exists, but no global symmetry !

Introduction

Lets look at molecules:



Superbiphenyl

R = *n*-dodecyl, *t*-butyl

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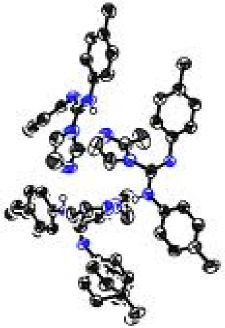

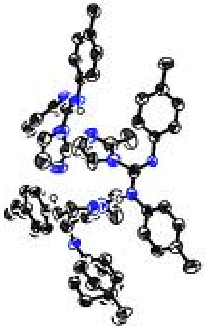

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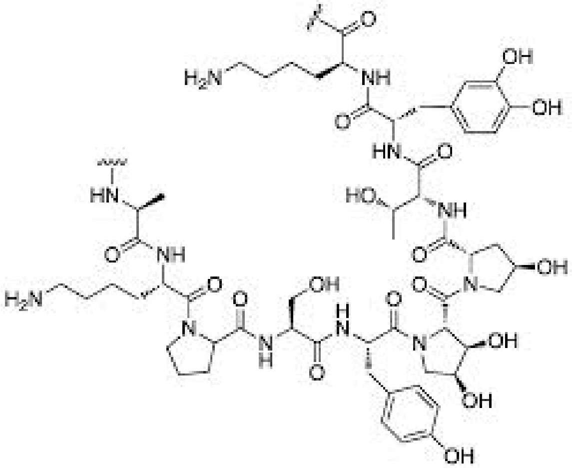

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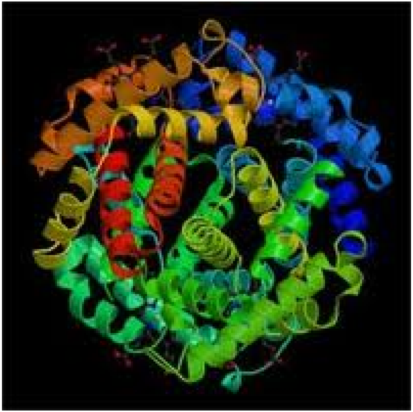
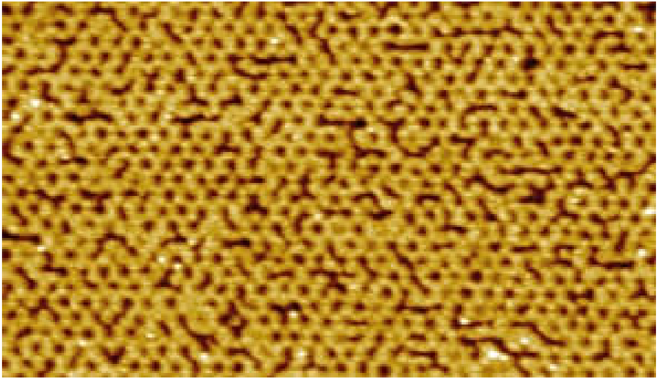
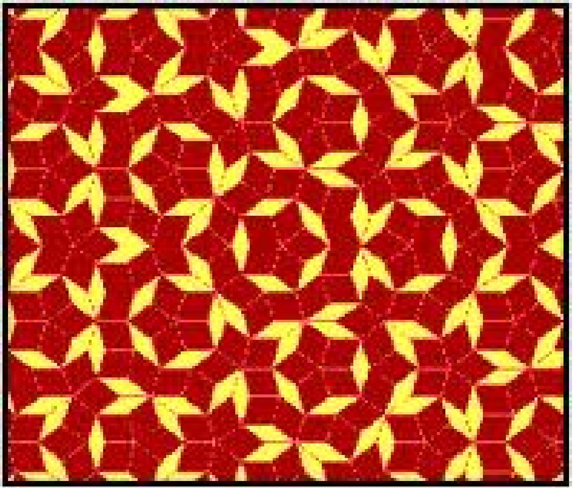


Lets look at surfaces:



Lets look at quasicrystals:



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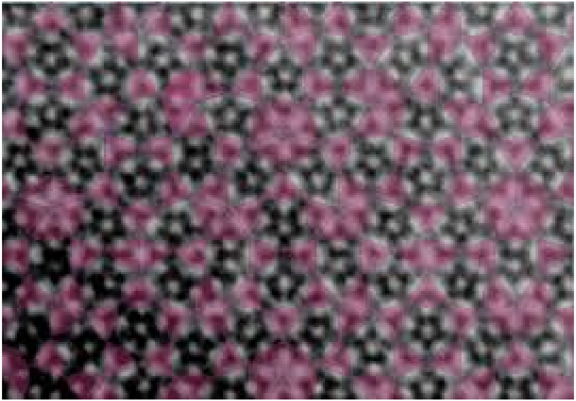
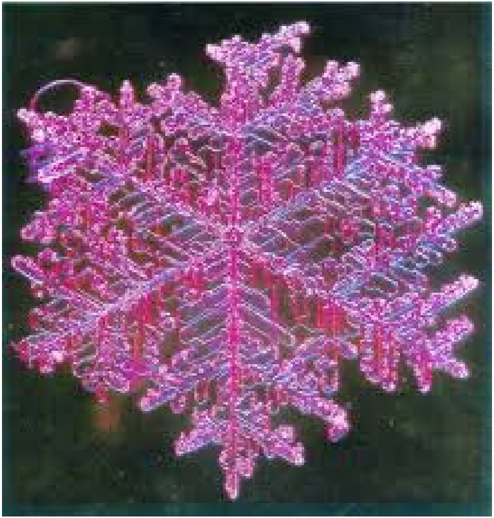


Introduction

Lets look at a snow-crystal:



Introduction

In sharp contrast to this:

There is no concept or theory of local spatial symmetries in physics !

Pathway of symmetry breaking

- global symmetry obeyed
  - inversion symmetry (parity): atoms, molecules, clusters ⇒ even/odd states
  - discrete translational symmetry: periodic crystals ⇒ Bloch phase and theorem
- introduce asymmetric boundary conditions: scattering setup breaks symmetry
- LOCAL SYMMETRY

Does any impact of symmetry on a local scale survive ?

Is there something like a generalized parity or Bloch theorem ? Or does symmetry breaking erase all signatures of the remnants of the symmetry ?

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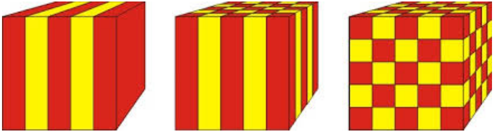
Focus on wave-mechanical systems:

- Acoustics (granular phononic crystals)
- Optics (photonic multilayers and crystals)
- Quantum Mechanics (electrons in semiconductor heterostructures, cold atoms ?)
- ....



2. Invariant Non-Local Currents

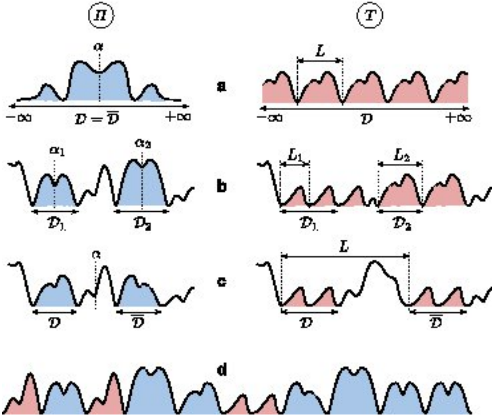
Wave equation of motion

Unified theoretical framework: Helmholtz equation with a complex wave field $\mathcal{A}(x)$

$$\mathcal{A}''(x) + U(x)\mathcal{A}(x) = 0$$

- optics - electromagnetic wave: $U(x) = \frac{\omega^2 n^2(x)}{c^2}$
- matter wave: quantum mechanics $U(x) = \frac{2m}{\hbar^2}(E - V(x))$
  $\mathcal{A}(x)$ wave function
- acoustics: sound waves
- focus on scattering

Complexity emerges due to $U(x)$: From global to local symmetries



Come back to the corresponding classification later !

Symmetry transformations

Consider the following (linear) spatial symmetry transformations:

$$F: \; x \rightarrow \overline{x} = F(x) = \sigma x + \rho,$$

$$\begin{aligned} \sigma = -1, \quad \rho = 2\alpha \; &\Rightarrow F = \Pi \quad &: \text{inversion through } \alpha \\ \sigma = +1, \quad \rho = L \; &\Rightarrow F = T \quad &: \text{translation by } L \end{aligned}$$

Assume now the following symmetry of $U(x)$

$$U(x) = U(F(x)) \quad \forall \; x \in \mathcal{D}$$

If $\mathcal{D} = \mathbb{R}$, then the above symmetry is global, otherwise the symmetry is called local.

$F(\mathcal{D}) = \overline{\mathcal{D}} \neq \mathcal{D}$ in general, but not for local inversion and parity.

Invariant nonlocal currents

Exploit the equation of motion and construct the difference $\mathcal{A}(\overline{x})\mathcal{A}''(x) - \mathcal{A}(x)\mathcal{A}''(\overline{x})$. One can show then:

$$\mathcal{A}(\overline{x})\mathcal{A}''(x) - \mathcal{A}(x)\mathcal{A}''(\overline{x}) = 2iQ'(x) = 0,$$

which implies that the complex quantity

$$Q = \frac{1}{2i}\left[\sigma\mathcal{A}(x)\mathcal{A}'(\overline{x}) - \mathcal{A}(\overline{x})\mathcal{A}'(x)\right] = \textit{constant}$$

is spatially invariant (constant in x) within the domain $\mathcal{D}$.
Repeating the procedure with the complex conjugation yields

$$\widetilde{Q} = \frac{1}{2i}\left[\sigma\mathcal{A}^{*}(x)\mathcal{A}'(\overline{x}) - \mathcal{A}(\overline{x})\mathcal{A}'^{*}(x)\right]$$

Invariant non-local currents $\leftrightarrow$ Invariant two-point correlators at symmetry related points !

Invariant nonlocal currents

Additionally we have, of course, the global current J (probability (QM), energy (optics,acoustics))

$$J = \frac{1}{2i}\left[\mathcal{A}^*(x)\mathcal{A}'(x) - \mathcal{A}(x)\mathcal{A}'^*(x)\right]$$

Some algebra shows that the non-local currents are related to the global current within each symmetry domain $\mathcal{D}$

$$|\widetilde{Q}|^2 - |Q|^2 = \sigma J^2$$

$|\widetilde{Q}| > |Q|$ for local translations and $|\widetilde{Q}| < |Q|$ for local parity

3. Generalized Parity and Bloch Theorems

Preliminaries

A brief reminder: **Global discrete symmetries**

Inversion symmetry leads to the **parity theorem**: $\psi(-x) = \pm\psi(x)$

Periodicity leads to the **Bloch theorem**: $\psi(x) = exp(ikx)\phi_k(x)$ with $\phi_k(x + L) = \phi_k(x)$ being periodic

with the Bloch phase $exp(ikL)$

(alternatively $\psi(x + L) = exp(ikL)\psi(x)$)

Generalized parity and Bloch theorems

Goal:
Use the invariants Q, $\widetilde{Q}$ to obtain a definite relation between the wave field $\mathcal{A}(x)$ and its image $\mathcal{A}(\overline{x})$ under a symmetry transformation.

This would generalize the usual parity and Bloch theorems to the case where global inversion and translation symmetry, respectively, is broken.

Herefore: define an operator $\hat{O}_F$ which acts on $\mathcal{A}(x)$ by transforming its argument through $F = \Pi$ or T: $\hat{O}_F \mathcal{A}(x) = \mathcal{A}(\overline{x} = F(x))$.

Some algebra then yields:

$$\hat{O}_F \mathcal{A}(x) = \mathcal{A}(\overline{x}) = \frac{1}{J} \left[\widetilde{Q} \mathcal{A}(x) - Q \mathcal{A}^*(x) \right]$$

for all $x \in \mathcal{D}$.

Central result providing a generalized symmetry image !

Generalized parity and Bloch theorems

$$\hat{O}_F \mathcal{A}(x) = \mathcal{A}(\overline{x}) = \frac{1}{J}\left[\widetilde{Q}\mathcal{A}(x) - Q\mathcal{A}^*(x)\right]$$

for all $x \in \mathcal{D}$.

Invariant non-local currents Q, $\widetilde{Q}$, induced by the generic symmetry of $U(x)$, provide the mapping between the field amplitudes at points related by this symmetry, regardless if the symmetry is global or not.

This generalized transformation of the field can therefore be identified as a remnant of symmetry in the case when it is globally broken.

P.A. Kalozoumis, C. Morfonios, F.K. Diakonos and P. S., PRL 113, 050403 (2014)

UHH

In a nutshell

Mapping relation

$$\begin{pmatrix} \mathcal{A}(\overline{x}) \\ \mathcal{A}^*(\overline{x}) \end{pmatrix} = \frac{1}{J} \begin{pmatrix} \widetilde{Q} & -Q \\ -Q^* & \widetilde{Q}^* \end{pmatrix} \begin{pmatrix} \mathcal{A}(x) \\ \mathcal{A}^*(x) \end{pmatrix}$$

$$det \frac{1}{J} \begin{pmatrix} \widetilde{Q} & -Q \\ -Q^* & \widetilde{Q}^* \end{pmatrix} = \sigma$$

- The $\underline{\underline{Q}}$-matrix belongs to the U(1,1) group
- However note: The above is a nonlinear identity
- Local basis renders the above relation diagonal

Back to global symmetry

$$\hat{O}_F \mathcal{A}(x) = \mathcal{A}(\overline{x}) = \frac{1}{J}\left[\widetilde{Q}\mathcal{A}(x) - Q\mathcal{A}^*(x)\right]$$

A nonvanishing Q is a manifestation of broken global symmetry under the discrete transformation F.

$\Rightarrow$ Recovery of the usual parity and Bloch theorems for globally Π- and T-symmetric systems

When $Q = 0$, the field $\mathcal{A}(x)$ becomes an eigenfunction of $\hat{O}_{F=\Pi,T}$.

$$\hat{O}_F \mathcal{A}(x) = \frac{\widetilde{Q}}{J}\mathcal{A}(x) \equiv \lambda_F \mathcal{A}(x)$$

Back to global symmetry

$$\hat{O}_F \mathcal{A}(x) = \frac{\widetilde{Q}}{J}\mathcal{A}(x) \equiv \lambda_F \mathcal{A}(x)$$

One can immediately see that $|\frac{\widetilde{Q}}{J}| = 1$, so that any eigenvalue of $\hat{O}_F$ is restricted to the unit circle $\lambda_F = e^{i\theta_F}$!

In more detail:

- For inversion Π we get $\lambda_\Pi = \pm 1$
- For translation $\widetilde{Q} = \pm|J|e^{i\theta_{\widetilde{Q}}} = \pm|J|e^{ikL}$ which constitutes the Bloch theorem

$Q = 0$: Global symmetry (note on BC).
$Q \neq 0$: Locally broken symmetry.
Q is a symmetry breaking (order) parameter !

4. Locally Symmetric Potentials

Locally symmetric potentials

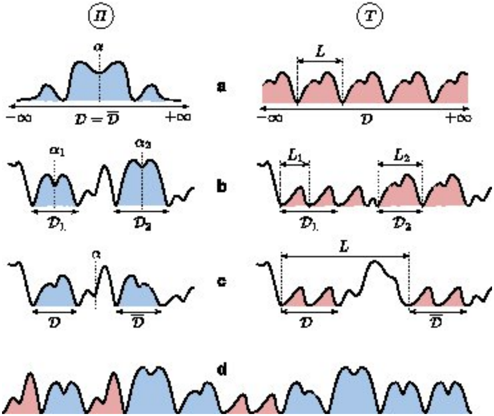
Invariance $U(x) = U(F(x))$ on limited domains: Local parity or translation invariance.

$\Rightarrow \hat{O}_F$ does not commute with $\hat{H}$!

Local symmetry impact is analyzed in terms of invariants Q and $\widetilde{Q}$.

Distinguish different cases !

Classification of locally symmetric potentials



1. Global symmetries

2. Non-gapped local symmetries - for every domain there exist the invariants Q and $\widetilde{Q}$ which map the wave function.

3. Gapped local symmetries - a domain $\mathcal{D}$ has no overlap with its symmetry-related image ($\overline{\mathcal{D}} \cap \mathcal{D} = \varnothing$). Gaps can be symmetry elements or not. Qs connect wave functions of distant elements.

4. Complete local symmetries - intertwined symmetry domains possible on different spatial scales - long range order.

The latter suggests a new class of materials with unique properties !

CLS - Local parity symmetric potentials

Local $\mathit{\Pi}$-symmetric potential $U(x) = \sum_{i=1}^{N} U_i(x)$ on successive non-overlapping domains $\mathcal{D}_i$ with centers α_i such that $U_i(2\alpha_i - x) = U_i(x)$ for $x \in \mathcal{D}_i$ and $U_i(x) = 0$ for $x \notin \mathcal{D}_i$.

The field in one half of the entire configuration space is mapped to the other half, though the domains of the source $\mathcal{A}(x)$ are topologically different.

Relation of the Q_i, $\widetilde{Q}_i$ to the globally invariant current J provides: different domains,

$$\frac{|Q_{i+1}|^2 - |\widetilde{Q}_{i+1}|^2}{|Q_i|^2 - |\widetilde{Q}_i|^2} = 1, \quad i = 1, 2, ..., N-1. \tag{1}$$

Overall piecewise constant functions $Q_c(x)$ and $\widetilde{Q}_c(x)$, which characterize the CLS of the structure at a given energy (or frequency) of the field.

CLS - Local parity symmetric potentials

CLS material structures generalize the notion of periodic or aperiodic crystals.

Classification:

- Periodic crystals
- Quasicrystals
- Disordered systems
- Locally symmetric materials
  - Nongapped, gapped or completely locally symmetric materials

Note: Quasicrystals are a special case - quasiperiodic dynamics of local symmetries generate quasicrystals !
See P.S. *et al*, Nonlinear Dynamics (2014).

5. Summary: Theoretical Foundations of Local Symmetries

Summary - theoretical foundations

- Existence of non-local invariant currents, Q and $\widetilde{Q}$, that characterize generic wave propagation within arbitrary (local) symmetry domains
- These invariant currents comprise the information necessary to map the wave function from a spatial subdomain to any symmetry-related subdomain
- Our theoretical framework generalizes the parity and Bloch theorems from global to local symmetries.
- Both invariant currents represent a (local) remnant of the corresponding global symmetry, and nonvanishing Q is identified as the key to the breaking of global symmetry

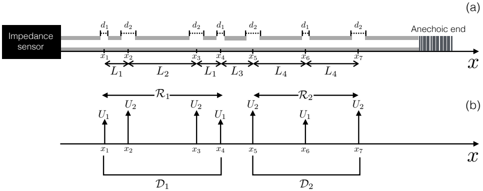
see P.A. Kalozoumis, C. Morfonios, F.K. Diakonos and P. S., PRL 113, 050403 (2014)

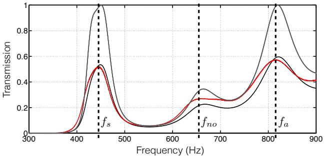
Summary - theoretical foundations

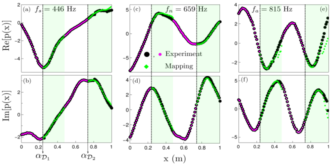
- Applies to any wave mechanical system: Acoustics, optics, quantum mechanics,....
  - Nanoelectronic devices, photonic crystals and multilayers or acoustic channels
  - Emergence of novel wave behaviour due to local symmetries
- New class of structures (artificial materials) consisting exclusively of locally symmetric building blocks
- PT Symmetry
- discrete systems (spin systems, optical waveguides, ...)
- Nonlinear dynamics of local symmetries: Generating new types of locally symmetric materials (chaotic, intermittent, quasiperiodic local symmetry devices)

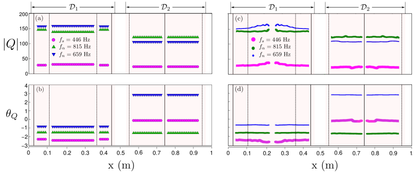
see P.A. Kalozoumis, C. Morfonios, F.K. Diakonos and P. S., PRL 113, 050403 (2014)

Acoustics - Experiment









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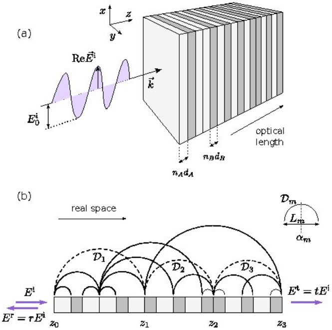
Summary - theoretical foundations

- Higher dimensions
- Interacting systems
- Periodically driven explicitly time-dependent systems
- Emergent phenomena
- Lossy systems: acoustics
- wave control by local symmetries (localization, perfect transmission, etc)
- ....
- Gauge theories ???

see P.A. Kalozoumis, C. Morfonios, F.K. Diakonos and P. S., PRL 113, 050403 (2014)

6. Application to Photonic Multilayers

Setup Photonic Multilayers



- Schematic of an aperiodic multilayer comprised of 16 planar slabs of materials A and B with $n_A d_A = n_B d_B = \lambda_0/4$. The scattered monochromatic plane light wave of stationary electric field amplitude E propagates along the z-axis, perpendicularly to the xy-plane of the slabs.
- 1D cross section of the multilayer in real space, showing its local symmetries. The arcs depict locally symmetric domains $\mathcal{D}_m$ of the device.

EOM, Invariants and Resonances

Helmholtz equation for light propagation

$$\hat{\Omega}(z,\omega)E(z) = \frac{\omega^2}{c^2}E(z)$$

with

$$\hat{\Omega}(z,\omega) = -\frac{d^2}{dz^2} + \left[1 - n^2(z)\right]\frac{\omega^2}{c^2}$$

with the non-local invariant currents

$$E(2\alpha_m - z)E'(z) + E(z)E'(2\alpha_m - z) \equiv Q_m$$

Important: the Q_m provide a classification of the resonances, i.e. of the corresponding field configurations in terms of local symmetries.

Perfectly Transmitting Resonances

We define

$$\mathcal{V}_m \equiv \frac{Q_m}{E(z_{m-1})\, E(z_m)}$$

and the sum

$$\mathcal{L} = \sum_{m=1}^{N} (-1)^{m-1} \mathcal{V}_m$$

Where the $E(z_m)$ at the boundaries of each domain are provided by the $Q_m, \widetilde{Q_m}$ via the symmetry mapping.

It can be shown that perfect transmission $T = 1$ leads to

$$\mathcal{L} = iJ[1 - (-1)^N] = \begin{cases} 0, & N \text{ even} \\ 2ik, & N \text{ odd} \end{cases}$$

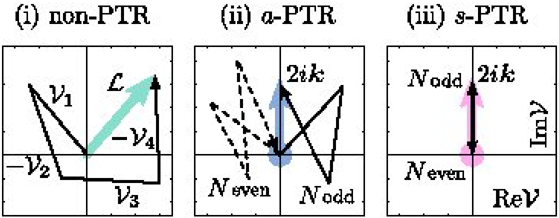
Sum rule for perfect transmission !

see PRA 87, 032113 (2013); PRA 88, 033857 (2013)

Perfectly Transmitting Resonances

The global quantity $\mathcal{L}$, together with the non-local invariants Q_m, can be utilized to classify the perfectly transmitting resonances (PTR).

- *Non-PTR*: Transmission $T < 1$, $\mathcal{V}_m$ add up to a complex vector $\mathcal{L} \neq 0, 2ik$. Open trajectory in the complex plane.
- *Asymmetric PTR*: $T = 1$ stationary light wave with electric field magnitude $E_0(z)$ which is *not* completely LP symmetric, does not follow the symmetries of $U(x)$. $\mathcal{V}_m$ take on arbitrary values in the N local symmetry domains.
  - Even N: closed trajectory in the complex plane, starting and ending at the origin.
  - Odd N: open trajectory ends at $2ik$.
- *symmetric PTR*: $T_m = 1$ in *each* subdomain $\mathcal{D}_m$. All local invariants *align* to the single, 'N-fold degenerate' value $Q_m = V_m = 2ik$. Trajectory representing $\mathcal{L}$ is restricted to the imaginary axis, oscillating between 0 and $2ik$.

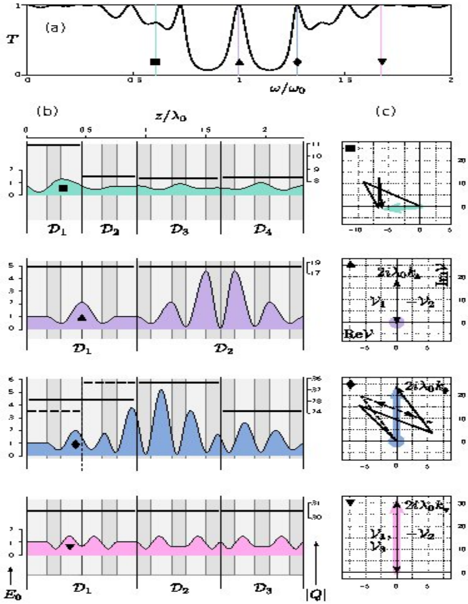


Geometric representation of scattering in locally symmetric media.

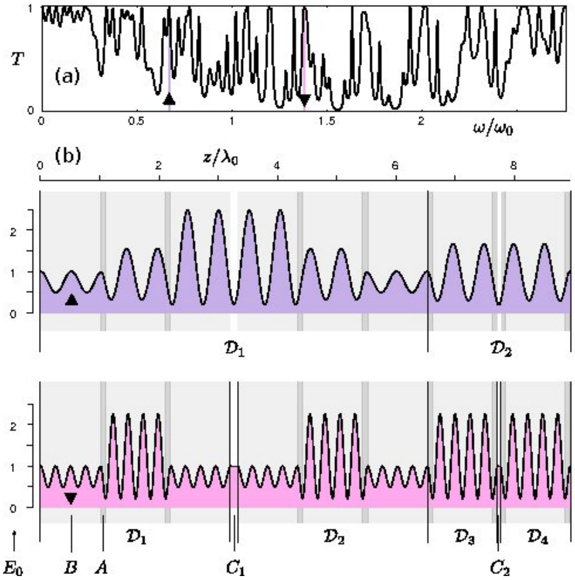
- Non-PTR, open trajectory with arbitrary end $\neq 2ik$.
- Asymmetric PTRs the trajectory explores the complex plane.
- Symmetric PTRs trajectory oscillates between 0 and $2ik$.

see PRA 87, 032113 (2013); PRA 88, 033857 (2013)

Transmission spectra in loc.symm. media



Transmission spectra in loc.symm. media



Construction principle for PTRs at desired energies based on the invariants !

The story of local symmetries just begins ....

Thank you for your attention!