Approximate Dynamics in Slowly Modulated Photonic Crystals

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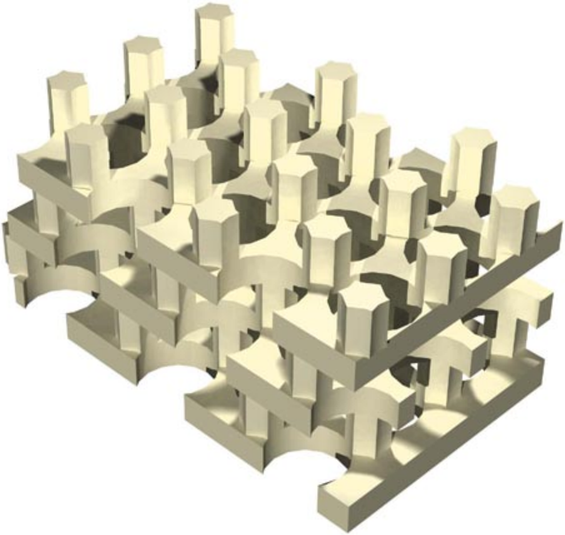
2013.09.27@UofT



Talk based on

- *The Perturbed Maxwell Operator as Pseudodifferential Operator*, with Giuseppe De Nittis (arxiv:1302.1956)
- *Effective Light Dynamics in Photonic Crystals: Isotropic Perturbations*, with Giuseppe De Nittis (arxiv:1307.1642)

Reformulate source-free Maxwell equations ($d = 3$)

1. *Field energy*

$$\mathcal{E}\big(\mathbf{E}, \mathbf{H}\big) = \frac{1}{2} \int_{\mathbb{R}^3} \mathrm{d}x \, \Big(\big\langle \mathbf{E}(x), \varepsilon(x) \mathbf{E}(x) \big\rangle_{\mathbb{C}^3} + \big\langle \mathbf{H}(x), \mu(x) \mathbf{H}(x) \big\rangle_{\mathbb{C}^3} \Big)$$

$$= \mathcal{E}\big(\mathbf{E}(t), \mathbf{H}(t)\big)$$

2. *Dynamical equations*

$$-\varepsilon \frac{\partial}{\partial t} \mathbf{E}(t) = \nabla_x \times \mathbf{H}(t), \qquad \mathbf{E}(0) = \mathbf{E}$$

$$+\mu \frac{\partial}{\partial t} \mathbf{H}(t) = \nabla_x \times \mathbf{E}(t), \qquad \mathbf{H}(0) = \mathbf{H}$$

3. *No sources*

$$\nabla_x \cdot \varepsilon \mathbf{E}(t) = 0$$

$$\nabla_x \cdot \mu \mathbf{H}(t) = 0$$

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2. *Dynamical equations* $\rightsquigarrow$ "Schrödinger-type equation"

$$\mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} \mathbf{E}(t) \\ \mathbf{H}(t) \end{pmatrix} = \begin{pmatrix} 0 & +\varepsilon^{-1} \, (-\mathrm{i}\nabla_x)^{\times} \\ -\mu^{-1} \, (-\mathrm{i}\nabla_x)^{\times} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E}(t) \\ \mathbf{H}(t) \end{pmatrix}$$

3. *No sources* $\rightsquigarrow$ "physical states"

$$\mathbf{J}(\varepsilon, \mu) := \Big\{ (\mathbf{E}, \mathbf{H}) \in \mathfrak{H}(\varepsilon, \mu) \; \big| \; \nabla_x \cdot \varepsilon \mathbf{E} = 0 \wedge \nabla_x \cdot \mu \mathbf{H} = 0 \Big\}$$

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Domain and invariant subspaces

Assumption

$\varepsilon, \mu \in L^\infty\big(\mathbb{R}^3, \mathrm{Mat}_{\mathbb{R}}(3)\big)$, $0 < c\, \mathbf{1}_{\mathbb{R}^3} \leq \varepsilon, \mu \leq C\, \mathbf{1}_{\mathbb{R}^3}$

Domain and invariant subspaces

Maxwell operator

$$\mathbf{M}(\varepsilon,\mu) := \begin{pmatrix} 0 & +\varepsilon^{-1}\,(-\mathrm{i}\nabla_x)^{\times} \\ -\mu^{-1}\,(-\mathrm{i}\nabla_x)^{\times} & 0 \end{pmatrix}$$
$$= \begin{pmatrix} \varepsilon^{-1} & 0 \\ 0 & \mu^{-1} \end{pmatrix} \begin{pmatrix} 0 & +(-\mathrm{i}\nabla_x)^{\times} \\ -(-\mathrm{i}\nabla_x)^{\times} & 0 \end{pmatrix}$$
$$= W\,\mathrm{Rot}$$

W bounded, bounded inverse

$\Rightarrow \mathcal{D} = \mathcal{D}(\mathrm{Rot})$ $\rightsquigarrow$ independent of choice of ε, μ!

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$\mathbf{M}(\varepsilon,\mu)^* = \mathbf{M}(\varepsilon,\mu)$ on $\mathcal{D}$ [Birman & Solomyak (1987)]

Domain and invariant subspaces

Decomposition of $\mathfrak{H}(\varepsilon, \mu)$ into invariant orthogonal subspaces

$$\begin{aligned}\mathfrak{H}(\varepsilon, \mu) &= \big(\mathrm{ran}\,\mathrm{Grad}\big)^{\perp_{\mathfrak{H}(\varepsilon,\mu)}} \oplus_{\perp} \mathrm{ran}\,\mathrm{Grad} \\ &=: \mathbf{J}(\varepsilon, \mu) \oplus_{\perp} \mathbf{G}\end{aligned}$$

$\rightsquigarrow$ identifies physical and unphysical subspaces

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Maxwell operator is block diagonal [Birman & Solomyak (1987)]

$$\mathbf{M}(\varepsilon, \mu) = \mathbf{M}(\varepsilon, \mu)|_{\mathbf{J}(\varepsilon,\mu)} \oplus 0|_{\mathbf{G}}$$

$\Rightarrow$ many authors study $\mathbf{M}(\varepsilon, \mu)|_{\mathbf{J}(\varepsilon,\mu)}$ instead of $\mathbf{M}(\varepsilon, \mu)$

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Fundamental symmetry

ε, μ matrix-valued functions (*real entries!*): complex conjugation C

$$C\,\varepsilon\,C = \varepsilon \qquad C\,\mu\,C = \mu$$

$\mathbf{M}_W$ and C anti-commute:

$$\begin{aligned} \Rightarrow \quad C\,\mathbf{M}_W\,C &= C\,W\,\mathrm{Rot}\,C = W\,C\,\mathrm{Rot}\,C \\ &= -W\,\mathrm{Rot} = -\mathbf{M}_W \end{aligned}$$

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$$\Rightarrow \; C\,\mathrm{e}^{-\mathrm{i}t\,\mathbf{M}_w}\,C = \mathrm{e}^{+\mathrm{i}t\,C\,\mathbf{M}_w\,C} = \mathrm{e}^{-\mathrm{i}t\,\mathbf{M}_w}$$

$$\Leftrightarrow \; \left[C\,,\,\mathrm{e}^{-\mathrm{i}t\,\mathbf{M}_w}\right] = 0$$

$$\Rightarrow \; \left[\mathrm{Re}\,,\,\mathrm{e}^{-\mathrm{i}t\,\mathbf{M}_w}\right] = 0 \qquad \mathrm{Re} := \tfrac{1}{2}\big(\mathbf{1} + C\big)$$

Real-valued initial conditions ⇒ real-valued solutions

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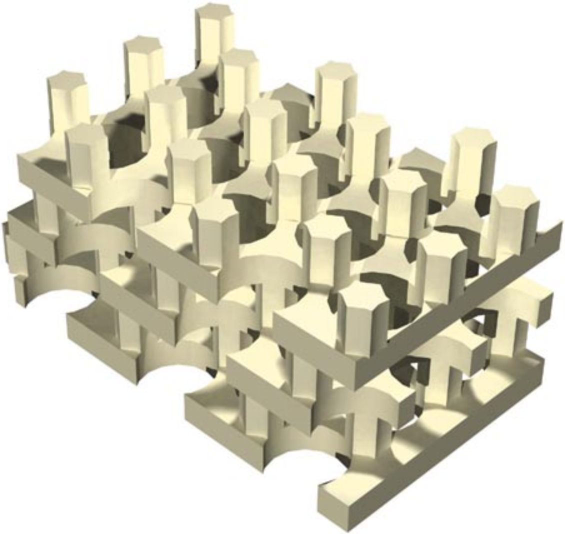
Structure of Maxwell operators

	Schrödinger operators	vs.	**Maxwell operators**
prototypical form	$H = -\Delta_x + V$	vs.	$M = W \, \mathrm{Rot}$
perturbations are	additive	vs.	multiplicative
Hilbert spaces are	not weighted	vs.	weighted
symmetry	$C H C = +H$	vs.	$C \mathbf{M}_w C = -\mathbf{M}_w$

Photonic crystals



taken from S. G. Johnson and J. D. Joannopoulos, APL 77, 3490-3492 (2000)

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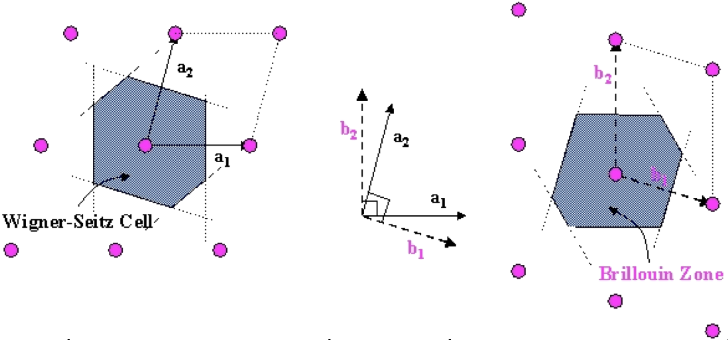

$\Gamma := \left\{ \gamma = \sum_{j=1}^{3} \beta_j \, a_j \mid \beta_1, \beta_2, \beta_3 \in \mathbb{Z} \right\}$

$\mathcal{W}$ Wigner-Seitz cell

$\Gamma^* := \left\{ \gamma^* = \sum_{j=1}^{3} \alpha_j \, b_j \mid \alpha_1, \alpha_2, \alpha_3 \in \mathbb{Z} \right\}$

$\mathcal{B}$ Brillouin zone

Photonic crystals

Assumption (Γ-periodicity)

In addition, assume $\varepsilon = \varepsilon_0$ and $\mu = \mu_0$ are Γ-periodic.

$\rightsquigarrow$ simplify notation: use $\mathfrak{H}_0 := \mathfrak{H}(\varepsilon_0, \mu_0)$, $\mathbf{M}_0 := \mathbf{M}(\varepsilon_0, \mu_0)$, etc.

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Fiber-decomposition of the spaces

Fibration via Zak transform:

$$(\mathcal{Z}\Psi)(k,y) := e^{-ik\cdot y} \, (\mathcal{F}\Psi)(k,y) = \sum_{\gamma\in\Gamma} e^{-ik\cdot(y+\gamma)} \, \Psi(y+\gamma)$$

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Zak transform: unitary map $\mathcal{Z} : \mathfrak{H}_0 \longrightarrow L^2(\mathcal{B}) \otimes \mathfrak{h}_0$ where

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$$\mathfrak{h}_0 \cong \mathbf{J}_0(k) \oplus \mathbf{G}_0(k)$$

$$\mathcal{Z}\mathbf{J}_0 \cong \bigsqcup_{k \in \mathcal{B}} \mathbf{J}_0(k) \qquad \text{physical}$$

$$\mathcal{Z}\mathbf{G}_0 \cong \bigsqcup_{k \in \mathcal{B}} \mathbf{G}_0(k) \qquad \text{unphysical}$$

Fibration of the periodic Maxwell operator

$$\mathbf{M}_0^{\mathcal{Z}} := \mathcal{Z}\,\mathbf{M}_0\,\mathcal{Z}^{-1} = \int_{\mathcal{B}}^{\oplus} \mathrm{d}k\,\mathbf{M}_0(k)$$

$$= \int_{\mathcal{B}}^{\oplus} \mathrm{d}k \begin{pmatrix} \varepsilon_0^{-1} & 0 \\ 0 & \mu_0^{-1} \end{pmatrix} \begin{pmatrix} 0 & +(-\mathrm{i}\nabla_y + k)^{\times} \\ -(-\mathrm{i}\nabla_y + k)^{\times} & 0 \end{pmatrix}$$

$\mathcal{D}\big(\mathbf{M}_0(k)\big) = \mathcal{D}\big(\mathrm{Rot}(0)\big) \subset \mathfrak{h}_0$

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Spectrum: physical and unphysical

- $\sigma\big(\mathbf{M}_0^{\mathcal{Z}}(k)|_{\mathbf{J}_0^{\mathcal{Z}}(k)}\big) = \sigma_{\mathrm{disc}}\big(\mathbf{M}_0^{\mathcal{Z}}(k)|_{\mathbf{J}_0^{\mathcal{Z}}(k)}\big)$ on **physical** subspace
- $\sigma\big(\mathbf{M}_0^{\mathcal{Z}}(k)|_{G^{\mathcal{Z}}(k)}\big) = \sigma_{\mathrm{pp}}\big(\mathbf{M}_0^{\mathcal{Z}}(k)|_{G^{\mathcal{Z}}(k)}\big) = \{0\}$ on **un**physical subspace

$\rightsquigarrow$ focus on non-trivial, physical part of spectrum

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Symmetry properties of $\mathbf{M}_0(k)$

Symmetry

$$\mathbf{M}_0(k)\varphi_n(k) = \omega_n(k)\,\varphi_n(k)$$
$$\Leftrightarrow$$
$$\mathbf{M}_0(k)\overline{\varphi_n(-k)} = -\omega_n(-k)\,\overline{\varphi_n(-k)}$$

To construct **real**-valued initial conditions:
symmetric pairs $\left\{\varphi_*(k), \overline{\varphi_*(-k)}\right\} \rightsquigarrow \left\{\omega_*(k), -\omega_*(-k)\right\}$

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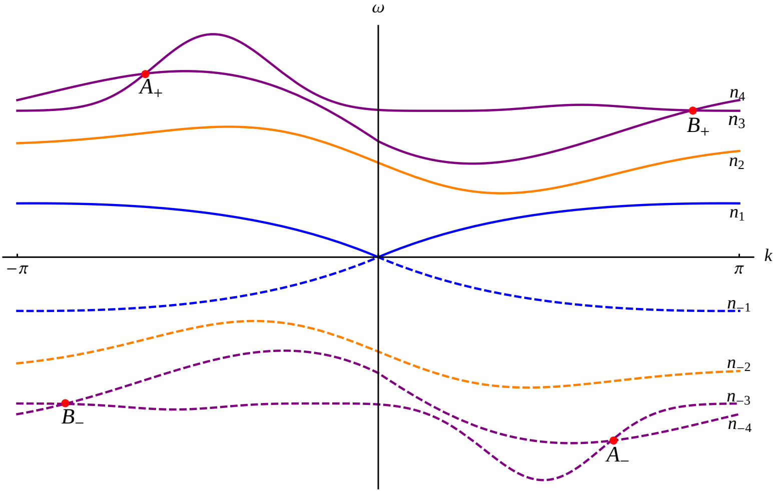
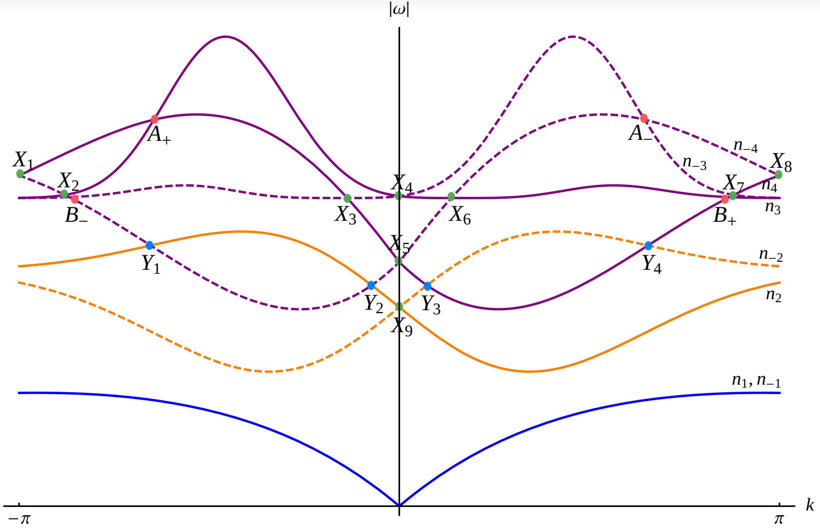
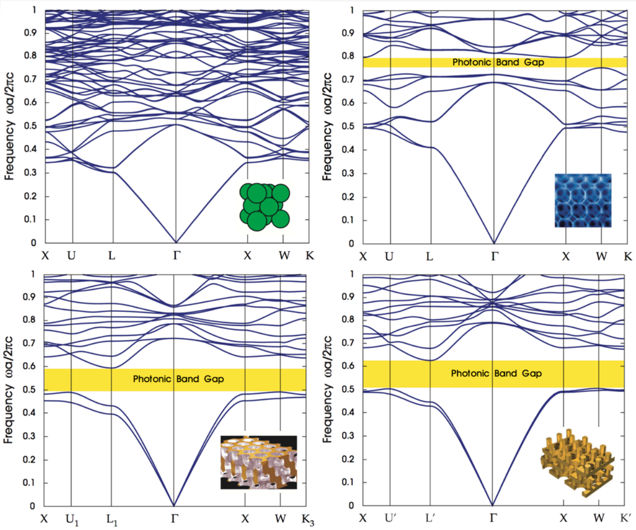


Theorem (De Nittis-L. 2013)


|ω|
X1
X2
B−
A+
X3
X4
X5
X6
X9
Y1
Y2
Y3
Y4
A−
n−4
n−3
X8
X7
n4
B+
n3
n−2
n2
n1, n−1
k
−π
π



3d, taken from *Photonic Crystals -- Molding the Flow of Light*

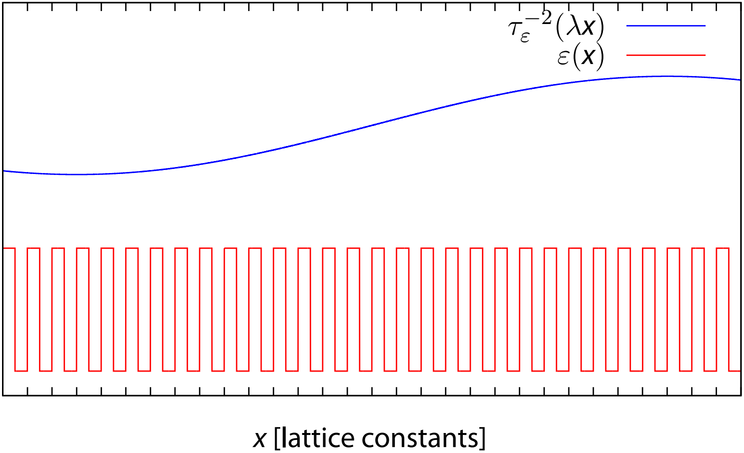
Perturbations of material weights

Assumption (Slow modulations of material weights)

$\tau_\varepsilon, \tau_\mu \in \mathcal{C}^\infty_{\mathrm{b}}(\mathbb{R}^3, \mathbb{R})$, $\tau_\varepsilon, \tau_\mu \geq c > 0$

$$\varepsilon_\lambda(x) := \frac{\varepsilon(x)}{\tau_\varepsilon(\lambda x)^2} \qquad \mu_\lambda(x) := \frac{\mu(x)}{\tau_\mu(\lambda x)^2}$$

Macroscopic and microscopic degrees of freedom



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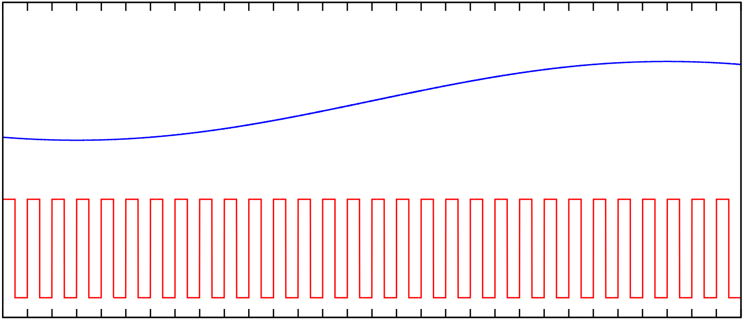
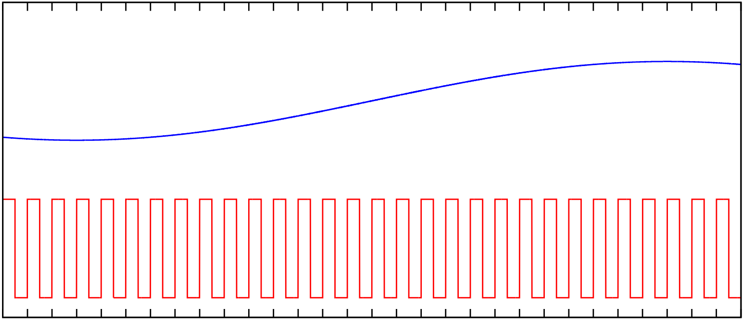


$\mathfrak{H}_0 \cong L^2(\mathcal{B}) \otimes \mathfrak{h}_0 = \mathfrak{H}_{\mathrm{macro}} \otimes \mathfrak{H}_{\mathrm{micro}}$

$\rightsquigarrow$ study macroscopic dynamics given a fixed microscopic state

Macroscopic and microscopic degrees of freedom



$\mathfrak{H}_0 \cong L^2(\mathcal{B}) \otimes \mathfrak{h}_0 = \mathfrak{H}_{\mathrm{macro}} \otimes \mathfrak{H}_{\mathrm{micro}}$
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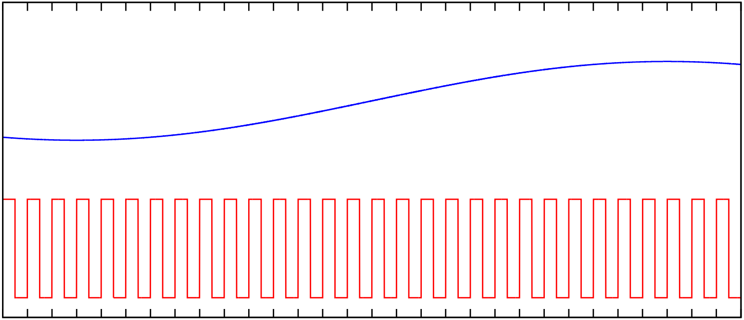

⇝ study macroscopic dynamics given a fixed microscopic state via space-adiabatic perturbation theory [PST (2002)]

Slowly modulated Maxwell operator

Maxwell operator

- $\mathbf{M}_\lambda := \mathbf{M}(\varepsilon_\lambda, \mu_\lambda)$
- $\mathcal{D} \subset \mathfrak{H}_\lambda := \mathfrak{H}(\varepsilon_\lambda, \mu_\lambda)$
- $\mathfrak{H}_\lambda = \mathbf{J}_\lambda \oplus_\perp \mathbf{G}$

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Maxwell operator

- $\mathbf{M}_\lambda := \mathbf{M}(\varepsilon_\lambda, \mu_\lambda)$
- $\mathcal{D} \subset \mathfrak{H}_\lambda := \mathfrak{H}(\varepsilon_\lambda, \mu_\lambda)$ $\rightsquigarrow$ Hilbert space depends on λ!
- $\mathfrak{H}_\lambda = \mathbf{J}_\lambda \oplus_\perp \mathbf{G}$

Effective dynamics

Goal

Approximate $e^{-it\mathbf{M}_\lambda}$ for **physical** states from a **narrow range of frequencies**, i. e. states which are

1. located in $\mathbf{J}_\lambda$,
2. *real-valued* states and
3. associated to specific frequency bands of $\mathbf{M}_0$

up to higher-order errors in λ.

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Physical states

Theorem (De Nittis-L. 2012)

There exist orthogonal projections

$$\mathbf{\Pi}_\lambda = \mathbf{\Pi}_{+\,\lambda} + \mathbf{\Pi}_{+\,\lambda} + \mathcal{O}_{\|\cdot\|}(\lambda^\infty)$$

associated to a symmetric family of bands so that

$$\big[\mathbf{M}_\lambda, \mathbf{\Pi}_{\pm\,\lambda}\big] = \mathcal{O}_{\|\cdot\|}(\lambda^\infty).$$

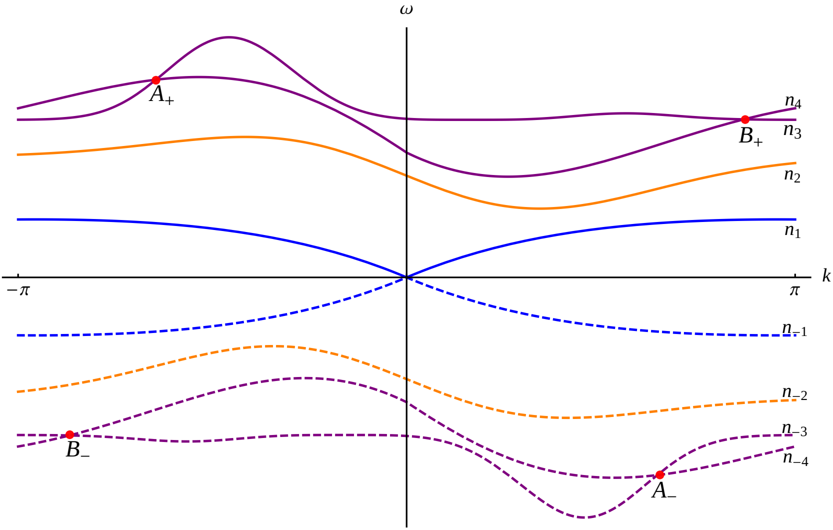
Effective *semiclassical* dynamics

Simplest case:

semiclassical dynamics

aka ray optics

Effective *semiclassical* dynamics



Effective *semiclassical* dynamics

Setup

- ω_* isolated, non-degenerate
  $\rightsquigarrow$ in actuality: consider the *pair* $\{\omega_*(k), -\omega_*(-k)\}$
- $\omega_*(k) \neq 0$ for all $k \in \mathbb{R}^3$ $\rightsquigarrow$ excludes ground state bands!
- Bloch function $k \mapsto \varphi_*(k)$
- projection $(r, k) \mapsto \pi_0(r, k) := S^{-1}(r) \, |\varphi_*(k)\rangle\langle\varphi_*(k)| \, S(r)$ smooth
- Chern number associated to $k \mapsto |\varphi_*(k)\rangle\langle\varphi_*(k)|$ need not be zero! (then $k \mapsto \varphi_*(k)$ cannot be chosen purely real)

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Effective semiclassical equations of motion

Semiclassical Maxwellian

$$\mathcal{M}_{\mathrm{sc}} = \tau_\varepsilon \, \tau_\mu \, \omega_* + \\ + \lambda \Big(\mathrm{i} \, \tau_\varepsilon \, \big\langle \varphi_*^E , \nabla_r \tau_\mu \times \varphi_*^H \big\rangle_{L^2} - \mathrm{i} \, \tau_\mu \, \big\langle \varphi_*^H , \nabla_r \tau_\varepsilon \times \varphi_*^E \big\rangle_{L^2} + \\ - \tfrac{\mathrm{i}}{2} \Big\langle \varphi_* , S \, \big\{ S^{-2} \, \mathbf{M}_0(\cdot) - \tau_\varepsilon \, \tau_\mu \, \omega_* \big\} \, S^{-1} \varphi_* \Big\rangle_{\mathfrak{h}_0} \Big)$$

Symbol $\mathbf{M}_\lambda$ and analog of Rammal-Wilkinson term

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Effective semiclassical equations of motion

$\mathcal{O}(\lambda)$-correction to symplectic form: Berry curvature

$\pi_0(r,k) = S^{-1}(r) \, |\varphi_*(k)\rangle\langle\varphi_*(k)| \, S(r)$

$$\Omega = \begin{pmatrix} \Omega^{rr} & \Omega^{rk} \\ \Omega^{kr} & \Omega^{kk} \end{pmatrix}$$

Effective semiclassical equations of motion

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$\boldsymbol{\pi}_0(r,k) = S^{-1}(r)\,|\varphi_*(k)\rangle\langle\varphi_*(k)|\,S(r)$

$$\Omega^{rr}_{jn} = -\mathrm{i}\Big\langle \varphi_*, S\left[\partial_{r_j}\boldsymbol{\pi}_0\,,\,\partial_{r_n}\boldsymbol{\pi}_0\right] S^{-1}\varphi_*\Big\rangle_{\mathfrak{h}_0} = 0$$

$$\Omega^{rk}_{jn} = -\mathrm{i}\Big\langle \varphi_*, S\left[\partial_{r_j}\boldsymbol{\pi}_0\,,\,\partial_{k_n}\boldsymbol{\pi}_0\right] S^{-1}\varphi_*\Big\rangle_{\mathfrak{h}_0} = -\Omega^{kr}_{nj} \neq 0$$

$$\Omega^{kk}_{jn} = -\mathrm{i}\Big\langle \varphi_*, S\left[\partial_{k_j}\boldsymbol{\pi}_0\,,\,\partial_{k_n}\boldsymbol{\pi}_0\right] S^{-1}\varphi_*\Big\rangle_{\mathfrak{h}_0}$$

$$= \partial_{k_j}\mathrm{i}\big\langle \varphi_*, \partial_{k_n}\varphi_*\big\rangle_{\mathfrak{h}_0} - \partial_{k_n}\mathrm{i}\big\langle \varphi_*, \partial_{k_j}\varphi_*\big\rangle_{\mathfrak{h}_0}$$

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Effective semiclassical equations of motion

Semiclassical dynamics

Φ^λ flow associated to

$$\begin{pmatrix} 0 & -\mathbf{1} + \lambda\,\Omega^{rk} \\ +\mathbf{1} + \lambda\,\Omega^{kr} & +\lambda\,\Omega^{kk} \end{pmatrix} \begin{pmatrix} \dot{r} \\ \dot{k} \end{pmatrix} = \begin{pmatrix} \nabla_r \mathcal{M}_{sc} \\ \nabla_k \mathcal{M}_{sc} \end{pmatrix}$$

Semiclassics: main result

Theorem (De Nittis-L. 2013)

For all suitable observables f, the following Egorov-type theorem holds:

$$\left\| \Pi_{\pm\,\lambda} \left(\mathrm{e}^{+\mathrm{i}t\,\mathbf{M}_\lambda} \, \mathrm{Op}_\lambda(f) \, \mathrm{e}^{-\mathrm{i}t\,\mathbf{M}_\lambda} - \mathrm{Op}_\lambda\big(f \circ \Phi^{\pm\lambda}\big) \right) \Pi_{\pm\,\lambda} \right\| = \mathcal{O}(\lambda^2)$$

$\Phi^{\pm\lambda}$ *flow associated to positive/negative frequency band*

Semiclassics: interpretation of main result

- first mathematically rigorous result
- previously unknown $\mathcal{O}(\lambda)$ terms
  - $\mathcal{O}(\lambda)$ term from symbol (change in field energy)
  - Teufel-Stiepan term ($\rightsquigarrow$ Rammal-Wilkinson term, geometric)
  - additional Berry curvature terms (geometric)
- assumption $\omega_*(k) \neq 0 \; \forall k \in \mathbb{R}^3$ excludes ground state bands
- »having to run two semiclassical dynamics« to approximate physical states
- Proof based on recent publication of Teufel & Stiepan

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  - states with $\omega_{\mathrm{gs}}(k) \approx 0$ at $k \approx 0$: wave length $\gg$ lattice spacing
  - do not see periodicity of photonic crystal
  - »universal« behavior $\rightsquigarrow$ *free waves* with modified v_{light}
  - $\Rightarrow$ multiscale ansatz breaks down!
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Semiclassics: comparison to notable previous results

Haldane & Raghu, Phys. Rev. A 78, 033834 (2008)

- »derivation by analogy« ($\dot{k}$ equation since derived by Esposito and Gerace)
- necessity of slow variation recognized, but small parameter λ not used
- equations of motion:

$$\dot{r} = +\nabla_k \big(\tau_\varepsilon \, \tau_\mu \, \omega_*\big) - \lambda \, \Omega^{kk} \, \dot{k}$$
$$\dot{k} = -\nabla_r \big(\tau_\varepsilon \, \tau_\mu \, \omega_*\big)$$

$\rightsquigarrow$ eom are missing $\mathcal{O}(\lambda)$ terms, only leading-order correct

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Onoda, Murakami, Nagaosa, Phys. Rev. E 76, 066610 (2006)

- use Sundaram–Niu variational technique + second quantization
- semiclassical states $\Psi(r,k,z)$ parametrized by $(r,k) \in T^*\mathbb{R}^3$, $z \in S^2 \rightsquigarrow$ find extremals of functional

$$L = \Big\langle \Psi(r,k,z) \Big| \mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}t} - M_\lambda^{\mathcal{Z}} \Big| \Psi(r,k,z) \Big\rangle$$

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- result is not readily comparable to ours

1 Rewriting the Maxwell equations

2 Fundamental properties

3 Periodic Maxwell operators

4 Perturbed periodic Maxwell operators

5 Open problems

Selection of few interesting questions

- Gyrotropic photonic crystals $\rightsquigarrow$ complex entries in offdiagonal entries of ε of μ
  $\Rightarrow$ topological effects analogous to quantum Hall effect
- Case $d = 2$
- Classification of symmetries of operators in the sense of Altlander and Zirnbauer $\Rightarrow$ existence of topological invariants
- **R**eal triviality of twin-band Bloch bundle
- Meta materials with negative refraction index
  $\rightsquigarrow \varepsilon$ and μ no longer positive-matrix-valued!

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