Approximate Dynamics in Slowly Modulated Photonic Crystals

in honor of Herbert's $(66 - \varepsilon)$th birthday where $\varepsilon \ll 1$

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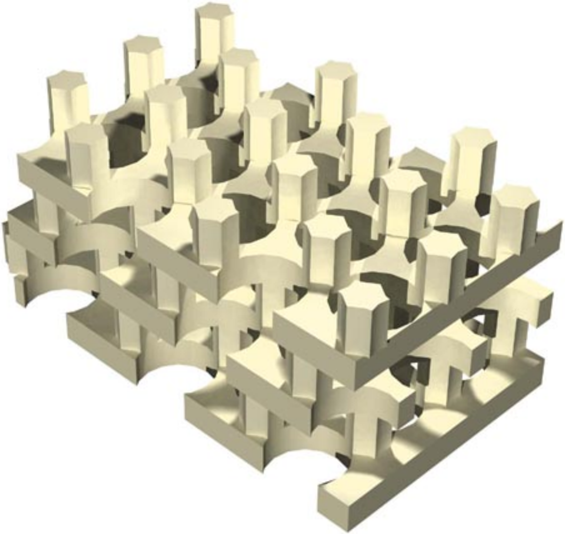
in collarboration with Giuseppe De Nittis

Kyushu University

2012.10@ESI



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

1. *Field energy*

$$\mathcal{E}\big(\mathbf{E},\mathbf{H}\big) = \int_{\mathbb{R}^3} \mathrm{d}x \,\big(\varepsilon(x)\,|\mathbf{E}(x)|^2 + \mu(x)\,|\mathbf{H}(x)|^2\big) = \mathcal{E}\big(\mathbf{E}(t),\mathbf{H}(t)\big)$$

2. *Dynamical equations*

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

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

3. *No sources*

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

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

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Domain and invariant subspaces

Assumption

$\varepsilon, \mu \in L^\infty(\mathbb{R}^3)$, $\varepsilon, \mu \geq c > 0$

Domain and invariant subspaces

Maxwell operator

$$M(\varepsilon,\mu) := \begin{pmatrix} 0 & +\varepsilon^{-1}(\hat{x})\,(-\mathrm{i}\nabla_x)^{\times} \\ -\mu^{-1}(\hat{x})\,(-\mathrm{i}\nabla_x)^{\times} & 0 \end{pmatrix}$$
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$$= \Xi(\hat{x})\,\mathrm{rot} \otimes \sigma_2$$

$\Xi(\hat{x})$ bounded, bounded inverse

$\Rightarrow \mathcal{D} = \mathcal{D}\big(\mathrm{rot} \otimes \sigma_2\big) = \ker \mathrm{Div} \oplus \mathrm{ran}\,\mathrm{Grad}$

⇝ independent of choice of ε, μ!

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$$\mathrm{Grad} := \mathrm{grad} \oplus \mathrm{grad} : H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3) \longrightarrow \mathcal{H}(\varepsilon,\mu)$$
$$\mathrm{Div} := \mathrm{div} \oplus \mathrm{div} : H^1(\mathbb{R}^3,\mathbb{C}^6) \subset \mathcal{H}(\varepsilon,\mu) \longrightarrow L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$$

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

Domain and invariant subspaces

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

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

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

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

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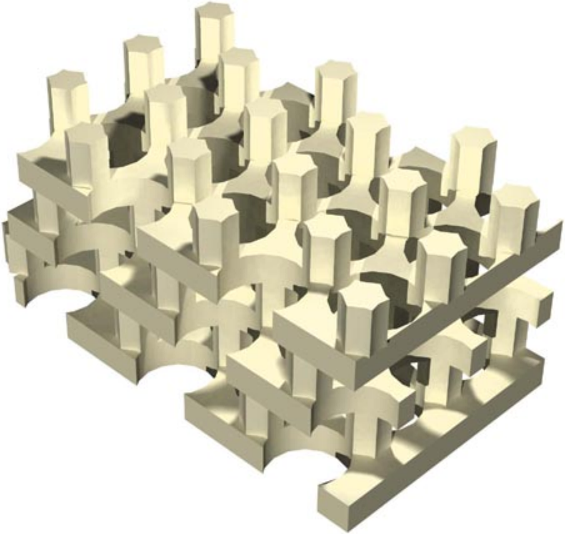
Photonic crystals



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

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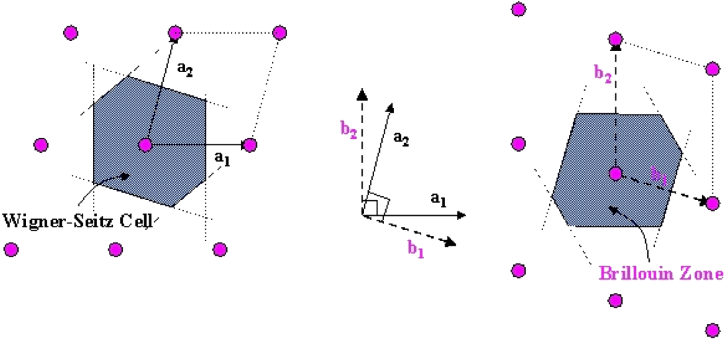

$\Gamma := \left\{ \gamma = \sum_{j=1}^{3} \beta_j \, a_j \;\middle|\; \beta_1, \beta_2, \beta_3 \in \mathbb{Z} \right\}$ $\Gamma^* := \left\{ \gamma^* = \sum_{j=1}^{3} \alpha_j \, b_j \;\middle|\; \alpha_1, \alpha_2, \alpha_3 \in \mathbb{Z} \right\}$

W Wigner-Seitz cell $\mathcal{B}$ Brillouin zone

Photonic crystals

Assumption (Γ-periodicity)

In addition, assume $\varepsilon = \varepsilon_\Gamma$ and $\mu = \mu_\Gamma$ are Γ-periodic.

⇝ simplify notation: use $\mathcal{H}_\Gamma := \mathcal{H}(\varepsilon_\Gamma, \mu_\Gamma)$, $M_\Gamma := M(\varepsilon_\Gamma, \mu_\Gamma)$, etc.

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Zak transform

$\Psi \in \mathcal{H}_\Gamma \cap \mathcal{C}_c^\infty(\mathbb{R}^3, \mathbb{C}^6)$

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

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Zak transform

Zak transform: unitary map $\mathcal{Z} : \mathcal{H}_\Gamma \longrightarrow L^2(\mathcal{B}) \otimes \mathcal{H}_\Gamma^{\mathbb{T}}$ where

$$\mathcal{H}_\Gamma^{\mathbb{T}} := L^2\big(\mathbb{T}^3, \varepsilon_\Gamma(y)\,\mathrm{d}y; \mathbb{C}^3\big) \oplus L^2\big(\mathbb{T}^3, \mu_\Gamma(y)\,\mathrm{d}y; \mathbb{C}^3\big)$$

The band picture

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

$$= \int_{\mathcal{B}}^{\oplus} \mathrm{d}k \begin{pmatrix} 0 & +\varepsilon_\Gamma^{-1}(\hat{y})\,(-\mathrm{i}\nabla_y + k)^{\times} \\ -\mu_\Gamma^{-1}(\hat{y})\,(-\mathrm{i}\nabla_y + k)^{\times} & 0 \end{pmatrix}$$

$$\mathcal{Z}\mathcal{D} = \mathcal{Z}\Big(\big(J_\Gamma \cap H^1(\mathbb{R}^3, \mathbb{C}^6)\big) \oplus G \Big)$$

$$\cong \bigsqcup_{k \in \mathcal{B}} \mathcal{D}^{\mathcal{Z}}(k) = \bigsqcup_{k \in \mathcal{B}} \Big(\big(H^1(\mathbb{T}^3, \mathbb{C}^6) \cap J_\Gamma^{\mathcal{Z}}(k)\big) \oplus G^{\mathcal{Z}}(k) \Big)$$

$\rightsquigarrow$ domain of $M_\Gamma^{\mathcal{Z}}(k)$ depends on k!

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- $\sigma\big(M_\Gamma^{\mathcal{Z}}(k)|_{J_\Gamma^{\mathcal{Z}}(k)}\big) = \sigma_{\mathrm{disc}}\big(M_\Gamma^{\mathcal{Z}}(k)|_{J_\Gamma^{\mathcal{Z}}(k)}\big)$ on **physical** subspace
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⇝ focus on non-trivial, physical part of spectrum

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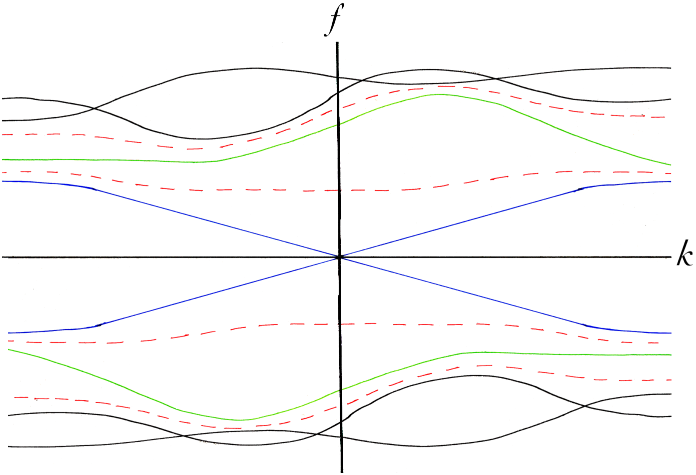

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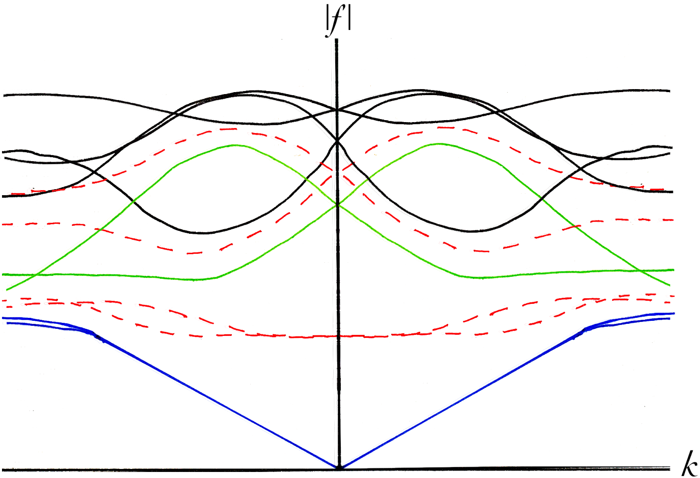
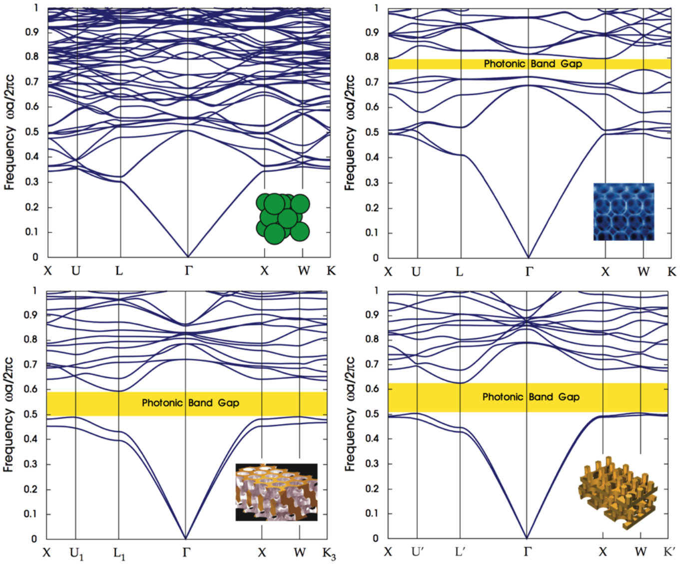


schematics of energy bands

The band picture



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

Non-analyticity

Question of analyticity

Easy: $k \mapsto M_{\Gamma}^{\mathcal{Z}}(k)$ is linear and thus analytic, right?

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Non-analyticity

Theorem

1. $k \mapsto M_\Gamma^{\mathcal{Z}}(k)$ *as well as their their restrictions to physical and unphysical subspaces are* ***analytic on*** $\mathbb{R}^3 \setminus \Gamma^*$
2. $k \mapsto M_\Gamma^{\mathcal{Z}}(k) \, 1_{\mathbb{R}\setminus(-\delta,+\delta)}\big(M_\Gamma^{\mathcal{Z}}(k)\big)$ *is* ***locally analytic on all of*** $\mathbb{R}^3$ *for* $\delta > 0$ *suitable*

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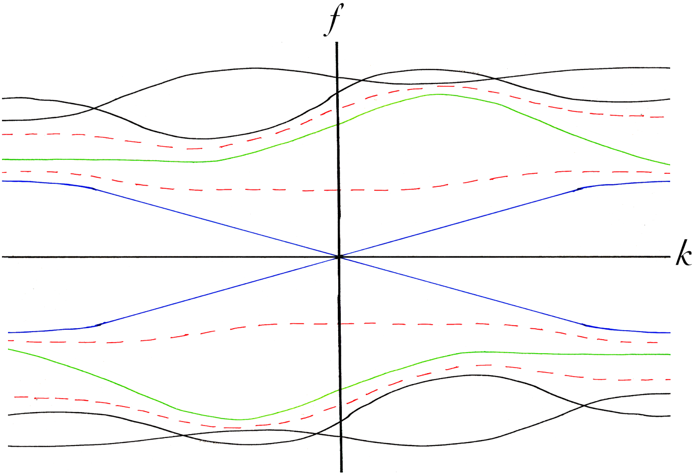
$\Rightarrow M_\Gamma^{\mathcal{Z}}$ is *not* a ΨDO! (but it's *very* close to a ΨDO)

Non-analyticity



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Perturbation multiplicative, not additive

Perturbation of material constants

$\lambda \ll 1$ small parameter, quantifies slow variation (lattice spacing vs. length scale of modulation)

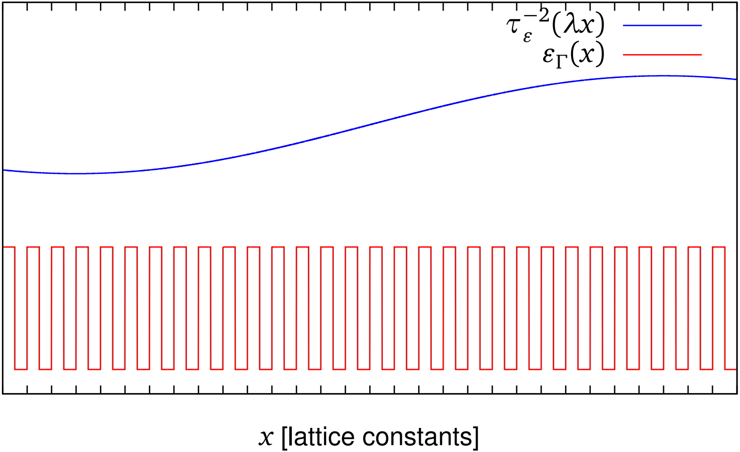
$$\varepsilon_\Gamma(x) \rightsquigarrow \varepsilon_\lambda(x) := \tau_\varepsilon^{-2}(\lambda x)\, \varepsilon_\Gamma(x)$$
$$\mu_\Gamma(x) \rightsquigarrow \mu_\lambda(x) := \tau_\mu^{-2}(\lambda x)\, \mu_\Gamma(x)$$

Perturbation multiplicative, not additive

Assumption (Slow modulation)

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

Macroscopic and microscopic degrees of freedom



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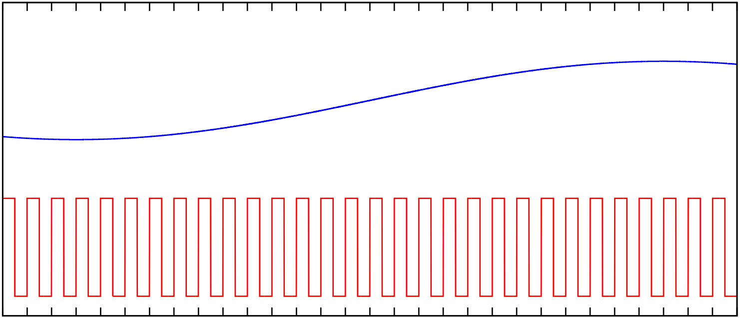

$$\mathcal{H}_\Gamma \cong L^2(\mathcal{B}) \otimes \mathcal{H}_\Gamma^{\mathbb{T}} = \mathcal{H}_{\text{macro}} \otimes \mathcal{H}_{\text{micro}}$$

⇝ study macroscopic dynamics given a fixed microscopic state

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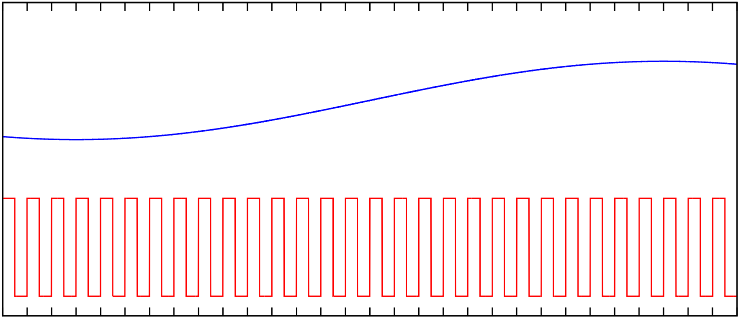

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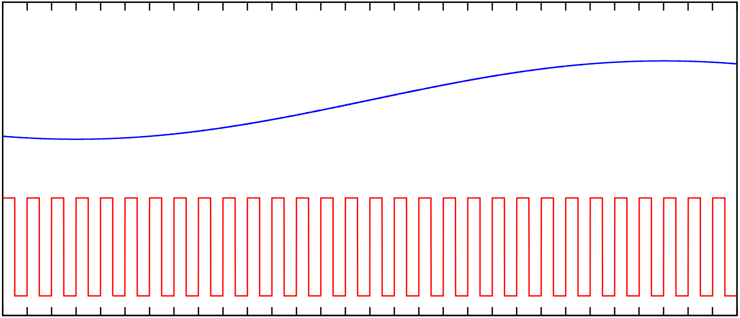

⇝ study macroscopic dynamics given a fixed microscopic state via space-adiabatic perturbation theory [PST (2002)]

Setup

Maxwell operator

- $M(\varepsilon_\lambda, \mu_\lambda)$ defined as before
- $\mathcal{D} \subset \mathcal{H}(\varepsilon_\lambda, \mu_\lambda)$
- $\mathcal{H}(\varepsilon_\lambda, \mu_\lambda) = J(\varepsilon_\lambda, \mu_\lambda) \oplus G$

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- $\mathcal{D} \subset \mathcal{H}(\varepsilon_\lambda, \mu_\lambda)$ $\rightsquigarrow$ Hilbert space depends on λ!
- $\mathcal{H}(\varepsilon_\lambda, \mu_\lambda) = J(\varepsilon_\lambda, \mu_\lambda) \oplus G$

Representation of M_λ on λ-independent Hilbert space

Preparation

How to compare Maxwell operators with different values of λ?

Representation of M_λ on λ-independent Hilbert space

$$\mathcal{H}(\varepsilon_\lambda, \mu_\lambda) \xrightarrow{S_\lambda} \mathcal{H}_\Gamma \xrightarrow{\mathcal{Z}} L^2(\mathcal{B}) \otimes \mathcal{H}_\Gamma^{\mathbb{T}}$$

where

$$S_\lambda = \begin{pmatrix} \tau_\varepsilon^{-1}(\lambda \hat{x}) & 0 \\ 0 & \tau_\mu^{-1}(\lambda \hat{x}) \end{pmatrix}$$

Representation of M_λ on λ-independent Hilbert space

Maxwell operator in new representation:

$$\begin{aligned} M_\lambda^{\mathcal{Z}} &:= \mathcal{Z}\, S_\lambda\, M(\varepsilon_\lambda, \mu_\lambda)\, S_\lambda^{-1}\, \mathcal{Z}^{-1} \\ &= \mathcal{Z}\, S_\lambda \begin{pmatrix} 0 & +\varepsilon_\Gamma^{-1}(\hat{x})\,(-\mathrm{i}\nabla_x)^\times \\ -\mu_\Gamma^{-1}(\hat{x})\,(-\mathrm{i}\nabla_x)^\times & 0 \end{pmatrix} S_\lambda^{-1}\, \mathcal{Z}^{-1} \end{aligned}$$

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&= \tau(\mathrm{i}\lambda\nabla_k) \, M_\Gamma^{\mathcal{Z}} + \lambda \, \tau(\mathrm{i}\lambda\nabla_k) \, \Upsilon(\mathrm{i}\lambda\nabla_k)
\end{aligned}
$$

Representation of M_λ on λ-independent Hilbert space

Hilbert space $L^2(\mathcal{B}) \otimes \mathcal{H}_\Gamma^{\mathbb{T}}$ splits

$$L^2(\mathcal{B}) \otimes \mathcal{H}_\Gamma^{\mathbb{T}} = J_\lambda^{\mathcal{Z}} \oplus_\perp G_\lambda^{\mathcal{Z}} := \big(\mathcal{Z} S_\lambda J(\varepsilon_\lambda, \mu_\lambda)\big) \oplus_\perp \big(\mathcal{Z} S_\lambda G\big)$$

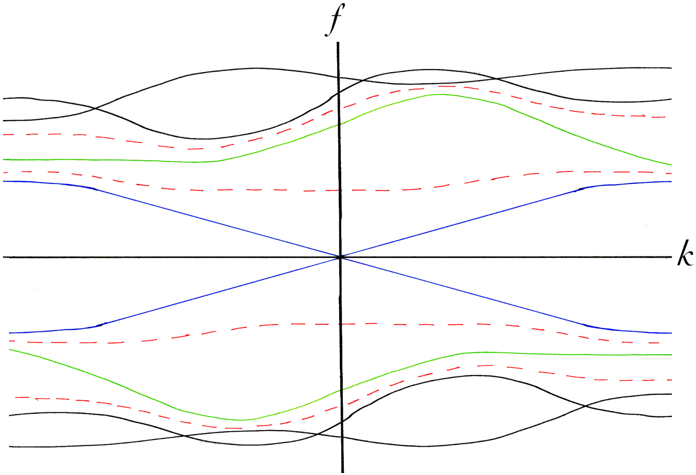
The Maxwell operator

$$\begin{aligned} M_\lambda^{\mathcal{Z}} &= M_0^{\mathcal{Z}} + \lambda\, M_1^{\mathcal{Z}} \\ &= \tau(\mathrm{i}\lambda\nabla_k)\, M_\Gamma^{\mathcal{Z}}(\hat{k}) + \lambda\, \tau(\mathrm{i}\lambda\nabla_k)\, \Upsilon(\mathrm{i}\lambda\nabla_k) \end{aligned}$$

is defined on the same λ-independent domain

$$\mathcal{Z}\mathcal{D} = \mathcal{Z}\big(\ker \mathrm{Div} \oplus G\big)$$

»Semiclassical« dynamics



»Semiclassical« dynamics

Setup

- $k \mapsto E_{\mathrm{b}}(k)$ isolated, non-degenerate
- $E_{\mathrm{b}}(k) \neq 0$ for all $k \in \mathbb{R}^3$ $\rightsquigarrow$ excludes ground state bands!
- Bloch function $k \mapsto \varphi_{\mathrm{b}}(k)$
- $\rightsquigarrow$ projection $k \mapsto |\varphi_{\mathrm{b}}(k)\rangle\langle\varphi_{\mathrm{b}}(k)|$ analytic
- Berry curvature $\Omega(k) := \mathrm{i}\,\nabla_k \wedge \big\langle \varphi_{\mathrm{b}}(k), \nabla_k \varphi_{\mathrm{b}}(k) \big\rangle_{\mathcal{H}_\Gamma^{\mathbb{T}}}$
- Chern number need not be zero! (then $k \mapsto \varphi(k)$ cannot be chosen purely real)

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»Semiclassical« dynamics

Semiclassical flow

Define $\Phi_\lambda : \mathbb{R} \times T^*\mathbb{R}^3 \longrightarrow T^*\mathbb{R}^3$ as flow associated to

$$\dot{r} = +\nabla_k \big(\tau \, E_{\mathrm{b}}\big) + \lambda \, \nabla_k \big\langle \varphi_{\mathrm{b}} \, , \, \tau \, \Upsilon \varphi_{\mathrm{b}} \big\rangle_{\mathcal{H}_\Gamma^{\mathbb{T}}} - \lambda \, \dot{k} \wedge \Omega$$

$$\dot{k} = -\nabla_r \big(\tau \, E_{\mathrm{b}}\big) - \lambda \nabla_r \big\langle \varphi_{\mathrm{b}} \, , \, \tau \, \Upsilon \varphi_{\mathrm{b}} \big\rangle_{\mathcal{H}_\Gamma^{\mathbb{T}}}$$

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»Semiclassical« dynamics

Theorem (Semiclassical dynamics, De Nittis & L. (2012))

There exists a projection

$$\Pi_\lambda = |\varphi_{\mathrm{b}}(\hat{k})\rangle\langle\varphi_{\mathrm{b}}(\hat{k})| + \lambda\,\pi_1 + \mathcal{O}_{\|\cdot\|}(\lambda^2)$$

such that $\forall\, f \in \mathcal{C}^\infty_{\mathrm{per}}(T^*\mathbb{R}^3;\mathbb{R})$ *and* $t = \mathcal{O}(1)$*:*

$$\left\| \Pi_\lambda \left(\mathrm{e}^{-\mathrm{i}\frac{t}{\lambda} M_\lambda^{\mathcal{Z}}}\, \mathrm{Op}(f)\, \mathrm{e}^{+\mathrm{i}\frac{t}{\lambda} M_\lambda^{\mathcal{Z}}} - \mathrm{Op}\big(f \circ \Phi_\lambda^t\big) \right) \Pi_\lambda \right\| = \mathcal{O}(\lambda^2).$$

Semiclassics: interpretation of result

- first mathematically rigorous result
- new term: $\mathcal{M}_1(r,k) = \langle \varphi_{\mathrm{b}}(k), \tau(r)\,\Upsilon(r)\varphi_{\mathrm{b}}(k)\rangle_{\mathcal{H}_\Gamma^{\mathbb{T}}}$ $\rightsquigarrow$ change in field energy
- assumption $E_{\mathrm{b}}(k) \neq 0\ \forall k \in \mathbb{R}^3$ excludes ground state bands
  - states with $E_{\mathrm{gs}}(k) \approx 0$ 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!
- Proof based on recent publication of Teufel & Stiepan
- uses mixture of operator-theoretic and ΨDO techniques (e. g. π_1 is *not* a ΨDO!)

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Semiclassics: comparison to notable previous results

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

- »derivation by analogy«
- necessity of slow variation recognized, but small parameter λ not used
- equations of motion:

$$\dot{r} = +\nabla_k(\tau E_{\mathrm{b}}) + \lambda\,(\nabla_k \mathcal{M}_1 - \dot{k} \wedge \Omega)$$
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- 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

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

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- involve incorrectly defined Berry connection**s** $\widetilde{\mathcal{A}}^E$ and $\widetilde{\mathcal{A}}^H$, Berry curvature $\widetilde{\Omega}$

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- result is not readily comparable to ours

Superadiabatic projection

Proposition

Suppose $\sigma_{\mathrm{rel}}(r,k) = \{\tau(r) E_n(k)\}_{n \in \mathcal{I}}$ consists of isolated bands. Then there exists an orthogonal projection

$$\Pi_\lambda = \sum_{n \in \mathcal{I}} |\varphi_n(\hat{k})\rangle\langle\varphi_n(\hat{k})| + \lambda\, \pi_1 + \mathcal{O}_{\|\cdot\|}(\lambda^2)$$

which commutes with $M_\lambda^{\mathcal{Z}}$ up to $\mathcal{O}_{\|\cdot\|}(\lambda^2)$,

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and maps onto states in the physical subspace up to $\mathcal{O}(\lambda^2)$,

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Superadiabatic projection

Proof.

- constructs *only first-order correction!*
- uses »defect construction« introduced in [Panati, Spohn & Teufel (2002)]
- explicit ansatz for π_1 $\rightsquigarrow$ only works for **isolated** bands
- construction *on the level of operators* $\rightsquigarrow$ tedious
- crucial: states in $\operatorname{ran} \Pi_\lambda$ are physically relevant states (up to errors of higher order)

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  - band crossings within $\sigma_{\mathrm{rel}}(r, k)$ can be treated
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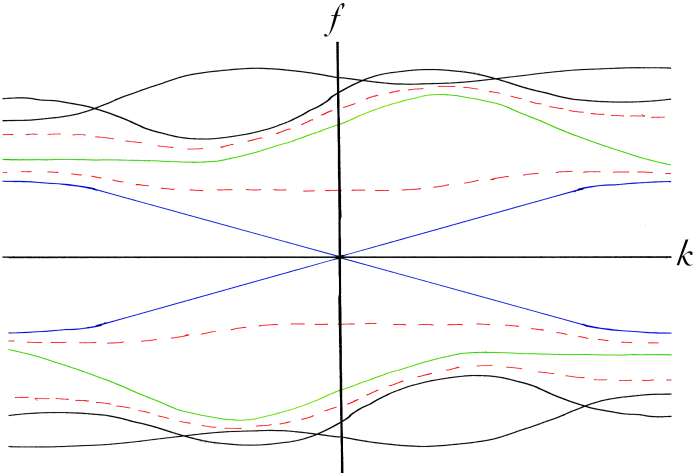

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Other questions

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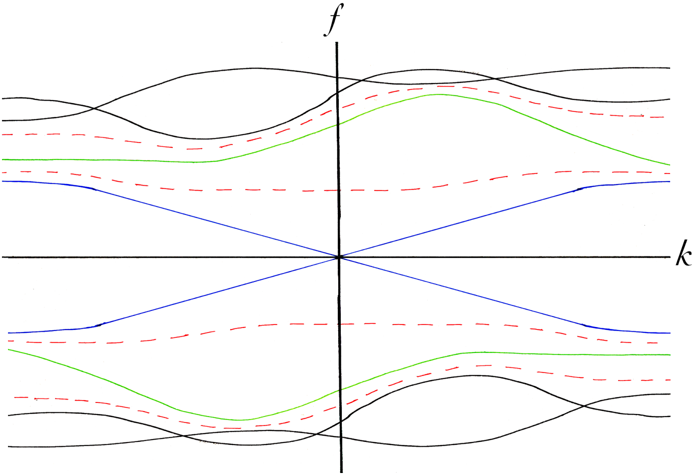

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Thank You for your attention!

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Multiband effective dynamics

Why is multiband dynamics interesting/necessary?

- If at least one of the Chern numbers

$$\mathrm{Ch}_j(|\varphi_{\mathrm{b}}\rangle\langle\varphi_{\mathrm{b}}|) = \frac{1}{2\pi}\int_{\mathcal{B}} \mathrm{d}k\,\Omega_j(k)$$

associated to the band E_{b} is non-zero $\Rightarrow$ *not* possible to choose $k \mapsto \varphi_{\mathrm{b}}(k)$ real everywhere!

- Physical fields $(\mathbf{E}, \mathbf{H})$ must be real!
- $\rightsquigarrow$ use $k \mapsto \frac{1}{2}\big(\varphi_{\mathrm{b}}(k) + \overline{\varphi_{\mathrm{b}}(-k)}\big)$ and $k \mapsto \frac{1}{2\mathrm{i}}\big(\varphi_{\mathrm{b}}(k) - \overline{\varphi_{\mathrm{b}}(-k)}\big)$!?
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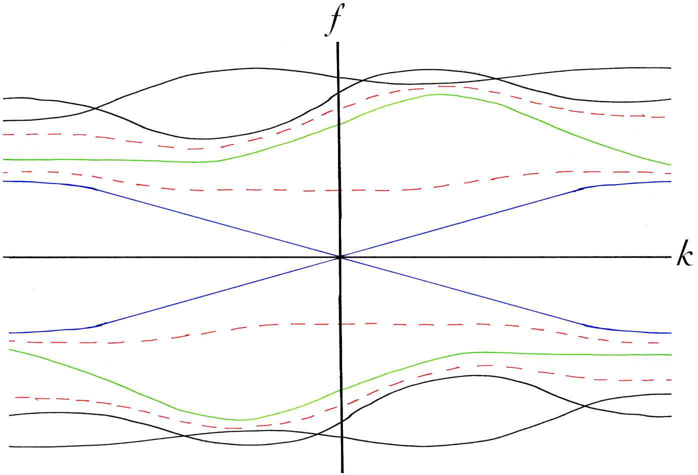

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- particle-hole symmetry (complex conjugation in original representation) ⇒ $\overline{\varphi_{\mathrm{b}}(k)}$ solution to eigenvalue equation $-E_{\mathrm{b}}(-k)$
- also $k \mapsto -E_{\mathrm{b}}(-k)$ is an isolated band!

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- upper and lower bands $E_{\pm}(k)$ with eigenfunctions $\varphi_{\pm}(k)$, $\varphi_{-}(k) = \overline{\varphi_{+}(-k)}$
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Theorem (De Nittis & L. (2012))

There exists a projection $\Pi_\lambda = \sum_{n=\pm} |\varphi_n(\hat{k})\rangle\langle\varphi_n(\hat{k})| + \lambda \pi_1$ *and an intertwining unitary* $U_\lambda = u_0(\hat{k}) + \lambda U_1$ *such the dynamics generated by the* Ψ*DO associated to*

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approximates the full Maxwell dynamics up to $\mathcal{O}(\lambda^2)$ *in norm:*

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