Homogenization of 'micro-resonances' and localization of waves.

Valery Smyshlyaev

University College London, UK

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(joint work with Ilia Kamotski UCL, and Shane Cooper Bath/ Cardiff)

Outline:

- Classical homogenization for waves (= low frequencies)

- Higher frequencies + higher contrasts ('degeneracies')

 \longrightarrow 'resonant' homogenization

- ${\bf Effects}:$ (frequency/wavenumber) band gaps, dispersion, 'negative' materials, etc.

- 'Partial' degeneracies and resonances (more of effects; general theory)

- Photonic Crystal Fibers as an example of **partial degeneracies** \rightarrow Band gaps in PCFs. (Cooper, Kamotski, V.S., 2012).





$$\rho^{\varepsilon}(x)u_{tt} - \operatorname{div}\left(a^{\varepsilon}(x)\nabla u^{\varepsilon}\right) = f(x,t)$$

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$$ho^{\varepsilon}(x)u_{tt} - \operatorname{div}\left(a^{\varepsilon}(x)\nabla u^{\varepsilon}\right)\right) = f(x,t)$$

$$\begin{split} f(x,t) &\equiv 0, \ t \leq 0; \quad u(x,t) \equiv 0, \ t \leq 0. \\ a^{\varepsilon}(x) &= a(x/\varepsilon), \ \rho^{\varepsilon} = \rho(x/\varepsilon) \\ \rho(y), \ \rho(y) \ \text{Q-periodic in y} \end{split}$$



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Asymptotic expansion

$$u^{\varepsilon}(x,t) \sim u^{0}(x,x/\varepsilon,t) + \varepsilon u^{1}(x,x/\varepsilon,t) + \dots u^{0}(x,y,t), u^{1}(x,y,t) Q$$
-periodic in y

$$arepsilon^{-2}: \ u^0 = u(x,t)$$
 (\equiv 'long wavelengths' \equiv 'low frequencies')

$$\begin{split} \varepsilon^{-2} : & u^0 = u(x,t) \quad (\equiv \text{`long wavelengths'} \equiv \text{`low frequencies'}) \\ \varepsilon^{-1} : & u^1 = \sum_j N_j(y) \frac{\partial u^0}{\partial x_j}(x,t) \end{split}$$

N solutions of "cell problem" $\operatorname{div}_{y}(a(y)(e^{j} + \nabla_{y}N_{j})) = 0$

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The Homogenisation Theorem

C>0 independent of ε such that $\|u^{\varepsilon} - (u^0 + \varepsilon u^1)\|_{\mathcal{H}^1} \leq C \varepsilon^{1/2}$

High-contrast (= 'micro-resonant') homogenization and 'non-classical' two-scale limits (Zhikov 2000, 2004)



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Contrast $\delta \sim \varepsilon^2$ is a **critical scaling** giving rise to 'non-classical' effects (Khruslov 1980s; Arbogast, Douglas, Hornung 1990; Panasenko 1991; Allaire 1992; Sandrakov 1999; Brianne 2002; Bourget, Mikelic, Piatnitski 2003; Bouchitte & Felbaq 2004, ...): elliptic, spectral, parabolic, hyperbolic, nonlinear, non-periodic/ random,

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WHY?

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Two-scale formal asymptotic expansion: div $(a^{\varepsilon}(x)\nabla u^{\varepsilon}) + \rho\omega^2 u^{\varepsilon} = 0$ (timeharmonicwaves) $\iff A^{\varepsilon}u^{\varepsilon} = \lambda u^{\varepsilon}, \ \lambda = \rho\omega^2$ (spectral problem). Seek $u^{\varepsilon}(x) \sim u^0(x, x/\varepsilon) + \varepsilon u^1(x, x/\varepsilon) + \dots u^j(x, y) Q$ – periodic in y.

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THEN:

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$$\begin{cases} \text{Then} & u^{0}(x, y) = \\ u^{0}(x) & \text{in } Q_{1} \quad (\text{still low frequency}) \\ w(x, y) & \text{in } Q_{0} \quad (\text{`resonance' frequency}) \end{cases}$$



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(u^{0}, w), w(x, y) := u^{0}(x) + v(x, y), \\
\text{solves the two-scale limit spectral problem:}
\end{cases}$$



Image: A math a math

$$-\operatorname{div}_{x}(a^{hom}\nabla_{x}u(x)) = \lambda u(x) + \lambda < v > (x) \text{ in } \Omega$$

$$-\operatorname{div}_{y}(a^{(0)}\nabla_{y}v(x,y)) = \lambda(u(x) + v(x,y)) \text{ in } Q_{0}$$

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Decouple it \downarrow

Two-scale limit spectral problem Decouple by choosing $v(x, y) = \lambda u(x)b(y)$ $-\operatorname{div}_{y}(a^{(0)}\nabla_{y}b(y)) - \lambda u = 1 \quad \text{in } Q_{0}$ $b(y) = 0 \quad \text{on } \partial Q_{0}$ $-\operatorname{div}_{x}(a^{hom}\nabla u(x)) = \beta(\lambda)u(x), \quad \text{in } \Omega,$ where $\beta(\lambda) = \lambda + \lambda^{2} \sum_{i=1}^{\infty} \frac{\langle \phi_{j} \rangle_{y}^{2}}{\lambda_{j} - \lambda},$

 (λ_j, ϕ_j) Dirichlet eigenvalues/functions of inclusion Q_0 (= "micro-resonances": $\beta < 0$ "negative denstity/magnetism" etc)



Rigorous analysis: Two-scale Convergence

Definition

1. Let $u_{\varepsilon}(x)$ be a bounded sequence in $L^{2}(\Omega)$. We say (u_{ε}) weakly two-scale converges to $u_{0}(x, y) \in L^{2}(\Omega \times Q)$, denoted by $u_{\varepsilon} \xrightarrow{2} u_{0}$, if for all $\phi \in C_{0}^{\infty}(\Omega)$, $\psi \in C_{\#}^{\infty}(Q)$

$$\int_{\Omega} u_{\varepsilon}(x)\phi(x)\psi\left(\frac{x}{\varepsilon}\right) \mathrm{d}x \longrightarrow \int_{\Omega} \int_{Q} u_{0}(x,y)\phi(x)\psi(y) \, \mathrm{d}x \mathrm{d}y$$

as $\varepsilon \to 0$.

2. We say $(u_{\varepsilon}) \xrightarrow{\text{strongly}}$ two-scale converges to $u_0 \in L^2(\Omega \times Q)$, denoted by $u_{\varepsilon} \xrightarrow{2} u_0$, if for all $v_{\varepsilon} \xrightarrow{2} v_0(x, y)$,

$$\int_{\Omega} u_{\varepsilon}(x) v_{\varepsilon}(x) \mathrm{d} x \longrightarrow \int_{\Omega} \int_{Q} u_{0}(x, y) v_{0}(x, y) \, \mathrm{d} x \mathrm{d} y$$

as $\varepsilon \rightarrow 0$. (implies convergence of norms upon sufficient regularity)

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1. Two-scale resolvent convergence:

 $\begin{array}{ll} \alpha > 0, \quad A^{\varepsilon}u^{\varepsilon} + \alpha u^{\varepsilon} = f^{\varepsilon} \in L^{2}(\Omega); \quad u^{\varepsilon} \in H^{1}_{0}(\Omega). \\ \text{If } f^{\varepsilon} \stackrel{2}{\rightarrow} f_{0}(x,y) \text{ then } u^{\varepsilon} \stackrel{2}{\rightarrow} u_{0}(x,y). (\text{If } f^{\varepsilon} \stackrel{2}{\rightarrow} f_{0}(x,y) \text{ then } u^{\varepsilon} \stackrel{2}{\rightarrow} u_{0}(x,y).) \\ \text{Here } u_{0} \text{ solves "two-scale limit problem" } A_{0}u_{0} + \alpha u_{0} = f_{0}. \end{array}$

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2. Spectral band gaps: (Let $\Omega = \mathbb{R}^d$.)

A₀ self-adjoint in $H \subset L^2(\mathbb{R} \times Q_0)$, with a band-gap spectrum $\sigma(A_0)$. $\sigma(A^{\varepsilon}) \to \sigma(A_0)$ in the sense of Hausdorff. (Hence a Band-gap effect: For small enough ε waves of certain frequencies do not propagate, in any direction). The proof is based on a "two-scale spectral compactness"

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Limit band gaps ={ $\lambda : \beta(\lambda) < 0$ }. Interpretation : $\beta(\lambda) = \mu(\omega) < 0 \leftrightarrow$ negative magnetism/density (Bouchitte & Felbacq, 2004).

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 $\beta(\lambda) > 0$ - propagation with (high) dispersion ($\lambda \rightarrow \lambda_j -$), due to "coupled resonances"' (V.S. & P. Kuchment, 2007).

'Frequency' vs ''directional'' gaps and 'partial' degeneracies Cherednichenko, V.S., Zhikov (2006): spatial nonlocality for homogenised limit with highly anisotropic fibers.



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V.S. (2009): a "directional localization" (via formal asymptotic expansions): for certain frequencies waves can propagate in some directions (e.g. along the fibers above) but cannot in others (e.g. orthogonal to the fibers).

'Frequency' vs ''directional'' gaps and 'partial' degeneracies Cherednichenko, V.S., Zhikov (2006): spatial nonlocality for homogenised limit with highly anisotropic fibers.

$$a^{\varepsilon}(x) = \begin{cases} \sim 1 & \text{in } Q_1(matrix) \\ \sim \varepsilon^2 & \text{in } Q_0 \text{ "across" fibers} \\ \sim 1 & \text{in } Q_0 \text{ "along" fibers} \end{cases}$$

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Notice, in the above fibres, $a^{\varepsilon}(x) = a^{(1)}(x/\varepsilon) + \varepsilon^2 a^{(0)}(x/\varepsilon)$, where $a^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, *i.e. is partially degenerate.*

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Photonic crystal fibers: A partially degenerate problem (Cooper, I. Kamotski, V.S. 2012); cf scalar prototype problem I.Kamotski V.S. 2006; M. Cherdantsev 2009 ('full' contrast)



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Photonic crystal fibers: Problem Formulation



$$\begin{aligned} \nabla \times E &= i\omega\mu H, \\ \nabla \times H &= -i\omega\epsilon E \\ \epsilon &= \epsilon_0\chi_0(x/\varepsilon) + \epsilon_1\chi_1(x/\varepsilon) \\ \epsilon_0 &> \epsilon_1, \quad \mu \text{ constant} \\ \text{E} &= \exp(ikx_3)E(x_1, x_2), \\ \text{H} &= \exp(ikx_3)H(x_1, x_2) \end{aligned}$$

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Photonic crystal fibers: Problem Formulation



In each phase E_3 and H_3 satisfy the following equations

$$\Delta E_3 + a^{\varepsilon} E_3 = 0, \qquad \qquad \Delta H_3 + a^{\varepsilon} H_3 = 0$$

where $a^{\varepsilon} = \omega^2 \mu \epsilon(x/\varepsilon)$ - k². E₃ and H₃ coupled across interface Γ^{ε} :

$$\omega \left[\frac{\epsilon}{a^{\varepsilon}} \nabla E_3 \cdot \mathbf{n} \right] = -k \left[\frac{1}{a^{\varepsilon}} \nabla H_3 \cdot \mathbf{n}^{\perp} \right], \quad k \left[\frac{1}{a^{\varepsilon}} \nabla E_3 \cdot \mathbf{n}^{\perp} \right] = \omega \left[\frac{\mu}{a^{\varepsilon}} \nabla H_3 \cdot \mathbf{n} \right]$$

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Photonic crystal fibers: A partially degenerate problem Consider the problem in its weak form:

$$\partial_{1}\left(\frac{\omega\epsilon}{a^{\varepsilon}}E_{3,1}\right) + \partial_{2}\left(\frac{\omega\epsilon}{a^{\varepsilon}}E_{3,2}\right) + \partial_{1}\left(\frac{k}{a^{\varepsilon}}H_{3,2}\right) - \partial_{2}\left(\frac{k}{a^{\varepsilon}}H_{3,1}\right) = -\omega\epsilon E_{3}$$
$$\partial_{1}\left(\frac{k}{a^{\varepsilon}}E_{3,2}\right) - \partial_{2}\left(\frac{k}{a^{\varepsilon}}E_{3,1}\right) - \partial_{1}\left(\frac{\omega\mu}{a^{\varepsilon}}H_{3,1}\right) - \partial_{2}\left(\frac{\omega\mu}{a^{\varepsilon}}H_{3,2}\right) = \omega\mu H_{3}.$$

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For $u = (E_3, H_3)$, find u such that

$$\begin{split} \int_{\mathbb{R}^2} \frac{\omega}{a^{\varepsilon}} \left(\epsilon \nabla u_1 \cdot \overline{\nabla \phi_1} + \mu \nabla u_2 \cdot \overline{\nabla \phi_2} \right) + \frac{k}{a^{\varepsilon}} \left(\left\{ \overline{\phi_1}, u_2 \right\} + \left\{ u_1, \overline{\phi_2} \right\} \right) \, \mathrm{d}x \\ &= \int_{\mathbb{R}^2} \omega \rho(x/\varepsilon) u \cdot \overline{\phi} \quad \forall \phi \in C_0^{\infty}(\mathbb{R}^2) \\ \{u, v\} &:= u_{,1} v_{,2} - v_{,1} u_{,2} \text{ (Poisson bracket);} \quad \rho(y) = \begin{pmatrix} \epsilon(y) & 0 \\ 0 & \mu \end{pmatrix} \end{split}$$

Form positive if $k^2 < \omega^2 \mu \epsilon_1$.

Photonic crystal fibers: A partially degenerate problem Consider the problem in its weak form:

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$$= \int_{\mathbb{R}^2} \omega \rho(x/\varepsilon) u \cdot \overline{\phi} \quad \forall \phi \in C_0^{\infty}(\mathbb{R}^2)$$

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Form positive if $k^2 < \omega^2 \mu \epsilon_1$. Consider a 'near critical' k: $k^2 = \omega^2 \mu (\epsilon_1 - \epsilon^2), \ \omega^2 \mu = \lambda$ Photonic crystal fibers: a partially degenerate problem

An 'emergent' high contrast:

$$\int_{\mathbb{R}^2} A_{\varepsilon}(x) \nabla u \cdot \overline{\nabla \phi} \, \mathrm{d}x = \lambda \int_{\mathbb{R}^2} \rho(x/\varepsilon) u \cdot \overline{\phi} \mathrm{d}x \quad \forall \phi \in C_0^{\infty}(\mathbb{R}^2)$$

Here $A_{\varepsilon}(x) = A(x/\varepsilon)$ where $A(y) = a^{(1)}(y) + \varepsilon^2 a^{(0)}(y) + O(\varepsilon^4)$.

$$a^{(1)} \ge 0 \text{ BUT } a^{(1)}(y) + a^{(0)}(y) > \nu I, \ \nu > 0$$

 $a^{(1)}(y)\nabla u \cdot \nabla u = \chi_1(y) \left(|u_{1,1} + u_{2,2}|^2 + |u_{1,2} - u_{2,1}|^2 \right)$ (partially) DEGENERATES for *u* s.t. RHS zero. i.e. satisfies Cauchy-Riemann type equations in matrix phase.

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Moral: This appears a particular case of homogenization for partially degenerating PDE systems \downarrow

General 'Partial' Degeneracies (I. Kamotski and V.S. 2012) Consider a 'resolvent' problem:



$$\begin{split} &\Omega \in \mathbb{R}^{d}, \ \alpha > 0, \\ &- \operatorname{div} \left(a^{\varepsilon}(x) \nabla u^{\varepsilon} \right) + \alpha \rho^{\varepsilon} u^{\varepsilon} = f^{\varepsilon} \in \\ &L^{2}(\Omega), \\ &u^{\varepsilon} \in \left(H^{1}_{0}(\Omega) \right)^{n}, \ n \geq 1. \end{split}$$

A general degeneracy

$$egin{array}{lll} \mathsf{a}^arepsilon(x) &= \ \mathsf{a}^{(1)}\left(rac{\mathsf{x}}{arepsilon}
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ight)^{n imes d imes n imes d}, \quad \mathsf{a}^{(1)} \geq 0, \ \ \mathsf{a}^{(1)} + \mathsf{a}^{(0)} > 0, \end{array}$$

Weak formulation:

$$\begin{split} \int_{\Omega} \left[a^{(1)} \left(\frac{x}{\varepsilon} \right) \nabla u \cdot \nabla \phi(x) + \varepsilon^2 \, a^{(0)} \left(\frac{x}{\varepsilon} \right) \nabla u \cdot \nabla \phi(x) + \alpha \, \rho^{\varepsilon}(x) \, u \cdot \phi(x) \right] dx \\ &= \int_{\Omega} f^{\varepsilon}(x) \cdot \phi(x) \, dx, \ \forall \phi \in \left(H^1_0(\Omega) \right)^d. \end{split}$$

General 'Partial' Degeneracies (I. Kamotski and V.S. 2012) Consider a 'resolvent' problem:



$$\begin{split} &\Omega \in \mathbb{R}^{d}, \ \alpha > 0, \\ &- \operatorname{div} \left(a^{\varepsilon}(x) \nabla u^{\varepsilon} \right) + \alpha \rho^{\varepsilon} u^{\varepsilon} = f^{\varepsilon} \in \\ &L^{2}(\Omega), \\ &u^{\varepsilon} \in \left(H^{1}_{0}(\Omega) \right)^{n}, \ n \geq 1. \end{split}$$

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A priori estimates:

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Weak two-scale limits. Key assumption on the degeneracy Introduce

$$\mathbf{V} := \left\{ v \in \left(H^1_{\#}(Q) \right)^n \middle| a^{(1)}(y) \nabla_y v = 0 \right\}.$$

(subspace of "microscopic oscillations"), and

$$\mathsf{W}:=\left\{\psi \in \left(L^2_{\#}(Q)\right)^{n\times d} \mid \operatorname{div}_{y}\left(\left(a^{(1)}(y)\right)^{1/2}\psi(y)\right) = 0 \text{ in } \left(H^{-1}_{\#}(Q)\right)^{n}\right\}$$

("microscopic fluxes")

Then, up to a subsequence, $u^{\varepsilon} \stackrel{2}{\rightharpoonup} u_0(x, y) \in L^2(\Omega; V)$

$$\begin{split} \varepsilon \nabla u^{\varepsilon} & \stackrel{2}{\rightharpoonup} & \nabla_{y} u_{0}(x, y) \\ \xi^{\varepsilon}(x) &:= \left(a^{(1)}(x/\varepsilon)\right)^{1/2} \nabla u^{\varepsilon} & \stackrel{2}{\rightharpoonup} & \xi_{0}(x, y) \in L^{2}(\Omega; \mathcal{W}) \end{split}$$

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Key assumption

There exists a constant C > 0 such that for all $v \in (H^1_{\#}(Q))^n$ $\|P_{V^{\perp}}v\|_{(H^1_{\#}(Q))^n} \leq C \|a^{(1)}(y)\nabla_y v\|_{L^2}$

The two-scale Limit Operator

Let Ω be bounded Lipschitz, or $\Omega = \mathbb{R}^d$. Introduce $U \subset L^2(\Omega; V)$:

$$U := \left\{ u(x,y) \in L^2(\Omega; V) \middle| \exists \xi(x,y) \in L^2(\Omega; W) \text{ s.t., } \forall \Psi(x,y) \in C^{\infty} \right\}$$

$$\int_{\Omega} \int_{Q} \xi(x, y) \cdot \Psi(x, y) dx dy = -\int_{\Omega} \int_{Q} u(x, y) \cdot \nabla_{x} \cdot \left(\left(a^{(1)}(y) \right)^{1/2} \Psi(x, y) \right)$$

Define $T: U \to L^2$ by $Tu = \xi$.

Strong two-scale resolvent convergence: Let $f^{\varepsilon} \xrightarrow{2} f_0(x, y)$. Then $u^{\varepsilon} \xrightarrow{2} u_0(x, y)$ solving:

Find $u_0 \in U$ such that $\forall \phi \in U$

$$\int_{\Omega} \int_{Q} \left\{ Tu_0(x,y) \cdot T\phi_0(x,y) + a^{(0)}(y) \nabla_y u_0(x,y) \cdot \nabla_y \phi_0(x,y) + \alpha \rho(y) u_0(x,y) \cdot \phi_0(x,y) \right\} dy \, dx = \int_{\Omega} \int_{Q} f_0(x,y) \cdot \phi_0(x,y) \, dy \, dx.$$

Back to Photonic Crystals



satisfy Cauchy-Riemann type equations

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satisfy Cauchy-Riemann type equations

Theorem 1 (Key assumption holds)

There exists a constant c > 0 such that for any $u \in H^1_{\theta}(Q)$ $\|P_{V^{\perp}_{\theta}}u\|_{H^1(Q)} \le c \left(\|u_{1,1} + u_{2,2}\|_{L^2(Q_0)} + \|u_{1,2} - u_{2,1}\|_{L^2(Q_0)}\right).$

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Second Result

The generalised flux $\xi =: Tu$ is zero. i.e. $Tu = 0 \ \forall u \in U$. (Two-scale limit solution u_0 determined by miscroscopic behaviour only)

Limit Spectral problem:

Find $u \in V_{\theta}$ such that

$$\int_{Q} a^{(0)}(y) \nabla_{y} u(y) \cdot \overline{\nabla_{y}(\phi(y))} \, \mathrm{d}y = \lambda \int_{Q} \rho(y) u(y) \cdot \overline{\phi(y)} \, \mathrm{d}y \ \forall \phi \in V_{\theta}.$$

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Theorem 2 (Spectral compactness: not trivial)

Let $\lambda_{\varepsilon} \in \sigma(A^{\varepsilon})$ (Bloch spectrum). Let u^{ε} be associated normalized Bloch's waves: $A^{\varepsilon}u^{\varepsilon} = \lambda^{\varepsilon}u^{\varepsilon}$, $u^{\varepsilon}(x) = e^{i\theta^{\varepsilon} \cdot x/\varepsilon}v^{\varepsilon}(x/\varepsilon)$, $\|v^{\varepsilon}(y)\|_{L^{2}(Q)} = 1$, $\theta^{\varepsilon} \in (-\pi, \pi]^{d}$. Let $\lambda \to \lambda_{0}$ and $\theta^{\varepsilon} \to \theta_{0}$. Then $\lambda_{0} \in \sigma_{0}(A_{0}, \theta_{0})$ (spectrum of the Limit operator), and $u^{\varepsilon} \to u_{0}(y)$, eigenfunction of $A_{0}(\theta)$. Hence the spectra converge.

Implication: If the limit problem displays a band-gap, the original problem must also have a gap for small enough ε .

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Example: Band gaps in 'ARROW' fibres

An extreme problem: Q_0 a circle of small radius δ



Theorem:

There exist constants c_1 , $c_2 > 0$ independent of δ , such that, for all quasimomenta θ_0 ,

$$\lambda_2(heta_0) \leq -rac{c_1}{\delta^2 \ln \delta}, \qquad \lambda_3(heta_0) \geq c_2 \delta^{-2}.$$

This implies that, for small enough δ , there is a wide spectral gap in the limit spectrum, and therefore also for small enough ε for the original problem by the spectral compactness.

+ Higher gaps: $\lambda \sim \lambda_j^D(Q_0^\delta) \sim \delta^{-2}$ (re 'micro-resonances')

The band gaps in a Photonic Crystal Fiber:



Summary:

- Homogenization for a critical high contrast scaling $\delta\sim\varepsilon^2$ gives rise to numerous "non-classical" effects described by two-scale limit problems due to "micro-resonances".

- **'Partial' degeneracies** often happen in physical problems, and give rise to more of such effects (e.g. **Band Gaps in Photonic Crystal Fibers**). These however have to be analysed in a new way.

- A general two-scale homogenization theory can be constructed for such partial degeneracies, under a generically held decomposition condition. Resulting limit (homogenized) operator is generically two-scale (and 'non-local').

- Associated two-scale operator and spectral convergence and compactness are held generally or for particular physical examples.

- In principle, some of this applies also to nonlinear (cf Cherednichenko & Cherdantsev 2011), discrete-to-continuous, as well as non-periodic problems.