Simplicity of Spectral Edges and Applications to Homogenization

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- Perturbation Theory for Periodic Elliptic Operators
  - Local Simplicity
  - Global Simplicity
  - Simplicity of Spectral Edge
- Applications to theory of Homogenization
  - General Theory
  - Bloch Wave Homogenization
  - Internal Edge Homogenization

Introduction

- Eigenvalue Problems that depend on parameters arise in a variety of physical problems.
- Examples include motion of electrons in semiconductors, wave motion in periodic media, etc.
- Knowledge of dependence of eigenvalues and eigenfunctions on parameters is crucial for understanding physics.
- Such problems pose significant mathematical challenges.

Spectral Theory of Periodic Elliptic Operators

Periodic Elliptic Operators

- We shall consider operators $\mathcal{A} : \mathcal{D}(\mathcal{A}) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ defined by

$$\mathcal{A}u := -\frac{\partial}{\partial y_k}\left(a_{kl}(y)\frac{\partial u}{\partial y_l}\right)$$

where $A = (a_{kl})$ is a coercive real symmetric matrix with entries in $L^\infty_\sharp(Y)$, $Y = [0, 2\pi)^d$.

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- The spectrum of $\mathcal{A}$ has a band structure.

Spectral Theory of Periodic Operators

The periodic symmetry of the operator induces a direct integral decomposition of the space

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$$\mathcal{A} = \int_{Y'}^{\oplus} \mathcal{A}(\eta) d\eta$$

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where $\mathcal{A}(\eta) = -(\nabla + i\eta) \cdot (A(\nabla + i\eta))$ is an unbounded operator in $L^2_\sharp(Y)$.

As a consequence, the spectrum of $\mathcal{A}$ is the union of spectra of $\mathcal{A}(\eta)$ as η varies over $Y' = \left[-\frac{1}{2}, \frac{1}{2}\right)^d$.

Bloch Spectrum of $\mathcal{A}$

- For $\eta \in Y^{'}$, the operator $\mathcal{A}(\eta) = -\left(\nabla + i\eta\right) \cdot \left(A\left(\nabla + i\eta\right)\right).$ is an unbounded self-adjoint operator on $L^2_\sharp(Y)$ with a compact resolvent.

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- By the spectral theorem of compact self-adjoint operators, $\mathcal{A}(\eta)$ has a sequence of countably many eigenvalues diverging to ∞,

$$0 \leq \lambda_1(\eta) \leq \lambda_2(\eta) \leq \ldots \lambda_n(\eta) \leq \ldots$$

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- The functions $\eta \mapsto \lambda_m(\eta), m \in \mathbb{N}$ are known as Bloch eigenvalues of the operator $\mathcal{A}$.

Spectral gaps of $\mathcal{A}$

- Let $\sigma_n^- = \min_{\eta \in Y'} \lambda_n(\eta)$ and $\sigma_n^+ = \max_{\eta \in Y'} \lambda_n(\eta)$, then

spectrum of the operator $\mathcal{A}$, $\sigma(\mathcal{A}) = \bigcup_{n \in \mathbb{N}} [\sigma_n^-, \sigma_n^+]$

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- The complement is a union of open intervals known as spectral gaps, whose endpoints are called spectral edges.

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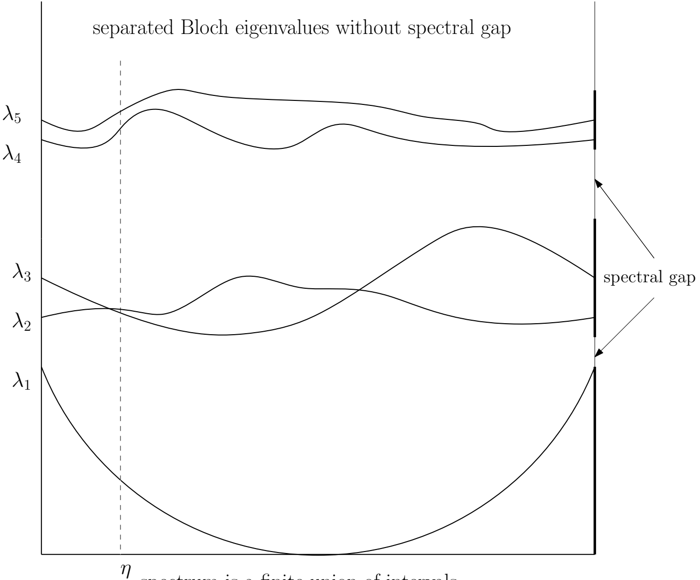

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Spectral Edges

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- In material science, homogenization is interpreted as a spectral edge phenomena, whereas in solid state physics, spectral edges are attached to the notion of effective mass and localization.
- In Solid State Physics, electric and magnetic potentials V are objects of interest, whereas in material science, the coefficients of the elliptic operator are important.
- The regularity properties of spectral edges determine the physical phenomena.

Regularity Properties of Spectral edges

A spectral edge is expected to have the following regularity properties generically[2].

- Spectral edge is isolated, i.e., the spectral edge is attained at finitely many points by the Bloch eigenvalues.

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- Spectral edge is non-degenerate, i.e., The Bloch eigenvalue is strongly convex when it is close to the spectral edge.

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What is known?

- Filonov & Kachkovskiy[3] proved that the spectral edge is isolated for periodic operators in dimension 2.

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- Parnovski and Shterenberg[5] proved that in dimension 2, a perturbation by a potential of a larger period makes a spectral edge non-degenerate.

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Perturbation Theory of Periodic Operators

- Local Simplicity
- Global Simplicity
- Simplicity of Spectral Edge

Local Simplicity

Theorem (S. Sivaji Ganesh & T., 2018)
Let $A = (a_{ij}) \in L^\infty_\sharp(Y)$ be a positive definite matrix. Let $\eta_0 \in Y'$ and $\lambda_m(\eta_0)$ be a Bloch eigenvalue of the operator $-\nabla \cdot (A\nabla)$ of multiplicty h. Then, there exists a diagonal matrix $B = (b_{ij}) \in L^\infty_\sharp(Y)$ such that the Bloch eigenvalue $\tilde{\lambda}_m(\eta_0)$ of the perturbed operator $-\nabla \cdot (A + tB)\nabla$ is simple for small $t > 0$.

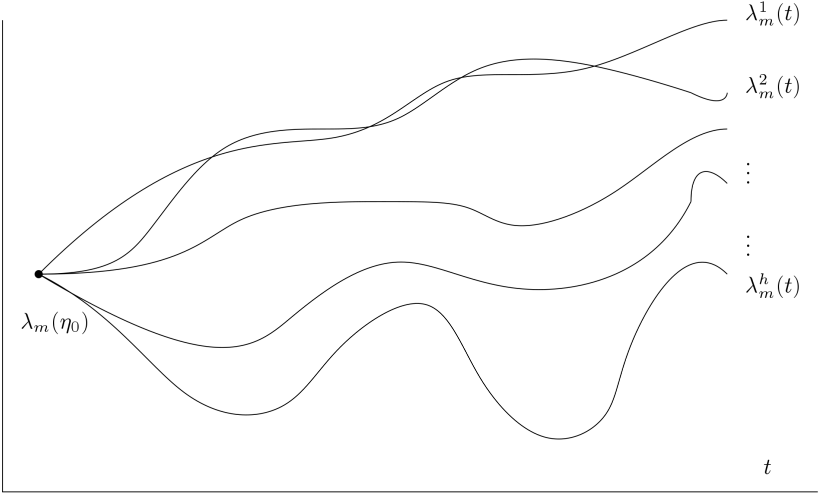

Figure: Perturbed Eigenvalues

Global Simplicity

Theorem (S. Sivaji Ganesh & T., 2018)

Let $A = (a_{ij}) \in L^\infty_\sharp(Y)$ be a real symmetric positive definite matrix. Let $\lambda_m(\eta)$ be a Bloch eigenvalue of the operator $-\nabla \cdot (A\nabla) = \int_{Y'}^{\oplus} \mathcal{A}(\eta)$. Then, there is a measurable family of matrices B_η, such that the perturbed operator $\int_{Y'}^{\oplus} \tilde{\mathcal{A}}(\eta)$ has simple Bloch eigenvalue $\tilde{\lambda}_m(\eta)$ for all $\eta \in Y'$ for small $\tau > 0$, where

$$\tilde{\mathcal{A}}(\eta) := -(\nabla + i\eta) \cdot (A + \tau B_\eta)(\nabla + i\eta)$$

Simplicity of Spectral Edge

Theorem (S. Sivaji Ganesh & T., 2018)
Let $A = (a_{ij})$ be a positive definite real symmetric matrix. Let (λ_-, λ_+) be a spectral gap of the operator $-\nabla \cdot (A\nabla)$. Suppose that either

- $a_{ij} \in W^{1,\infty}_\sharp(Y)$, or
- $a_{ij} \in L^\infty_\sharp(Y)$ and the spectral edge is attained at finitely many points.

Then, there exists a diagonal matrix $B = (b_{ij}) \in L^\infty_\sharp(Y)$ such that the new spectral edge $\tilde{\lambda}_+$ of the perturbed operator $\nabla \cdot (A + tB)\nabla$ is simple for small $t > 0$.

Ideas behind the proof

- For $a_{ij} \in W_\sharp^{1,\infty}(Y)$, a global perturbation is obtained. The proof relies on the interior Hölder continuity of the eigenfunctions and its derivatives. Hence the requirement of $W_\sharp^{1,\infty}(Y)$ coefficients.

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- For $a_{ij} \in W^{1,\infty}_{\sharp}(Y)$, a global perturbation is obtained. The proof relies on the interior Hölder continuity of the eigenfunctions and its derivatives. Hence the requirement of $W^{1,\infty}_{\sharp}(Y)$ coefficients.

- For $a_{ij} \in L^{\infty}_{\sharp}(Y)$, fiberwise perturbations are used to obtain simplicity of the spectral edge.

- Variational characterization of the eigenvalues (Courant-Fischer minmax principle) and perturbation theory is used.

Consequences of Simplicity

Simplicity implies Differentiability

- Given an eigenvalue problem depending smoothly (or C^1, C^ω) on multiple parameters, simplicity of the eigenvalue ensures smoothness (or C^1, C^ω) of the eigenvalues.

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- This may be generalized to operators in the von Neumann-Schatten class of operators, where a notion of determinant exists[6].

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Analytic Eigenvectors

- For a closed operator A, if λ is an isolated point of the spectrum $\sigma(A)$, the Projection operator

$$P_\lambda = -\frac{1}{2\pi i}\oint_{|\lambda-\mu|=r}(A-\mu)^{-1}d\mu$$

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exists, where r is the radius of a circle containing λ alone.

- For an analytic family of operators, the family of projection operators, $P_\lambda(\eta)$, is also analytic.

- If the eigenspace is one-dimensional, we obtain an analytic choice of eigenvectors by defining $\phi(y,\eta) = P_\lambda(\eta)\phi(y,0)$.

Applications to Bloch wave homogenization

Introduction to homogenization

- Homogenization is the study of the limits of solutions to equations with highly oscillatory coefficients.

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- For example, consider the problem

$$-div(A\left(\frac{x}{\epsilon}\right)\nabla u^{\epsilon}(x)) = f \text{ in } \Omega$$
$$u^{\epsilon} = 0 \text{ on } \partial\Omega$$

where A is a periodic matrix with bounded measurable coefficients.

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- The sequence of solutions u^{ϵ} is bounded in $H_0^1(\Omega)$ independent of ϵ, hence converges for a subsequence to u^0.

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- The sequence of solutions u^ϵ is bounded in $H_0^1(\Omega)$ independent of ϵ, hence converges for a subsequence to u^0.
- The theory of homogenization identifies matrices A^* such that the limit u^0 satisfies the equation

$$-div(A^* \nabla u^0(x)) = f \text{ in } \Omega$$
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Bloch wave homogenization

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- In particular, Bloch wave homogenization identifies the homogenized tensor with the Hessian of the first Bloch eigenvalue at $0 \in Y^{'}$.

$$a^*_{kl} = \frac{1}{2}\frac{\partial^2 \lambda_1}{\partial \eta_k \eta_l}(0).$$

Internal edge homogenization

- Hessian of the lowest Bloch eigenvalue is a measure of the convexity of the lowest spectral edge. Hence, homogenization may be interpreted as a phenomena governed by the regularity properties of the lowest spectral edge.

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Internal edge homogenization

- Hessian of the lowest Bloch eigenvalue is a measure of the convexity of the lowest spectral edge. Hence, homogenization may be interpreted as a phenomena governed by the regularity properties of the lowest spectral edge.

- Birman and Suslina[7] extended the notion of homogenization to internal edges of the spectrum by proposing an effective operator to the highly oscillating operator at internal edges.

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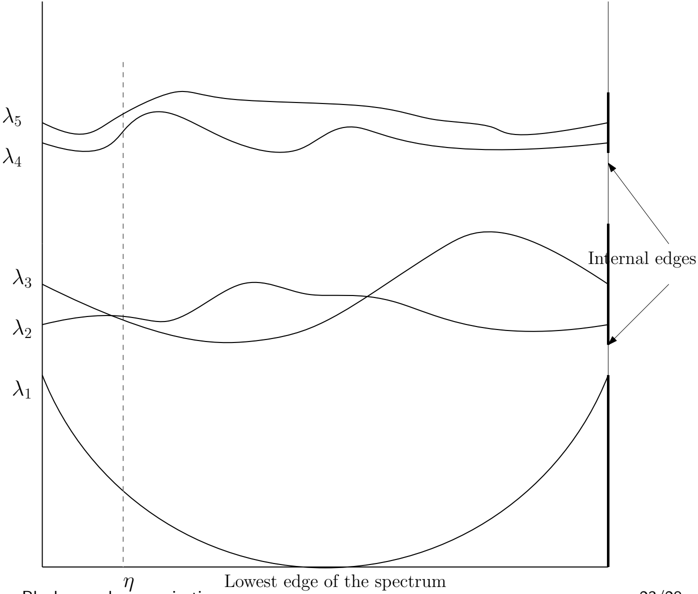
λ_5
λ_4
λ_3
λ_2
λ_1
Internal edges
η
Lowest edge of the spectrum

Internal edge homogenization

- Convergence to the effective operator depends on the regularity properties of the spectral edge. In particular, Birman and Suslina assume that the internal spectral edge is simple, isolated and non-degenerate.

Internal edge homogenization

- Convergence to the effective operator depends on the regularity properties of the spectral edge. In particular, Birman and Suslina assume that the internal spectral edge is simple, isolated and non-degenerate.
- We have extended the theorem of Birman and Suslina to spectral edges with multiplicity greater than 1 by using a perturbation of the operator which renders the multiple edge simple.

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- Given a microstructure A, how does one physically or geometrically realize the perturbed media $A + B$?
- These questions seem to point towards regularity of A?

Questions

- The elasticity operator with periodic coefficients has a multiple spectral edge with multiplicity 3. In particular, the lowest Bloch eigenvalue may not be smooth enough to compute its Hessian. This difficulty was circumvented earlier by using directional smoothness of the Bloch eigenvalues[8].

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- A proposal is to consider a zeroth order perturbation of the elasticity operator which would make its spectral edge simple and use the corresponding Hessian to approximate the homogenized coefficients for the elasticity operator.

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Genericity Results on Bloch Spectrum of Periodic Elliptic Operators and Applications to Homogenization.
arXiv:1807.00917

Thank you