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Eigenvalues in Gaps of the Essential Spectrum — an Overview.

Thank you, Percy, for a wonderful collaboration!

Contents.

- Introduction: Color of Crystals/doped semi-conductors
- The existence problem
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1. Introduction.

3 types of solid matter: metals, semi-conductors, insulators.

- Periodic Schrödinger operator $H = -\Delta + V(x)$ in $\mathbb{R}^d$;

  Bloch decomposition, spectral bands;

  Fermi level, gap length above Fermi level.

- Role of impurities: eigenvalues in gaps; selective absorption of e.m. radiation in crystals; transport properties of doped semi-conductors

  Ruby and Sapphire

  Simple model: $W \in C_c(\mathbb{R}^d)$ impurity potential, $W(x) \to 0$ at ∞.

  Question: Does $H - W$ have eigenvalues inside a given gap of H?

  Easier question: Does $H - \lambda W$ have eigenvalues in the gap H for suitable coupling $\lambda \in \mathbb{R}$?

1. Existence of eigenvalues.

- **Main difficulty:** Can't use min-max (variational principle)

  What do we get for granted? Perturbation theory implies that

- eigenvalues of $H - \lambda W$ in the gap are organized in **analytic branches** $E_i(\lambda)$.
- $E_i'(\lambda) = \langle W u_i, u_i \rangle$

Two simple examples

(1) Matrix example:

$$H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad W = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

No eigenvalue of $H - \lambda W$ enters the "gap" $(-1, 1)$.

(2) o.d.e. example:

Let $H = -\frac{d^2}{dx^2} + q(x)$, with $q\colon \mathbb{R} \to \mathbb{R}$ periodic, and let $W = \delta_{x_0}$ (Dirac distribution).

Suppose H has a spectral gap (α, β). Let $\alpha < E < \beta$ and let $\psi_\pm(x, E)$ denote the generalized eigenfunctions of H that decay exponentially at $\pm\infty$.

If x_0 is a zero of either ψ_+ or ψ_-, then no eigenvalue branch of $H - \lambda\delta_{x_0}$ will ever cross E.

Now consider $H = -\Delta + V(x)$ and perturbation $W(x)$ in $\mathbb{R}^d$. V need not be periodic. Let (α, β) be a spectral gap for H.

- Birman-Schwinger-principle

For $W \geq 0$, study the *Birman-Schwinger-operator*

$$B_E := \sqrt{W}(H - E)^{-1}\sqrt{W},$$

a compact, symmetric operator. Have:

$$E \in \sigma(H - \lambda W) \Longleftrightarrow 1/\lambda \in \sigma(B_E).$$

Klaus [Kl-82] used the BSP in 1-dim. to prove the existence of eigenvalues in gaps.

- Deift-H. [DH-86] study general case. E.g.:

Theorem I. *Suppose* $|x|^2 W(x) \to 0$ *at* ∞ *and* $W(x) \geq h > 0$ *on some ball. Then there is at most one* E_0 *which does not appear as an eivenvalue of* $H - \lambda W$*, for all* $\lambda \in \mathbb{R}$.

Approximating problems on large balls B_n,

$$H_n = -\Delta + V \quad \text{in } L_2(B_n),$$

with Dirichlet BC.

Problem: have to choose boundary conditions on ∂B_n; gap is not preserved.

Modify the H_n by projecting out the eigenstates related to the boundary, $H_n \longrightarrow \tilde{H}_n$.

Tools:

(1) Exponential decay of eigenfunctions

(2) Weyl's Law gives a polynomial bound on # of eigenstates

Compute (estimate) via min-max

$$\dim_E(\tilde{H}_n \pm \lambda W) - \dim_E(\tilde{H}_n).$$

- Potential wells $-\lambda W_+$ versus potential barriers λW_-, for $\lambda > 0$!
- Extensions and complements in the 80's: [H-87, 89], Alama-Deift-H. [ADH-89], Gesztesy-Simon [GS-88]

2. Asymptotics.

Question had been raised in [DH-86].

Further work in [Alama, PhD-thesis, 88], [H-87], [ADH-89].

For $E \in (\alpha, \beta)$ fixed, find the distribution of the couplings λ_i for which $E \in \sigma(H - \lambda W)$.

Phase space volume gives correct answer for $W \geq 0$, but not for $W \leq 0$.

Define

$$N_{\pm}(\lambda, H-E, W) := \#\{0 < \lambda_j < \lambda; E \in \sigma(H \mp \lambda_j W)\}$$

Theorem II. [H-87, ADH-89]

Let $0 \leq W(x) \leq c(1+|x|)^{-\alpha}$, *for some* $\alpha > 0$. *Then*

$$\begin{aligned}
&(2\pi)^d \lim_{\lambda\to\infty} \lambda^{-d/2} \cdot N_+(\lambda, H-E, W) \\
&= \lim_{\lambda\to\infty} \lambda^{-d/2} \mathrm{Vol}\{(x,p) \in \mathbb{R}^{2d}; 0 < p^2 + V - E < \lambda W\} \\
&= C_d \int W(x)^{d/2} dx.
\end{aligned}$$

Theorem III. [A-88, ADH-89]

Suppose $0 \leq W(x) \sim c|x|^{-\alpha}$, *as* $|x| \to \infty$, *for some* $c, \alpha > 0$. *Then*

$$\lim_{\lambda\to\infty} \lambda^{-d/\alpha} \cdot N_{-}(\lambda, H-E, W)$$

$$= \int_0^E \mathrm{Vol}\{y \in \mathbb{R}^d; -c|y|^{-\alpha} < t - E < 0\}\, d\varrho(t),$$

where $\varrho(.)$ *denotes the i.d.s. for* H.

- Weyl's Law; Fefferman-Phong (*Uncertainty Principle*)

Many results along these lines for $W = W_+ - W_-$.

Intuitively, expect

$$N_+(\lambda; H - E, W) \\ \geq |N_+(\lambda; H - E, W_+) - N_-(\lambda; H - E, W_-)|, \qquad (*)$$

cf. also Levendorskii [95]

Problem was taken up around 89/90 by M. Birman and his school.

Raikov, A. Sobolev, Weidl, Pushnitsky, Safronov ...

Almost exclusively $W \geq 0$ or $W \leq 0$, up to Safronov's tour de force.

Various extensions and refinements, e.g., study of the couplings where eigenvalue branches emerge from gap edges or are absorbed into a band.

Sobolev: number of eigenvalues in $[\alpha, \beta] \subset (a, b)$.

Birman applies the first resolvent equation to the BS-operator with $E \in (a, b)$, E_0 below the spectrum of H,

$$\begin{aligned}\sqrt{W}(H-E)^{-1}\sqrt{W} = {} & \sqrt{W}(H-E_0)^{-1}\sqrt{W} \\ & - \sqrt{W}(H-E)^{-1}(H-E_0)^{-1}\sqrt{W}.\end{aligned}$$

The two terms on the RHS belong to different weak trace ideals; in particular the spectral asymptotics are dominated by the first term on the RHS.

- Birman [91—] extends this to couplings where branches are created or merge into a band (ψ.d.o.-methods).

3. Eigenvalue trajectories.

Mainly o.d.e. results.

Write $W = W_+ - W_-$, where $W_\pm \geq 0$.

The eigenvalue trajectories for $H \pm \lambda W_\pm$ look as follows:

Figures!

The eigenvalue trajectories for $H - \lambda W$ are roughly a superposition of the 2 above pictures?

Trapping and Cascading [G^{2}HKS^{2}V-88]

2 phenomena in connection with trapping and cascading:

(1) Dirichlet decoupling along $\partial\{x; W_-(x) \neq 0\}$.

(2) generically, avoided crossings (figure)

Flat portions are close to eigenvalues of H considered in $L_2(\mathbb{R}^n \setminus \{W(x) \neq 0\})$.

Problem in P.D.E.-case: too many eigenvalues ("can of worms")

4. Extensions.

(1) Random Schrödinger operators H.-Kirsch [HK-94]

W of compact support $=$ potential of a single impurity.

Random distribution of impurities at periodic lattice sites, low density.

Spectral gaps disappear; i.d.s. concentrates at the eigenvalues of $H - W$ as density $\to 0$.

(2) Divergence type operators Alama, Avellaneda, Deift, H. [AADH-94], Birman [B-94]

$$A(\lambda) = -\nabla \cdot (\mathbf{a}(x) + \lambda \mathbf{b}(x))\nabla \quad \text{on } \mathbb{R}^d,$$

with

$\mathbf{a}$ uniformly positive definite,

$\mathbf{b} \geq 0$ and $\mathbf{b}(x) \to 0$ at ∞, $\mathbf{b}(x) \sim |x|^{-\beta}$ at ∞.

One approach uses *commutation formula* of Deift-Sakai.

Find asymptotics of couplings s.th. $E \in \sigma(A(\lambda))$.

Main mechanism: functions have to be almost constant on the support of $\mathbf{b}$, for λ large!

- Existence of $\mathbf{a}$, periodic, s.th. $-\nabla \cdot \mathbf{a}(x)\nabla$ has a spectral gap is of independent interest (photonic crystals,... Figotin-Kuchment [FK-96]), [H-92], H.-Lienau [HLi-00]

(3) Similar question as in (1) for Laplace-Beltrami-operators O. Post [P-01, etc.]

(4) Magnetic background can be easily accomodated. (Birman, Raikov [BR-91, R-91], H.-Levendorskii [HLe-98])

(5) Bohm-Aharonov Hamiltonians, i.e, perturbation of H by a (strong) magnetic field $\mathcal{B}$ of compact support.

- $\vec{a}$ vector field (vector potential) s.th. $\operatorname{curl} \vec{a} = \mathcal{B}$.

$$H(\lambda\vec{a}) = (-\mathrm{i}\nabla - \lambda\mathbf{a}(x))^2 + V(x), \qquad \lambda \in \mathbb{R},$$

$H_0 = -\Delta + V$, with a spectral gap (a, b).

- Note: eigenvalues of H_λ need not be monotonic!
- gauge invariance: $\vec{a} \to \vec{a} + \nabla f$ leaves spectrum inv.
- For large coupling λ, get natural DBC on ∂M,

$$M := \Omega^C, \qquad \Omega := \{x; \mathcal{B}(x) \neq 0\}.$$

Magnetic barriers, cyclotron radius!

Let $H_M(\lambda\vec{a})$ denote the operator with the same symbol as H_λ acting in $L_2(M)$ with DBC. Without restriction $V \geq 1$. Find

$$\left\| H(\lambda\vec{a})^{-1} - H_M(\lambda\vec{a})^{-1} \oplus 0 \right\| \to 0, \qquad \lambda \to \infty.$$

(H.-Herbst [HH-95], Herbst-Nakamura [HN-99]).

$\Longrightarrow$ for $\lambda \to \infty$, enough to study $\sigma(H_M(\lambda\vec{a}))$.

Simplification: there is $\mathbf{no}$ magnetic field on M.

- $\sigma(H(\lambda\mathbf{a}))$ approaches a quasi-periodic function of the fluxes through the components of Ω.

- Existence of eigenvalues in gap?

Easiest if Ω has a finite number of components. Find a sequence of couplings $\lambda_i \to \infty$ where $\lambda_i \vec{a}$ can be gauged away in M up to a small error. H.-Besch [HB-03], H. [H-06]

For such couplings, $\sigma(H(\lambda_i \vec{a}))$ is close to the spectrum of $-\Delta + V$ in $L_2(M)$ with DBC.

Use either Dirichlet's Theorem (number theory) or Ergodic Theory (Remark by B. Simon).

Connection with the case $H_0 + \mu\chi_\Omega$, Ω open.

Can handle some special cases with an ∞ number of components ([H-06]).

- Open Questions: Better understanding of infinite number of components?

(6) Nonlinear problems Alama-Li [92]