

SPECTRAL ANALYSIS OF A CONFINEMENT MODEL IN RELATIVISTIC QUANTUM MECHANICS

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MOTIVATION

Faber-Krahn inequality: $\Omega \subset \mathbb{R}^d$ open & bounded, $\Omega^* \subset \mathbb{R}^d$ ball with $|\Omega^*| = |\Omega|$, $\lambda_1(\Omega)$ lowest eigenvalue of the Dirichlet Laplacian $\begin{cases} -\Delta u = \lambda u & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$
 $\Rightarrow \lambda_1(\Omega) \geq \lambda_1(\Omega^*)$.

Among all membranes of a given area and with fixed boundary, the circular one produces the lowest fundamental tone.

Interpreting $\left\{ \begin{array}{l} \text{Laplacian} \rightarrow \text{free Schrödinger operator} \\ \text{Dirichlet boundary condition} \rightarrow \text{hard-wall boundary} \end{array} \right.$

The ground-state energy of a nonrelativistic quantum particle constrained to nanostructures of a given material is minimized by a ball.

In quantum mechanics:

- $-\Delta$ nonrelativistic \rightarrow Dirac operator $\left\{ \begin{array}{l} \text{relativistic} \\ \text{(\& local!)} \end{array} \right.$
- Dirichlet boundary condition $\left. \right\} \rightarrow$ MIT bag boundary condition (also called "infinite mass" boundary condition)

DIRAC OPERATORS

$$H := -i\alpha \cdot \nabla + m\beta$$

$$\Omega \subset \mathbb{R}^3$$

$$= -i(\alpha_1 \partial_1 + \alpha_2 \partial_2 + \alpha_3 \partial_3) + m\beta$$

• $m \geq 0$ mass.

• $\alpha_1, \alpha_2, \alpha_3, \beta$ 4×4 matrices $\begin{cases} \text{anticommute} \\ \alpha_i^2 = \alpha_j^2 = \alpha_k^2 = \beta^2 = \text{Id} \end{cases}$

$$\Rightarrow H^2 = (-\Delta + m^2)\text{Id} \quad (\text{in the spirit of } -\Delta = \frac{1}{4}\partial_z \partial_{\bar{z}} \text{ in } \mathbb{R}^2 \cong \mathbb{C})$$

$\Rightarrow H$ is a local version of $\sqrt{-\Delta + m^2}$ (not semibounded)

MIT bag boundary condition: $\mu = -i\beta(\alpha \cdot \vec{\nu})\mu$ on $\partial\Omega$
 $\vec{\nu}$ (normal vector field on $\partial\Omega$)

We study the family $\{H_\tau\}_{\tau \in \mathbb{R}}$:

$$\text{Dom}(H_\tau) := \{ \psi \in H^1(\Omega; \mathbb{C}^4) : \psi = i(\sinh \tau - \cosh \tau \beta)(\alpha \cdot \vec{\nu})\psi \text{ on } \partial\Omega \}$$

$$H_\tau \psi := (-i\alpha \cdot \nabla + m\beta)\psi \quad \forall \psi \in \text{Dom}(H_\tau)$$

Properties of the spectrum of H_τ :

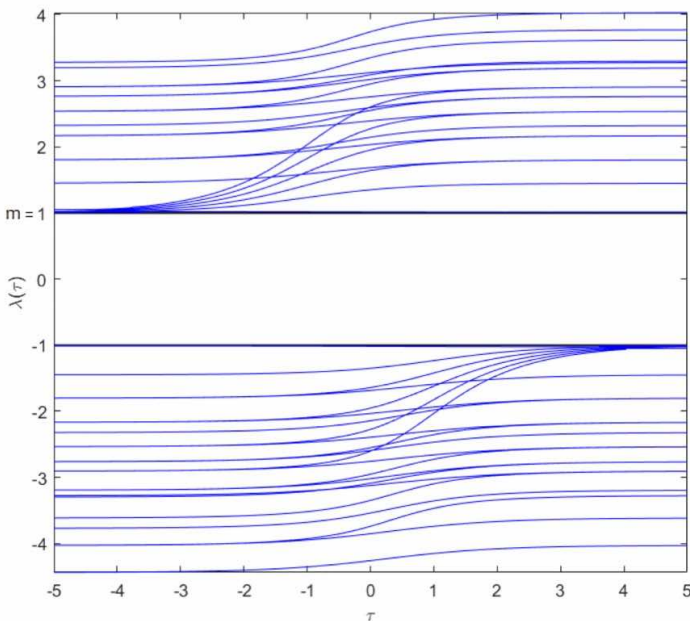
• $\sigma(H_\tau) \subset \mathbb{R} \cup [-m, m]$, purely discrete.

• $\lambda \in \sigma(H_\tau) \Leftrightarrow -\lambda \in \sigma(H_{-\tau})$.

\rightarrow (eigenvalues of H_τ)

We want to DESCRIBE the map $\tau \in \mathbb{R} \mapsto \lambda(\tau) \in \sigma(H_\tau) \cap (m, +\infty)$
 [eigenvalue curves]

THE BALL



The spectral study on a ball is "explicit" (Bessel functions):

Eigenvalue curves $\tau \mapsto \lambda(\tau)$ are:

* smooth

* increasing

* $\lambda(+\infty) \in \sqrt{\sigma(-\Delta_D) + m^2}$

* $\lambda(-\infty) \in \sqrt{\sigma(-\Delta_D) + m^2} \cup \{m\}$

RESULTS

$\Omega \subset \mathbb{R}^3$ bounded domain with C^2 boundary.

* $\tau \mapsto \lambda(\tau) \in \sigma(H_\tau)$ are real analytic & increasing:

• Perturbation theory (Kato) + Krein-type resolvent formula

$$(H_\tau - \xi)^{-1} = (H_0 - \xi)^{-1} + T(\tau, \xi)$$

(holomorphic in τ)

\Rightarrow parametrization & smoothness.

• Differentiate $H\psi = \lambda(\tau)\psi$ + integrate by parts

+ boundary condition for $\psi \in \text{Dom}(H_\tau) \Rightarrow \frac{d\lambda}{d\tau} > 0$.

* $\lim_{\tau \rightarrow \pm\infty} \lambda(\tau)$ & Dirichlet Laplacian $-\Delta_D$:

• Reproducing formula for $(H - \lambda)\psi = 0$ (like Cauchy formula for $\partial_{\bar{z}}f = 0$) + regularity estimates for (fractional and singular) integral operators on $\partial\Omega$

\Rightarrow uniform estimates for $\psi \Rightarrow$ compactness as $\tau \rightarrow \pm\infty$.

• $\left. \begin{array}{l} H^2 = -\Delta + u^2 \\ H\psi = \lambda\psi \end{array} \right\} \Rightarrow (-\Delta + u^2)\psi = H^2\psi = \lambda^2\psi \Rightarrow -\Delta\psi = (\lambda^2 - u^2)\psi$

• $\frac{d\lambda}{d\tau} > 0 \Rightarrow \exists \lambda(\pm\infty) := \lim_{\tau \rightarrow \pm\infty} \lambda(\tau) \in [u, +\infty]$

$[\psi = i(\sinh\tau - \cosh\tau\beta)(\alpha \cdot \nabla)\psi \text{ on } \partial\Omega, \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}]$

$\lim_{\tau \rightarrow \pm\infty} (\sinh\tau \mp \cosh\tau) = 0 \Rightarrow$ Some components of ψ vanish on $\partial\Omega$

\Rightarrow vanishing Dirichlet condition $\Rightarrow \begin{cases} \lambda(+\infty)^2 - u^2 \in \sigma(-\Delta_D) \cup \{+\infty\} \\ \lambda(-\infty)^2 - u^2 \in \sigma(-\Delta_D) \cup \{0\} \end{cases}$

SHAPE OPTIMIZATION

(indeed open for $H_\tau \forall \tau \in \mathbb{R}$)

Open problem [Faber-Krahn inequality for H_0 : MIT bag model]:

"Among all $\Omega \subset \mathbb{R}^3$ with same volume, the ball has the smallest positive eigenvalue of H_0 ".

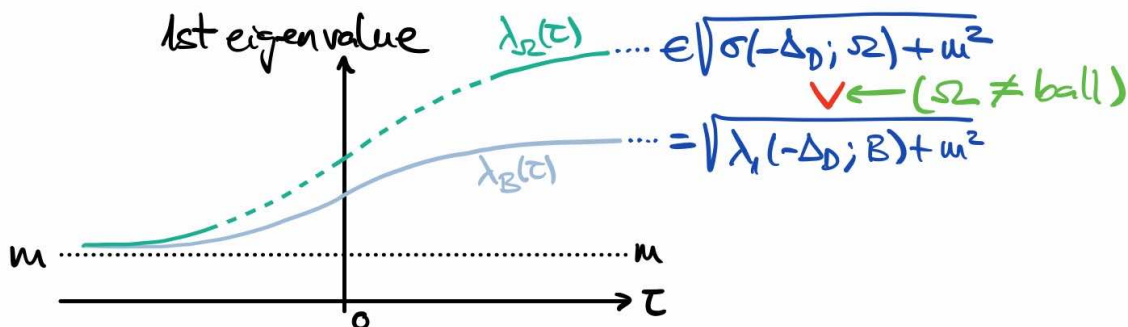
Set $\lambda_\Omega(\tau) :=$ "1st positive eigenvalue of H_τ on Ω ".

• On a ball $B \subset \mathbb{R}^3$ we have $\lambda_B(\tau) \xrightarrow{\tau \rightarrow +\infty} \sqrt{\lambda_1(-\Delta_D; B) + m^2}$
 (Bessel functions) \hookrightarrow (1st eigenvalue of $-\Delta_D$)

• For any $\Omega \subset \mathbb{R}^3$ we know that $\lambda(\tau)^2 - m^2 \in \sigma(-\Delta_D) \cup \{+\infty\}$.

$$\Rightarrow \lambda_\Omega(\tau) \xrightarrow{\tau \rightarrow +\infty} \lambda_\Omega(+\infty) \geq \sqrt{\lambda_1(-\Delta_D; \Omega) + m^2}$$

$$\left[\begin{array}{l} \text{Faber-Krahn inequality} \\ \text{for } -\Delta_D \text{ on } \Omega \text{ and } B \\ \text{with } |\Omega| = |B| \end{array} \right] \Rightarrow \sqrt{\lambda_1(-\Delta_D; \Omega) + m^2} \xrightarrow{\tau \rightarrow +\infty} \lambda_B(\tau)$$



Therefore, if $\Omega \subset \mathbb{R}^3$ is not a ball, and $|B| = |\Omega|$
 $\Rightarrow \lambda_B(\tau) < \lambda_\Omega(\tau)$ for all $\tau \in \mathbb{R}$ big enough.

The case $\tau \rightarrow -\infty$ is more difficult: $\lambda_\Omega(-\infty) = m \forall \Omega \subset \mathbb{R}^3$.

We expand $\lambda_\Omega(\tau) = m + L_\Omega e^\tau + o(e^\tau)$ as $\tau \rightarrow -\infty$
 \hookrightarrow ("slope at $-\infty$ ")

Description of L_Ω using a Rayleigh quotient:

$$\frac{1}{L_\Omega} \leq \sup_{u \in \text{Hardy space on } \partial\Omega} \frac{\int_{\partial\Omega} [\text{Single layer of } -\Delta] u \cdot u}{\int_{\partial\Omega} |u|^2}$$

[like "traces on $\partial\Omega$ of functions holomorphic on Ω "]