On the spectrum coming from “bending” a chain quantum graph

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- To motivate investigation of geometric effects in such a setting, I will present a simple model of describing a “bent chain” graph
- I will find the spectrum of the model and show how it depends on the parameters
- And since it is a birthday conference, I will add also something else . . .

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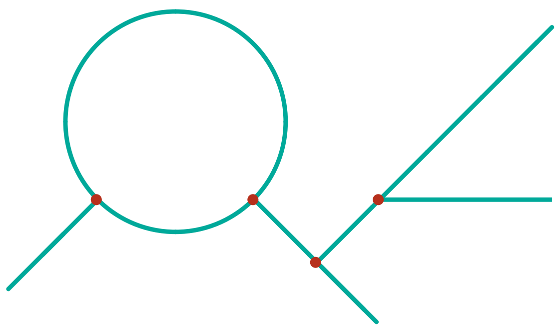
The concept extends, however, to graphs of *arbitrary shape*



Hamiltonian: $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

and what is important, it became *practically important* after experimentalists learned in the last two decades to fabricate tiny graph-like structure for which this is a good model

Remarks

- There are many graph-like systems based on *semiconductor* or *metallic* materials, *carbon nanotubes*, etc. The dynamics can be also simulated by *microwave network* built of optical cables – see [Hul et al.'04]

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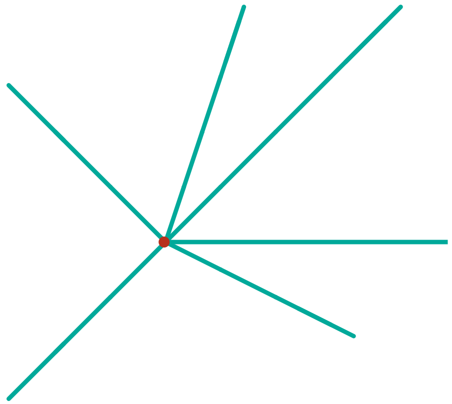
- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], [Bolte-Harrison'03], , and also recent applications to *graphene* and its derivates
- The graph literature is extensive; recall just a review [Kuchment'04], proceedings of Snowbird'05 conference, and the recent AGA Programme at INI Cambridge

Vertex coupling



The most simple example is a *star graph* with the state Hilbert space $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and the particle Hamiltonian acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j''$

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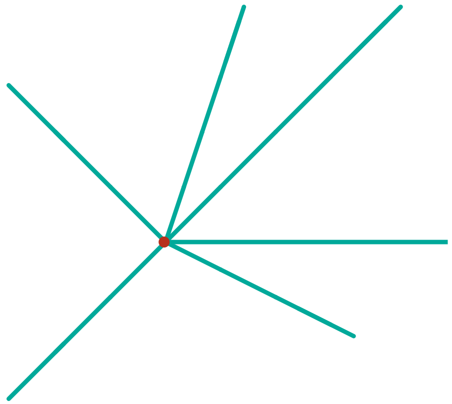

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

$$A\Psi(0) + B\Psi'(0) = 0\,;$$

by [Kostrykin-Schrader'99] the $n \times n$ matrices A, B give rise to a self-adjoint operator if they satisfy the conditions

- $\mathrm{rank}\,(A, B) = n$
- AB^* is self-adjoint

Unique boundary conditions

The non-uniqueness of the above b.c. can be removed:

Proposition [Harmer'00, K-S'00]: Vertex couplings are uniquely characterized by unitary $n \times n$ matrices U such that

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One can derive them modifying the argument used in [Fülöp-Tsutsui'00] for generalized point interactions, $n = 2$

Self-adjointness requires vanishing of the boundary form,

$$\sum_{j=1}^{n} (\bar{\psi}_j \psi'_j - \bar{\psi}'_j \psi_j)(0) = 0\,,$$

which occurs *iff* the norms $\|\Psi(0) \pm i\ell\Psi'(0)\|_{\mathbb{C}^n}$ with a fixed $\ell \neq 0$ coincide, so the vectors must be related by an $n \times n$ unitary matrix; this gives $(U - I)\Psi(0) + i\ell(U + I)\Psi'(0) = 0$

Examples of vertex coupling

- Denote by $\mathcal{J}$ the $n \times n$ matrix whose all entries are equal to one; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the standard δ *coupling*,

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,,\;\; j,k = 1,\dots,n\,,\;\; \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)$$

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- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ_s' coupling*

$$\psi_j'(0) = \psi_k'(0) =: \psi'(0)\,,\; j,k = 1,\dots,n\,,\;\; \sum_{j=1}^{n} \psi_j(0) = \beta\psi'(0)$$

  with $\beta \in \mathbb{R}$; for $\beta = \infty$ we get *Neumann* decoupling, etc.

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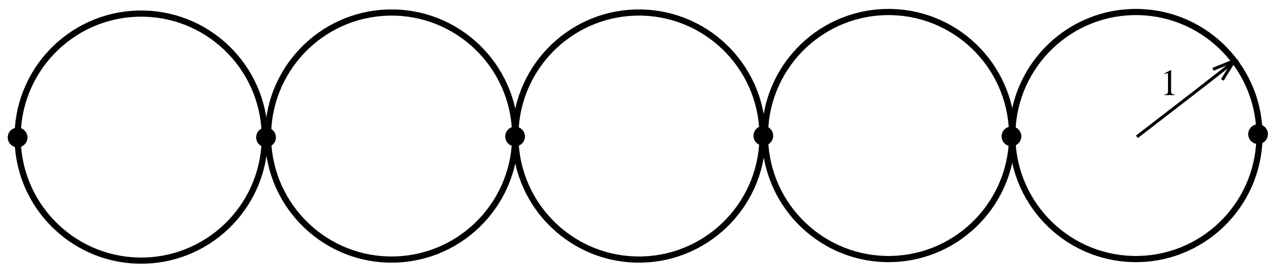
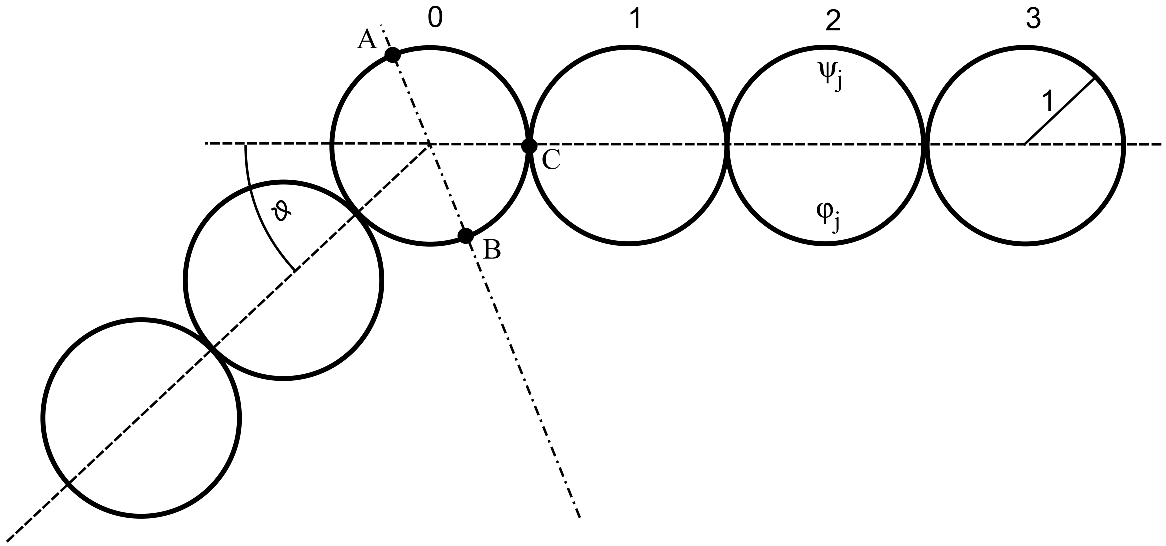
A simple model: analyze the *influence of a "bending" deformation* on a a "chain graph" which exhibits a one-dimensional periodicity



Without loss of generality we assume unit radii; the rings are connected by the δ-*coupling* of a strength $\alpha \neq 0$

Bending the chain

We will suppose that the chain is deformed as follows



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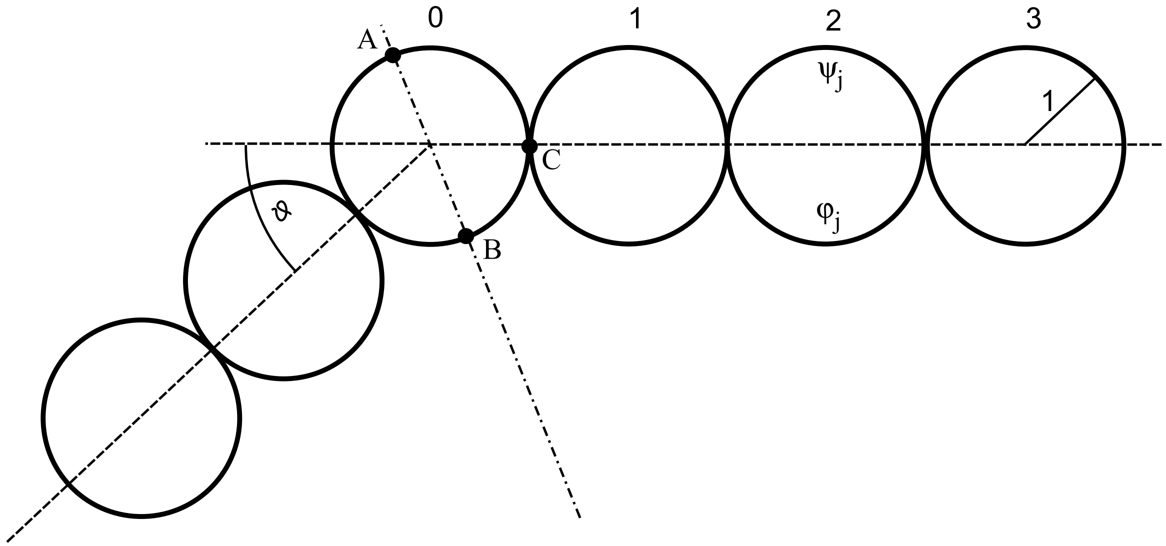
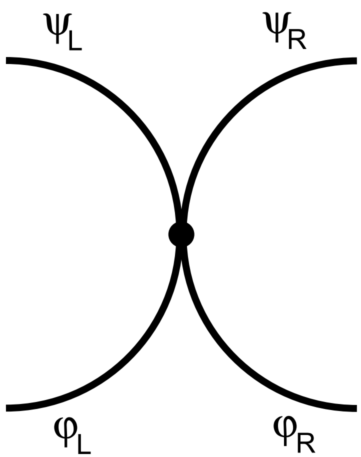


Our aim is to show that

- the band spectrum of the straight Γ is preserved
- there are *bend-induced eigenvalues*, we analyze their behavior with respect to model parameters
- the bent chain exhibits also *resonances*

An infinite periodic chain

The "straight" chain Γ_0 can be treated as a periodic system analyzing the spectrum of the elementary cell



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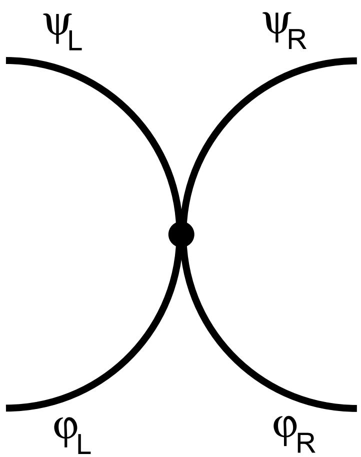

with Floquet-Bloch boundary conditions with the phase $\mathrm{e}^{2\mathrm{i}\theta}$

This yields the condition

$$\mathrm{e}^{2\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\theta}\left(2\cos k\pi + \frac{\alpha}{2k}\sin k\pi\right) + 1 = 0$$

Straight chain spectrum

A straightforward analysis leads to the following conclusion:

Proposition: $\sigma(H_0)$ consists of *infinitely degenerate eigenvalues* equal to n^2 with $n \in \mathbb{N}$, and *absolutely continuous spectral bands* such that

If $\alpha > 0$, then every spectral band is contained in $(n^2, (n+1)^2]$ with $n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, and its upper edge coincides with the value $(n+1)^2$.

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If $\alpha < 0$, then in each interval $[n^2, (n+1)^2)$ with $n \in \mathbb{N}$ there is exactly one band with the lower edge n^2. In addition, there is a band with the lower edge (the overall threshold) $-\kappa^2$, where κ is the largest solution of

$$\left| \cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa} \right| = 1$$

Straight chain spectrum

Proposition, cont'd: The upper edge of this band depends on α. If $-8/\pi < \alpha < 0$, it is k^2 where k solves

$$\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} = -1$$

in $(0, 1)$. On the other hand, for $\alpha < -8/\pi$ the upper edge is negative, $-\kappa^2$ with κ being the smallest solution of the condition, and for $\alpha = -8/\pi$ it equals zero.

Finally, $\sigma(H_0) = [0, +\infty)$ holds if $\alpha = 0$.

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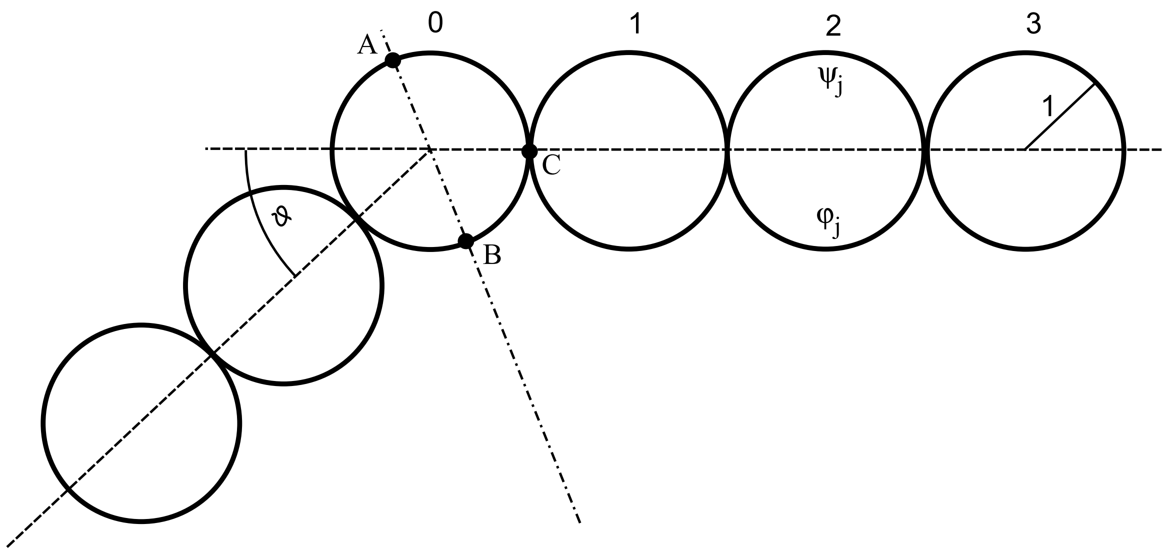
Let us add a couple of *remarks*:

- The bands correspond to *Kronig-Penney model* with the coupling $\frac{1}{2}\alpha$ instead of α, in addition one has here the *infinitely degenerate point spectrum*
- It is also an example of *gaps coming from decoration*

The bent chain spectrum

Now we pass to the bent chain denoted as Γ_ϑ:



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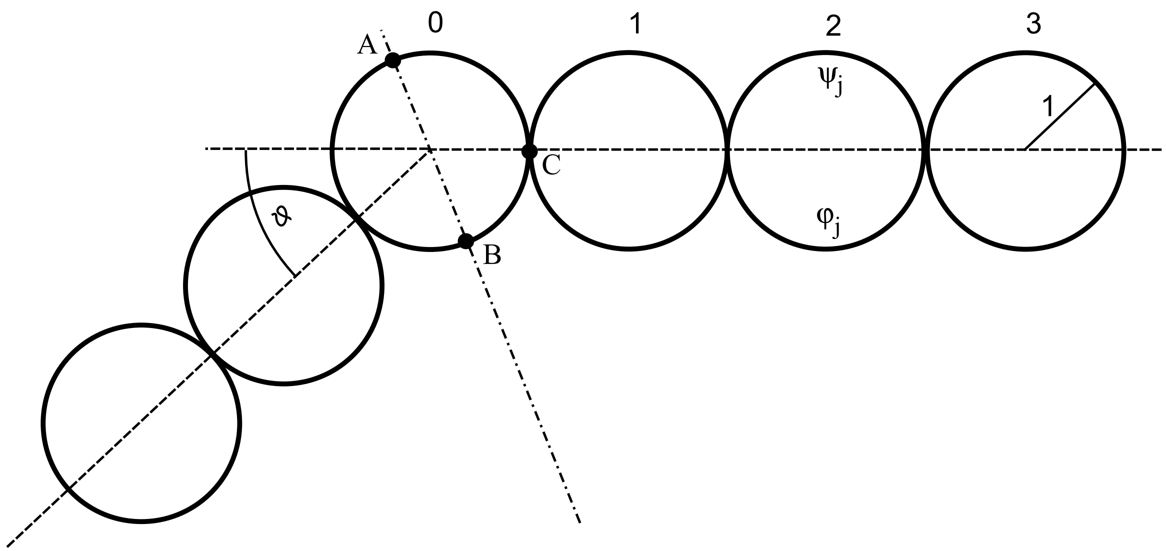

Since Γ_ϑ has mirror symmetry, the operator H_ϑ can be reduced by parity subspaces into a direct sum of an even part, H^+, and odd one, H^-; we drop mostly the subscript ϑ

Equivalently, we analyze the half-chain with *Neumann* and *Dirichlet* conditions at the points A, B, respectively

Eigenfunction components

At the energy k^2 they are are linear combinations of $\mathrm{e}^{\pm \mathrm{i}kx}$,

$$\begin{aligned} \psi_j(x) &= C_j^+ \mathrm{e}^{\mathrm{i}kx} + C_j^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0,\pi]\,, \\ \varphi_j(x) &= D_j^+ \mathrm{e}^{\mathrm{i}kx} + D_j^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0,\pi] \end{aligned}$$

for $j \in \mathbb{N}$. On the other hand, for $j = 0$ we have

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There are δ-couplings in the points of contact, i.e.

$$\psi_j(0) = \varphi_j(0)\,, \quad \psi_j(\pi) = \varphi_j(\pi)\,, \quad \text{and}$$

$$\psi_j(0) = \psi_{j-1}(\pi)\,; \quad \psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0)$$

Transfer matrix

Using the above relations we get for all $j \geq 2$

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = \underbrace{\begin{pmatrix} \left(1 + \frac{\alpha}{4\mathrm{i}k}\right) \mathrm{e}^{\mathrm{i}k\pi} & \frac{\alpha}{4\mathrm{i}k} \mathrm{e}^{-\mathrm{i}k\pi} \\ -\frac{\alpha}{4\mathrm{i}k} \mathrm{e}^{\mathrm{i}k\pi} & \left(1 - \frac{\alpha}{4\mathrm{i}k}\right) \mathrm{e}^{-\mathrm{i}k\pi} \end{pmatrix}}_{M} \cdot \begin{pmatrix} C_{j-1}^+ \\ C_{j-1}^- \end{pmatrix},$$

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To have eigenvalues, one eigenvalue of M has to be *less than one* (they satisfy $\lambda_1\lambda_2 = 1$); this happens *iff*

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Remark: By general arguments, σ_{ess} is preserved, and there are at most two eigenvalues in each gap

Spectrum of H^+

Combining the above with the Neumann condition at the mirror axis we get the spectral condition in this case,

$$\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}$$

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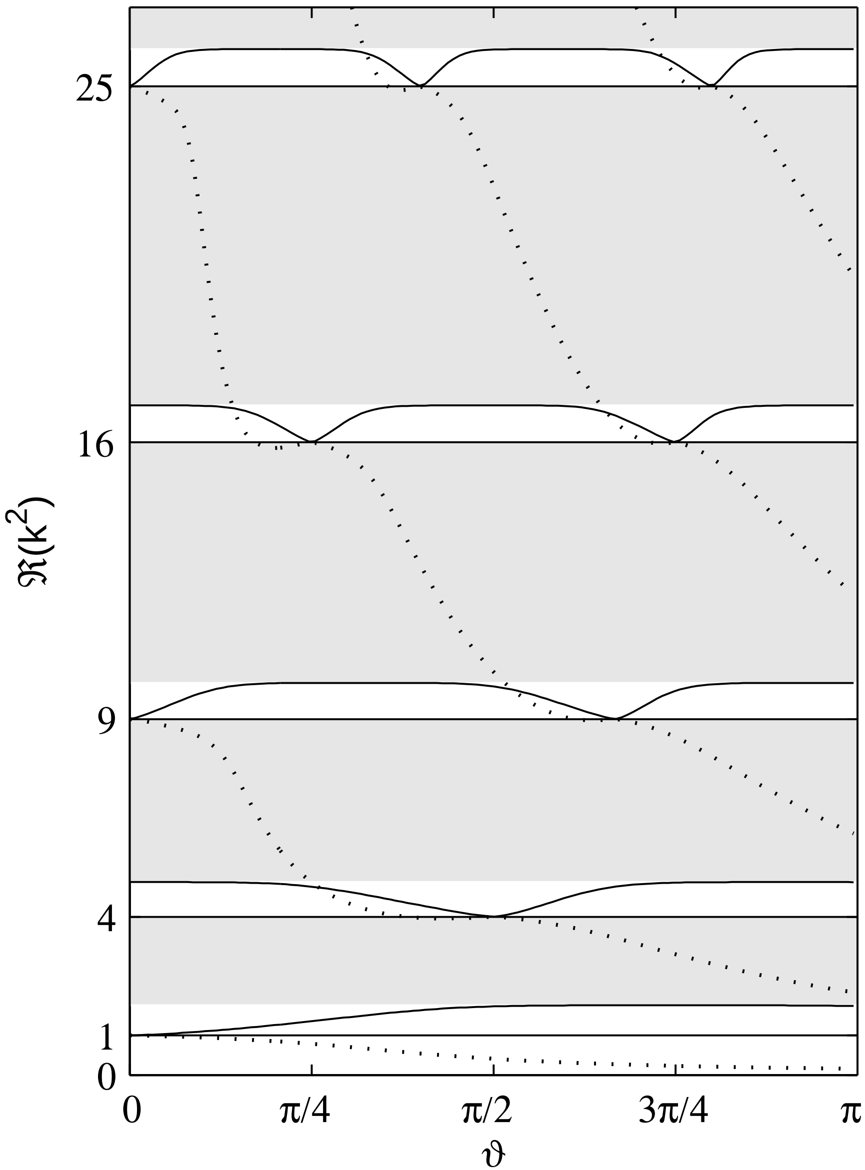
After a tiresome but straightforward analysis one arrives then at the following conclusion:

Proposition: If $\alpha \geq 0$, then H^+ has no negative eigenvalues. On the other hand, for $\alpha < 0$ the operator H^+ has at least one negative eigenvalue which lies under the lowest spectral band and above the number $-\kappa_0^2$, where κ_0 is the (unique) solution of $\kappa \cdot \tanh \kappa\pi = -\alpha/2$

Spectrum of H^+ for $\alpha = 3$



Spectrum of H^-

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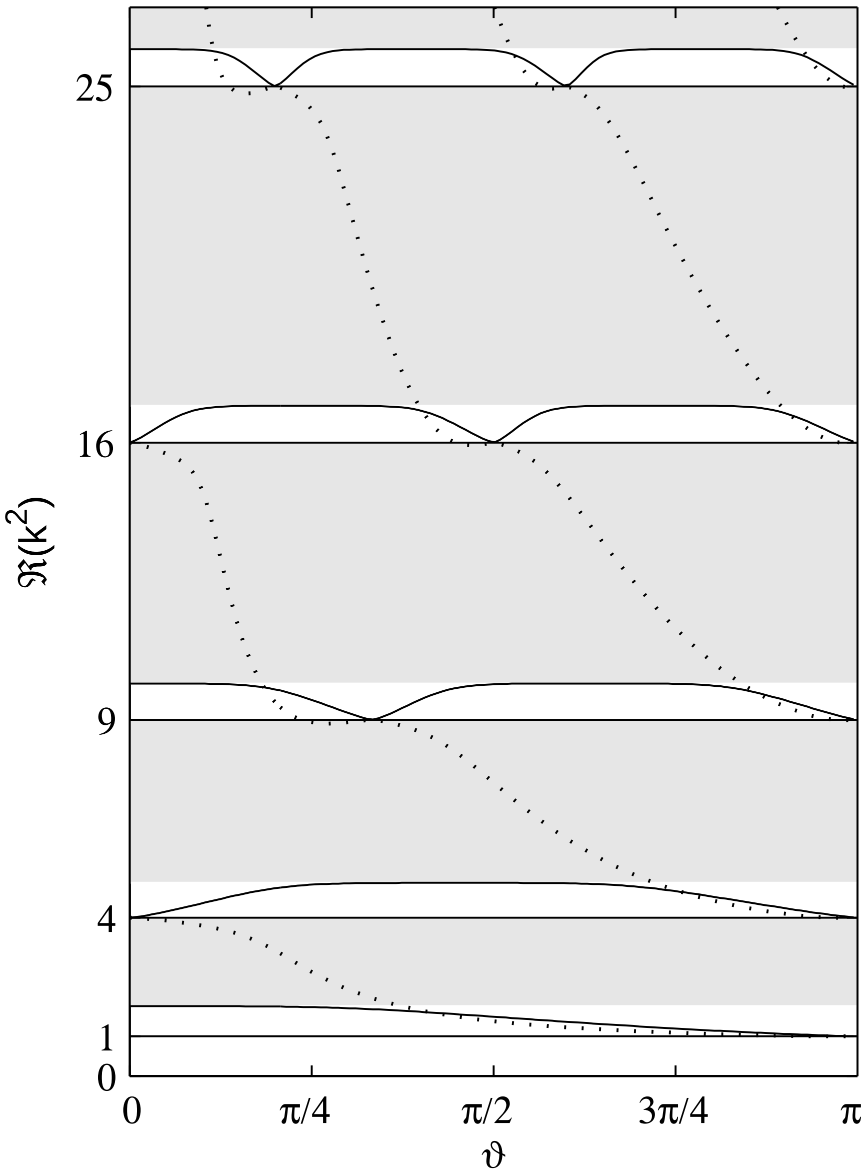
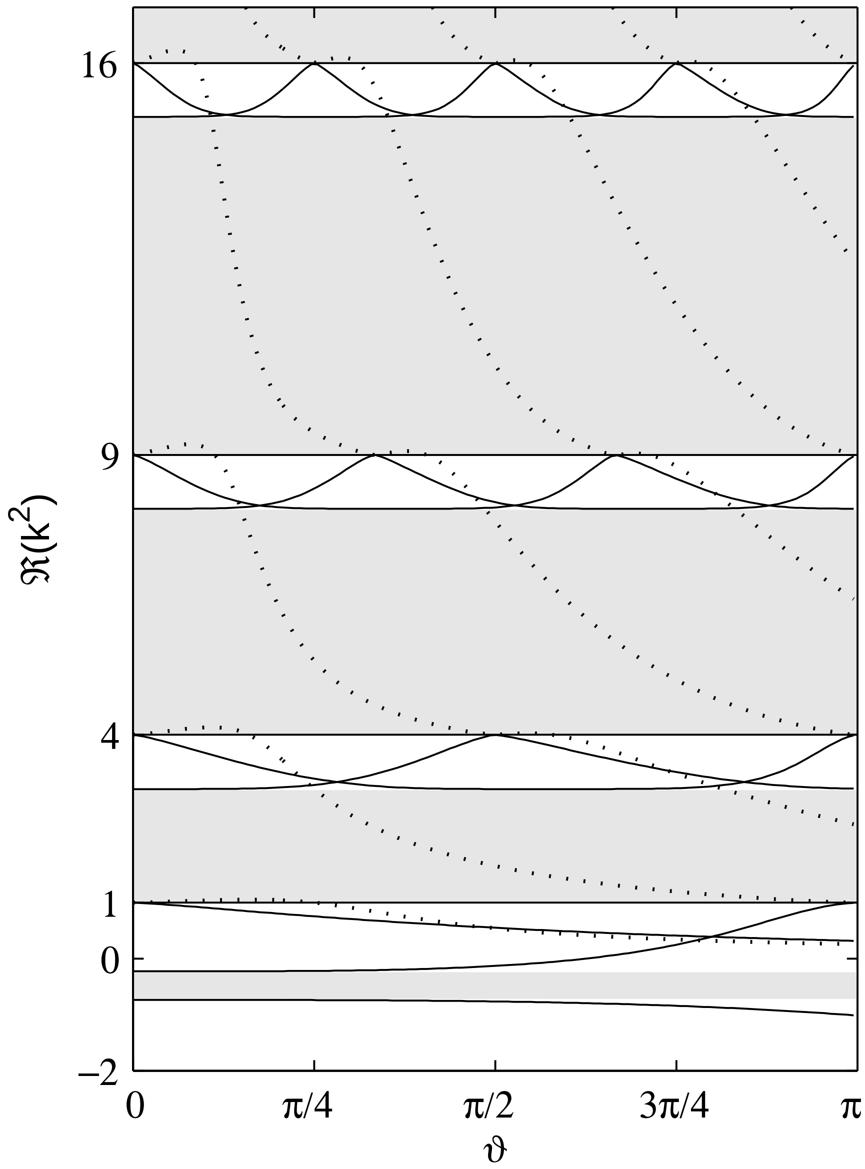
Summarizing, for each of the operators $H^\pm$ there is at least one eigenvalue in every spectral gap closure. It can lapse into a band edge n^2, $n \in \mathbb{N}$, and thus be in fact absent. The ev's of H^+ and H^- may coincide, becoming a single ev of multiplicity two; this happens only if

$$k \cdot \tan k\pi = \frac{\alpha}{2}$$

Spectrum of H^- for $\alpha = 3$



$\sigma(H)$ for attractive coupling, $\alpha = -3$



Resonances, analyticity

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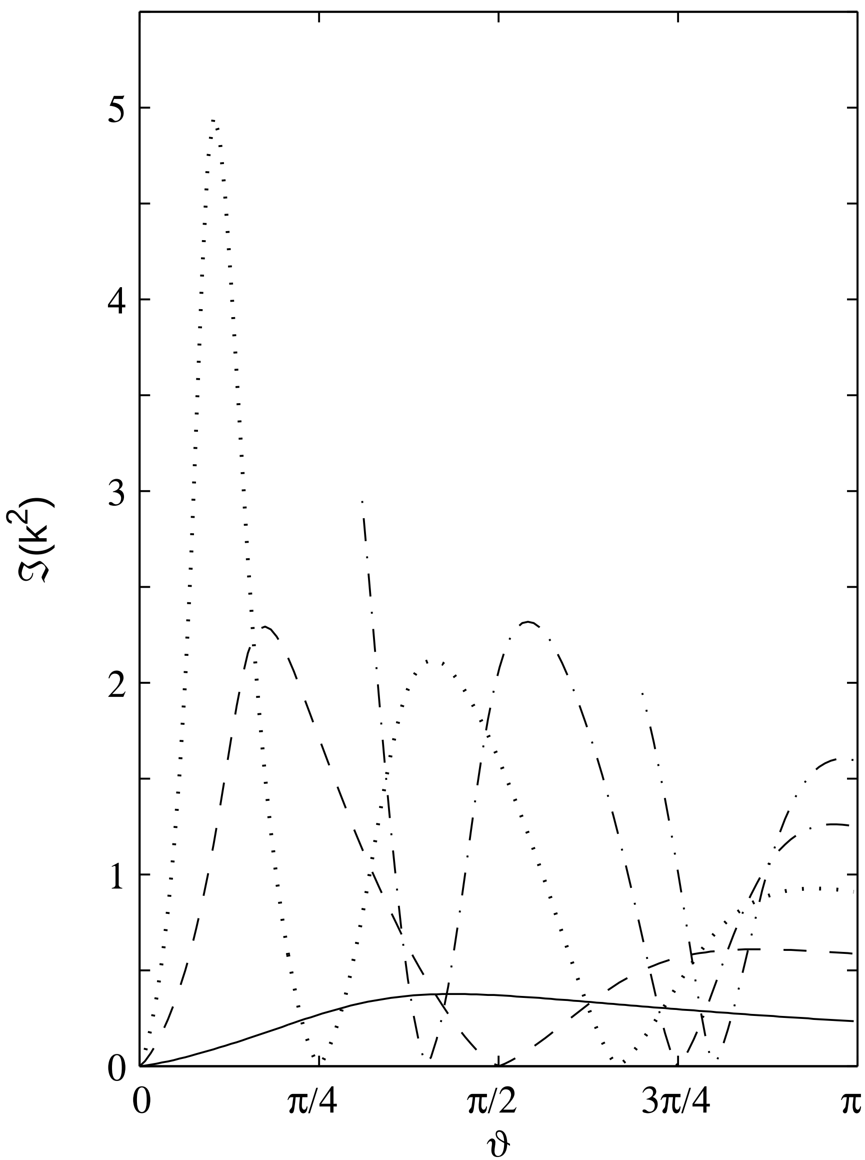
A further analysis of the spectral condition gives

Proposition: The eigenvalue and resonance curves for H^+ are *analytic* everywhere except at $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}_0$, $\ell \leq \left[\frac{n+1}{2}\right]$. Moreover, the real solution in the n-th spectral gap is given by a function $\vartheta \mapsto k$ which is *real-analytic*, except at the points $\frac{n+1-2\ell}{n}\pi$. Similar claims can be made for the odd part for H^-.

Imaginary parts of H^+ resonances, $\alpha = 3$



More on the angle dependence

For simplicity we take H^+ only, the results for H^- are analogous. Ask about the behavior of the curves at the points whe they touch bands and where eigenvalues and resonances may cross

If $\vartheta_0 := \frac{n+1-2\ell}{n}\pi > 0$ is such a point we find easily that in is vicinity we have

$$k \approx k_0 + \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\,|\vartheta - \vartheta_0|^{4/3}$$

so he curve is indeed non-analytic there. The same is true for $\vartheta_0 = 0$ provided the band-edge value k_0 is odd

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However, H^+ has an eigenvalue near $\vartheta_0 = 0$ also in the gaps adjacent to even numbers, when the curve starts at $(0, k_0)$ for k_0 solving $|\cos k\pi + \frac{\alpha}{4k}\sin k\pi| = 1$ in $(n, n+1)$, n even

Even threshold behavior

Proposition: Suppose that $n \in \mathbb{N}$ is even and k_0 is as described above, i.e. k_0^2 is the right endpoint of the spectral gap adjacent to n^2. Then the behavior of the solution in the vicinity of $(0, k_0)$ is given by

$$k = k_0 - C_{k_0,\alpha} \cdot \vartheta^4 + \mathcal{O}(\vartheta^5)\,,$$

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Remark: Notice that the fourth-power is the same as for the ground state of a *slightly bent Dirichlet tube* despite the fact that the dynamics is completely different in the two cases

The above results were taken from

[DET08] P. Duclos, P.E., O. Turek: On the spectrum of a bent chain graph, *J. Phys. A: Math. Theor.* **A41** (2008), 415206

see also, e.g.

[EKKTS08] P.E., J.P. Keating, P. Kuchment, T. Sunada, A. Teplyaev, eds.: Analysis on Graphs and Applications, *Proceedings of a Isaac Newton Institute programme*, January 8–June 29, 2007; 670 p.; AMS "Proceedings of Symposia in Pure Mathematics" Series, vol. 77, Providence, R.I., 2008

[EP07] P.E., O. Post: Quantum networks modelled by graphs, *Proceedings of the Joint Physics/Mathematics Workshop on "Few-Body Quantum System" (Aarhus 2007)*; AIP Conf. Proc., vol. 998; Melville, NY, 2008, pp. 1-17 `arXiv: 0706.0481v1`

[ET07] P.E., O. Turek: Approximations of singular vertex couplings in quantum graphs, *Rev. Math. Phys.* **19** (2007), 571-606

However, a birthday party needs a gift!

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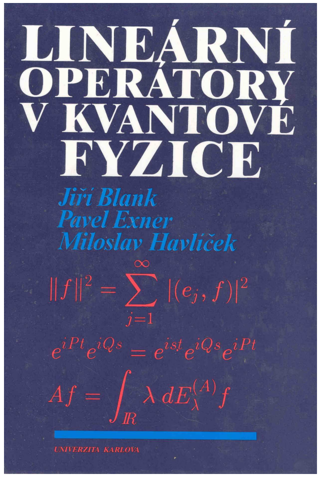

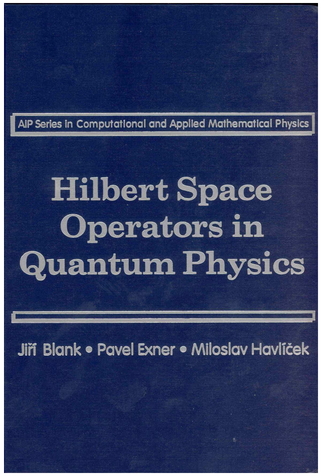

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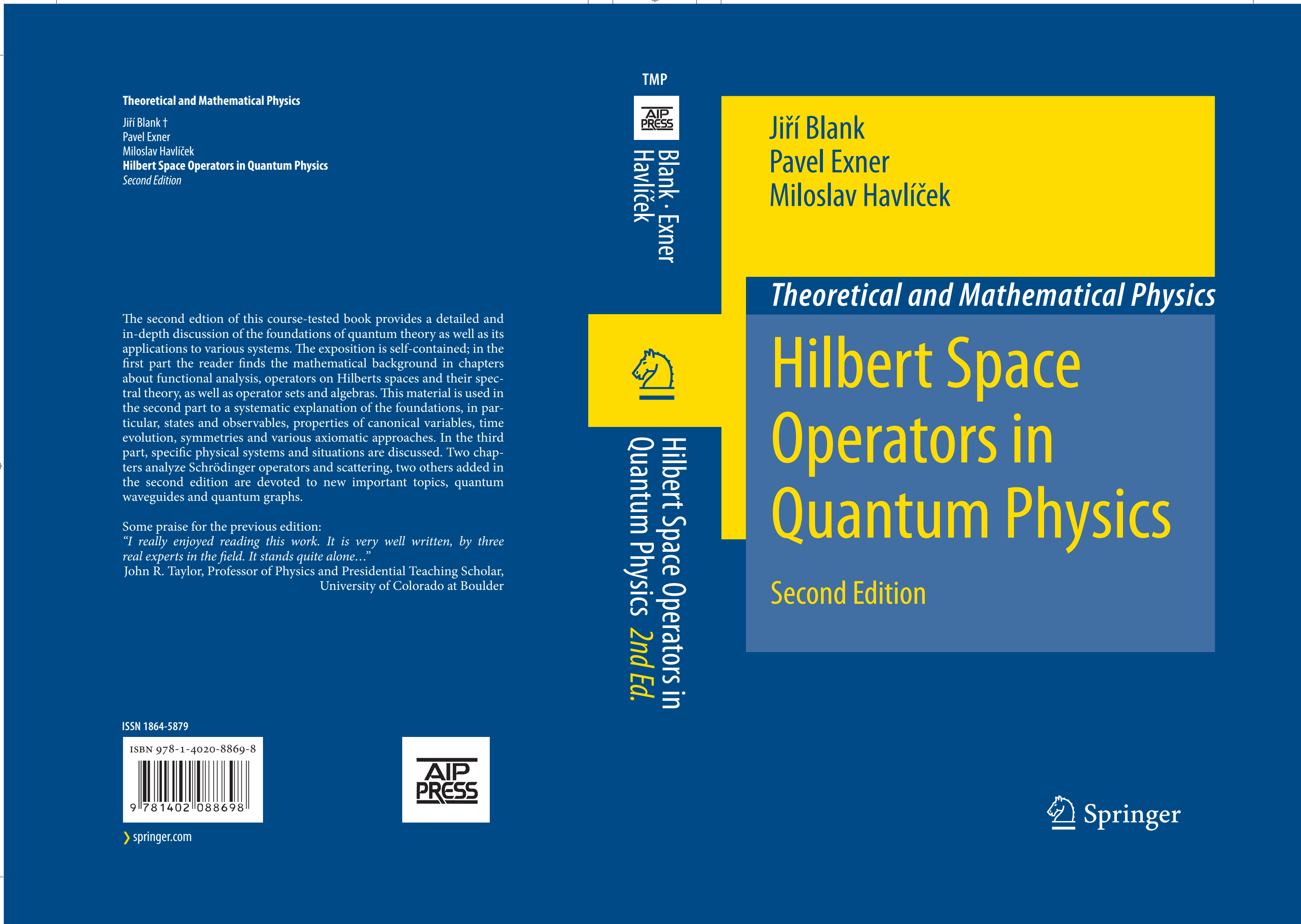

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Theoretical and Mathematical Physics

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