Reduction of quantum graphs to tight-binding Hamiltonians

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More general boundary conditions, more general edges

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von Below' 84: free Laplacian on finite graph, Kirchhoff b.c., essentially $\operatorname{spec} H = \{z : \cos\sqrt{z} \in \operatorname{spec} \Delta\}$.

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Pankrashkin' 06: $(i\partial + a_e)^2 + V$ on the edges, magnetic Kirchhoff boundary conditions: $\operatorname{spec} H = \{z : \eta(z) \in \operatorname{spec}\Delta_m\}$, η is the Hill discriminant for V, Δ_m is a discrete magnetic Laplacian (rigorous version later)

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Fourth order operators (networks of beams, elasticity theory), Nicaise, Dekoninck'00 et al.

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Enumeration of edges near each vertex v: the edges 1 to $\operatorname{outdeg} v$ are outgoing w.r.t. v, the edges $\operatorname{outdeg} + 1$ to $\deg v$ are ingoing. Notation: $e_j v$ is the edge with index j near v. Clear, $\iota e_j v = v$ for $j \le \operatorname{outdeg} v$ and $\tau e_j v = v$ for $j > \operatorname{outdeg} v$.

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For each edge e: $n_\iota(e)$ and $n_\tau(e)$ are the indices of e near ιe and τe, respectively. Clear, $n_\iota(e_j v) = j$ for $j \leq \operatorname{outdeg} v$ and $n_\tau(e_j v) = j$ for $j > \operatorname{outdeg} v$.

Metrization of edge

Let S_0 be a closed densely defined symmetric operator in $\mathscr{H}$ with deficiency indices $(2,2)$. Then for $S := S_0^*$ one can find two maps $\Gamma = (\Gamma_0, \Gamma_1), \Gamma' = (\Gamma_0', \Gamma_1') : \operatorname{dom} S \to \mathbb{C}^2$ such that

- $\langle f, Sg\rangle - \langle Sf, g\rangle = \langle \Gamma f, \Gamma' g\rangle - \langle \Gamma' f, \Gamma g\rangle$ for all f, g,
- $(\Gamma, \Gamma') : \operatorname{dom} S \to \mathbb{C}^2 \oplus \mathbb{C}^2$ is surjective: i.e. $(\mathbb{C}^2, \Gamma, \Gamma')$ is a boundary triple for S.

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Denote $H_0 := S|_{\ker \Gamma}$, self-adjoint. For z outside of $\operatorname{spec} H_0$ and any $\varphi \in \mathbb{C}^2$ one can find a unique f solving $(S - z) f = 0$ and $\Gamma f = \xi$. Consider the matrix m defined by $\Gamma' f = m(z) \Gamma f$.

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Typical example: $S = -\partial^2 + V$, $V \in L^2[0,1]$, in $L^2[0,1]$ with $\operatorname{dom} S = H^2[0,1]$. One can take $\Gamma f = \big(f(0), f(1)\big)$, $\Gamma' f = \big(f'(0), -f'(1)\big)$,

$$m(z) = \frac{1}{s(1;z)} \begin{pmatrix} c(1;z) & -1 \\ -1 & s'(1;z) \end{pmatrix},$$

where s, c solve $-y'' + Vy = zy$ with $s(0;z) = c'(0;z) = 1 - s'(0;z) = 1 - c(0;z) = 0$.

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Self-adjointness: $f_e \in \operatorname{dom} S$ + boundary conditions. The most general local boundary conditions: $\big(1 - U(v)\big) f(v) = i\big(1 + U(v)\big) f'(v)$ for all v. Here $U(v)$ is a unitary matrix of size $\deg v$,

$$f(v) := \big(\Gamma_0 f_{e_1 v}, \dots, \Gamma_0 f_{e_{\operatorname{outdeg} v} v}, \Gamma_1 f_{e_{\operatorname{outdeg} v+1} v}, \dots, \Gamma_1 f_{e_{\deg v} v}\big),$$

$$f'(v) := \big(\Gamma_0' f_{e_1 v}, \dots, \Gamma_0' f_{e_{\operatorname{outdeg} v} v}, \Gamma_1' f_{e_{\operatorname{outdeg} v+1} v}, \dots, \Gamma_1' f_{e_{\deg v} v}\big),$$

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Denote $N(v) := \deg v - \dim\ker\big(1 + U(v)\big)$.
Orthonormal basis of eigenvectors $\xi_j(v)$, $j = 1, \dots, N(v)$, in $\ker(1 + U(v))^{\perp}$.
Discrete space $\mathscr{L}$, "reduced l^2 space", $\big(\varphi(v)\big)$, $\varphi \in \mathbb{C}^{N(v)}$, $\sum \|\varphi(v)\|^2 < \infty$

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If $\bigcup_{v \in V} \operatorname{spec} U(v) \setminus \{-1\} = \{e^{i\Phi}\}$, then outside the spectrum of H_0 one has $\operatorname{spec}_\bullet H = \eta^{-1}(\operatorname{spec}_\bullet P)$, where $\bullet \in \{\mathrm{p}, \mathrm{pp}, \mathrm{disc}, \mathrm{ess}, \mathrm{ac}, \mathrm{sc}\}$, $\eta(z) := \dfrac{m_{11}(z) + \alpha}{m_{12}(z)}$, $\alpha := \dfrac{1 - e^{i\Phi}}{i(1 + e^{i\Phi})}$, and P is an operator acting on $\mathscr{L}$ as

$$\left(P\varphi\right)_j(v) = \sum_{k=1}^{\operatorname{outdeg} v} \sum_{s=1}^{N(\tau e_k v)} \xi_{jk}(v) \xi_{s n_\tau(e_k v)}(\tau e_k v) \varphi_s(\tau e_k v) + \sum_{k=\operatorname{outdeg} v+1}^{\deg v} \sum_{s=1}^{N(\iota e_k v)} \xi_{jk}(v) \xi_{s n_\tau(e_k v)}(\iota e_k v) \varphi_s(\iota e_k v).$$

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Note that η is the Hill discriminant for $L := -\partial^2 + V + \alpha \sum_{n\in\mathbb{Z}} \delta(\cdot - n)$ and that $\|P\| \le 1$. This provides (up to the Dirichlet levels) the inclusion $\operatorname{spec} H \subset \operatorname{spec} L$.

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L has infinitely many gaps $\Rightarrow$ the same for H (independent of the underlying graph!)

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$$U(v) = -E_{\deg v} + \frac{2}{\deg v + \alpha(v)} J_{\deg v}$$

($J_{\deg v}$ is the matrix whose all entries are 1. For $\alpha(v) = \alpha \deg v$ reduces to the transition operator $Pf(v) = D\Delta D$ in $l^2(V)$. Here D is the multiplication by $1/\sqrt{\deg v}$ and $\Delta f(v) = \sum_{w \sim v} f(w)$.

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Magnetic case: $(i\delta + a_e)^2 + V$ on each edge, f is continuous at each vertex, $\sum_{\iota e=v}(\partial - ia_e) f_e'(0) - \sum_{\tau e=v}(\partial - ia_e) f_e'(1) = \alpha(v) f(v)$, $\alpha(v)$ real. By the transformation $f_e(t) = \exp(\int_0^t a_e(s)ds) g_e(t)$ reduction to the considered situation. Again, for $\alpha(v) = \alpha \deg v$ reduction to a discrete operator (magnetic Laplacian) $Pf(v) = D\Delta D$ in $l^2(V)$ with $\Delta f(v) = \sum_{\iota e=v} e^{-i\beta(e)} f(\tau e) + \sum_{\tau e=v} e^{i\beta(e)} f(\iota e)$, $\beta(e) := \int_0^1 a_e(s)ds$, on $l^2(V)$.

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δ_p-type boundary conditions (Exner): $\sum_{e\sim v} f_e(0) = 0$,
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For $\alpha(v) = \alpha \deg v$ reduction to a discrete operator. Each vertex v has “degree of freedom” $\deg v - 1$.

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δ' and δ_s'-type boundary conditions can be considered. One has to change the boundary triple for S: $\Gamma f = \big(-f'(0), f'(1)\big)$, $\Gamma' f = \big(f(0), f(1)\big)$. The function η becomes $c(1;z) + \alpha c'(1;z)$, i.e. the Hill discriminant for $-\partial^2 + V + \alpha \sum_{n\in\mathbb{Z}} \delta'(\cdot - n)$. The same estimates for the gaps as above, and the Dirichlet spectrum is replaced by the Neumann spectrum.

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Further generalizations (for non-even V): bipartite graphs, uniformly directed graphs etc.

Hybrid spaces

Still $S_0 = -\Delta$ on a 2D sphere M with the domain $\{f \in \operatorname{dom}\Delta : f(a_0) = f(a_1) = 0\}$ ($a_0, a_1 \in M$ are fixed). Take $S := S_0^*$.

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For any $f \in \operatorname{dom} S$ one can define $\Gamma_j f = -\lim_{x\to a_j} \dfrac{2\pi}{\log d(x,a_j)} f(x)$ and $\Gamma'_j f = \lim_{x\to a_j} \Big(f(x) + \dfrac{\Gamma_j f}{2\pi} \log d(x,a_j)\Big)$. It is known that $(\mathbb{C}^2, \Gamma, \Gamma')$ is a boundary triple for S. The corresponding matrix m is

$$m(z) = \begin{pmatrix} G^r(a_0,a_0;z) & G(a_0,a_1;z) \\ G(a_1,a_0;z) & G^r(a_1,a_1;z) \end{pmatrix},$$

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Replace each edge by a copy of S. This results is a hybrid space (coupled spheres).

The study is as above, the function $\eta(z) := \dfrac{m_{11}(z) + \alpha}{m_{12}(z)}$ has poles, but the same discrete Hamiltonian!