Many-particle systems on quantum graphs with singular interactions

Analysis on Graphs and its Applications Follow-up Meeting

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Jens Bolte
Department of Mathematics
Royal Holloway, University of London
jens.bolte@rhul.ac.uk

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Introduction

Quantum Graphs (QG) are one dimensional models for the motion of a (single) particle along the edges of a graph (network of wires). QGs are, e.g., used as models for:

- Molecules
- Networks of waveguides
- Mesoscopic quantum systems
- Manifolds in spectral geometry
- Quantum chaos (QC)

Goal: Extend existing QG models to many-particle systems, study QC with many-particle interactions.

Previous work: non-interacting QFT-models on graphs (Bellanzini, Mintchev 2006; Schrader 2009)

What is a quantum graph?

- A finite, connected graph $\Gamma = (\mathcal{V}, \mathcal{E})$ with vertices $\mathcal{V} = \{v_1, \dots, v_V\}$, edges $\mathcal{E} = \{e_1, \dots, e_E\}$ and lengths $l_{e_1}, \dots, l_{e_E}$ assigned to edges.
- Functions F on Γ as collections of functions on the edges,

$$F = (f_1, \dots, f_E)^T \ , \quad \text{with} \quad f_e : (0, l_e) \to \mathbb{C} \ ,$$

  i.e., spaces of functions: $L^2(\Gamma)$, $C^\infty(\Gamma)$, $H^2(\Gamma)$, etc. as direct sums.
- A differential Laplacian acting on such functions,

$$-\Delta F = (-f_1'', \dots, -f_E'') \ , \quad F \in C^\infty(\Gamma) = \bigoplus_{e=1}^{E} C^\infty(0, l_e) \ .$$

One-particle quantum graphs

A quantum model requires self-adjoint operators on a Hilbert space $\mathcal{H}$. For a single, 'free' particle on a metric graph, the Laplacian can be realised as a self-adjoint operator:

Self-adjoint extensions of the symmetric operator

$$-\Delta \quad \text{on} \quad H_0^2(\Gamma) \subset \mathcal{H} = L^2(\Gamma) \ .$$

Domains of such extensions in terms of boundary conditions imposed on

$$F_{bv} = \big(f_1(0), \ldots, f_E(0), f_1(l_1), \ldots, f_E(l_E)\big)^T$$

$$F'_{bv} = \big(f'_1(0), \ldots, f'_E(0), -f'_1(l_1), \ldots, -f'_E(l_E)\big)^T \ ,$$

i.e.,

$$\mathcal{D}_{A,B} = \{F \in H^2(\Gamma);\ AF_{bv} + BF'_{bv} = 0\} \ ,$$

Theorem (Kostrykin, Schrader 1999)
$\mathcal{D}_{A,B}$ is a domain of a self-adjoint extension of the Laplacian, iff $A, B \in M_{2E}(\mathbb{C})$ satisfy

(i) $\mathrm{rank}(A, B) = 2E$,
(ii) AB^* self-adjoint.

Equivalent characterisation in terms of quadratic forms: projector P onto $\ker B$, $Q = I - P$ and self-adjoint map $L = (B|_{\mathrm{ran}\, B^*})^{-1} AQ$.

Theorem (Kuchment 2004)
The quadratic form associated with $-\Delta_1$ on $\mathcal{D}_{A,B}$ is

$$Q_{A,B}[F] = \sum_{e=1}^{E} \int_0^{l_e} |f_e'(x)|^2 \, dx - \big(F_{bv}, LF_{bv}\big)_{\mathbb{C}^{2E}} \ ,$$

with domain
$$\mathcal{D}_Q = \{F \in H^1(\Gamma);\ PF_{bv} = 0\} \ .$$

Some important and well known spectral properties:

- Discrete spectrum $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \to \infty$, (at most) finitely many negative eigenvalues
- Weyl's law

$$N(\lambda) = \#\{n;\ \lambda_n \leq \lambda\} \sim \frac{\mathcal{L}}{\pi}\sqrt{\lambda}\,, \quad \lambda \to \infty$$

- Eigenvalue correlations follow RMT predictions (Kottos, Smilansky 1997/99): quantum graphs as models in quantum chaos
- Trace formulae (Roth 1983; Kottos, Smilansky 1997/99; ...)
- Periodic orbit correlations leading to eigenvalues correlations (Berkolaiko, Keating 1999; Berkolaiko, Schanz, Whitey 2003; Altland, Gnutzmann 2004; ...)
- Inverse problems: 'Can you hear the shape of a graph' (Gutkin, Smilansky 2001)

Many-particle systems: Fock space

Fock space over the one-particle Hilbert space $\mathcal{H}_1 = L^2(\Gamma)$,

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} L^2(\Gamma)^{\otimes n} \ .$$

Fock-space vectors $\Psi = (\Psi_0, \Psi_1, \Psi_2, \dots)$ have n-particle components $\Psi_n = (\psi_{e_1,\dots,e_n}) \in L^2(\Gamma)^{\otimes n}$ that themselves have components

$$\psi_{e_1,\dots,e_n} \in L^2(0, l_{e_1}) \otimes \cdots \otimes L^2(0, l_{e_n}) \ ,$$

i.e., these are functions of n variables on n (not necessarily distinct) edges.

Identical particles (bosons): symmetric Fock space $\mathcal{F}_s \subset \mathcal{F}$ consisting of vectors $\Psi = (\Psi_0, \Psi_1, \Psi_2, \dots)$ where each Ψ_n is invariant under particle exchange.

Projector $\Pi_s : \mathcal{F} \to \mathcal{F}_s$,

$$(\Pi_s \Psi)_{e_1,\dots,e_n} = \frac{1}{n!} \sum_{\pi \in S_n} \psi_{e_{\pi(1)},\dots,e_{\pi(n)}} \ .$$

Creation and annihilation operators $a^*(\phi)$, $a(\phi)$ add or remove a one-particle state $\phi \in L^2(\Gamma)$ to/from a bosonic Fock state,

$$\big(a^*(\phi)\Psi\big)_{e_1,\dots,e_{n+1}} = \sqrt{n+1}\,\Pi_s\big[\psi_{e_1,\dots,e_n} \otimes \phi_{e_{n+1}}\big]$$

$$\big(a(\phi)\Psi\big)_{e_1,\dots,e_{n-1}} = \sqrt{n}\sum_{e=1}^{E}\int_0^{l_e} \overline{\phi_e(x_e)}\,\psi_{e_1,\dots,e_{n-1},e}(x_{e_1},\dots,x_{e_{n-1}},x_e)\ dx_e \ ,$$

and satisfy the canonical commutation relations (CCR),

$$\big[a(\phi), a^*(\psi)\big] = \langle \phi, \psi \rangle_{L^2(\Gamma)} \ .$$

This construction is generic and does not reflect specific properties of the graph.

Non-interacting (i.e., free) time-evolution generated by 2nd-quantised one-particle Laplacian,

$$\big(d\Gamma(-\Delta_1)\Psi\big)_{e_1,\dots,e_n} = -\sum_{j=1}^{n} \frac{\partial^2 \psi_{e_1,\dots,e_n}}{\partial x_{e_j}^2} \ .$$

This is defined on a suitable domain inherited from $\mathcal{D}(A,B)$, or in terms of the associated quadratic form $Q_{A,B}$, suitably lifted to Fock space; formally,

$$d\Gamma(-\Delta_1) = \int_\Gamma \nabla a^*(x) \cdot \nabla a(x)\ dx \ .$$

Then $a_t(\phi) = a\big(e^{it\Delta_1}\phi\big)$ is a solution of the Schrödinger equation

$$i\frac{\partial}{\partial t} a_t(\phi) = \big[a_t(\phi), d\Gamma(-\Delta_1)\big] \ , \qquad \text{with} \qquad a_{t=0}(\phi) = a(\phi) \ .$$

Two-particle interactions

One-particle (self-adjoint) operators A_1 can be lifted to the two-particle Hilbert space,

$$A_2 = A_1 \otimes I + I \otimes A_1 \ .$$

Operators of this type describe no interactions between the particles.

For a quantum graph, the two-particle Hilbert space is

$$\mathcal{H}_2 = \left(\bigoplus_{e=1}^{E} L^2(0, l_e) \right) \otimes \left(\bigoplus_{e=1}^{E} L^2(0, l_e) \right) \ ,$$

i.e., the vectors are functions with components

$$\Psi = \big(\psi_{ee'}\big) \ , \quad \psi_{ee'} \in L^2(0, l_e) \otimes L^2(0, l_{e'}) \ .$$

Formally, a two-particle Laplacian is given by

$$(-\Delta_2\Psi)_{ee'}(x_e, y_{e'}) = -\frac{\partial^2\psi_{ee'}}{\partial x_e^2}(x_e, y_{e'}) - \frac{\partial^2\psi_{ee'}}{\partial y_{e'}^2}(x_e, y_{e'}) \ ,$$

and appears to represent no particle interactions.

BUT: Unbounded operators need a domain specified.

Any two-particle Laplacian on a graph is a self-adjoint extension of the symmetric operator $-\Delta_{2,0}$ with domain

$$\left(\bigoplus_{e=1}^{E} H_0^2([0,l_e])\right) \otimes \left(\bigoplus_{e=1}^{E} H_0^2([0,l_e])\right) \ .$$

Some of the self-adjoint realisations are lifts of one-particle Laplacians and hence contain no two-particle interactions. *All other extensions represent interactions*; these are singular and localised in the vertices.

Interactions localised at vertices

Simple case: interval as graph with one edge ($E = 1$); $D = [0, l] \times [0, l]$

Theorem (JB, Kerner 2010)
The domains $\mathcal{D} \subset H^2(D)$ of self-adjoint, bosonic realisations of the two-particle Laplacian $-\Delta_2$ on an interval of length l can be characterised in terms of the boundary conditions

$$A(y) \begin{pmatrix} \psi(0, y) \\ \psi(l, y) \end{pmatrix} + B(y) \begin{pmatrix} \psi_x(0, y) \\ -\psi_x(l, y) \end{pmatrix} = 0$$

for a.e. $y \in (0, l)$. Here, for a.e. $y \in (0, l)$ the 2×2 matrices $A(y)$ and $B(y)$ satisfy

(i) $\text{rank}\big(A(y), B(y)\big) = 2$,
(ii) $A(y)B^*(y)$ self-adjoint.

The operator is a lift from a one-particle operator to the two-particle Hilbert space, iff A and B are independent of y.

Sketch of proof:
$-\Delta^*_{2,0}$ has domain $H^2(D)$, hence identify subspaces of $H^2(D)$ on which

$$\langle \phi, \Delta^*_{2,0}\psi \rangle - \langle \Delta^*_{2,0}\phi, \psi \rangle = 0 \ .$$

The difference can be determined through an integration by parts. Using bosonic symmetry this yields an integral over ∂D,

$$2\int_0^l \left[\bar{\phi}(x,y)\,\psi_x(x,y) - \bar{\phi}_x(x,y)\,\psi(x,y)\right]_{x=0}^{x=l} \, dy = 0 \ ,$$

To conclude when this vanishes one requires knowledge of the regularity of the functions on ∂D.

Theorem (Ding, 1996)
Ω bounded, simply connected Lipshitz domain. Then the trace operator $\gamma|_{\partial\Omega}$ is a bounded linear map

- from $H^s(\Omega)$ to $H^{s-\frac{1}{2}}(\partial\Omega)$ when $\frac{1}{2} < s < \frac{3}{2}$,
- from $H^s(\Omega)$ to $H^1(\partial\Omega)$ when $s > \frac{3}{2}$.

Hence, on the boundary ∂D the functions are of class H^1.

The boundary conditions imposed on $\psi(\cdot, y)$ in the Theorem, for a.e. $y \in (0, l)$, imply that these functions are in a domain for a one-particle, *self-adjoint* Laplacian Δ_x. Hence

$$\operatorname{ran}(\Delta_{1,x} + iI) = L^2(0, l) \ .$$

Apply this to above for a.e. y to conclude

$$\operatorname{ran}(\Delta_2^* + iI) = L^2(D) \ ,$$

hence the two-particle Laplacian with the prescribed boundary conditions is self-adjoint.

Extension to graphs:

On a general graph two-particle states are E^2-component functions on rectangles $(0, l_e) \times (0, l_{e'})$. Domains of self-adjoint Laplacians involve $2E^2$ boundary values, hence the notation becomes heavier. Otherwise, not much changes.

For convenience one rescales the intervals to have E copies of $(0, 1)$, i.e., the components of two-particle states are functions

$$\psi_{ee'}(l_e x, l_{e'} y) \ , \quad x, y \in (0, 1) \ .$$

Theorem (JB, Kerner 2010)
The domains $\mathcal{D}$ of self-adjoint, bosonic realisations of the two-particle Laplacian $-\Delta_2$ on a finite, metric graph can be characterised in terms of the boundary conditions

$$A(y)\begin{pmatrix}\big(\sqrt{l_{e'}}\psi_{ee'}(0,l_{e'}y)\big)\\ \big(\sqrt{l_{e'}}\psi_{ee'}(l_e,l_{e'}y)\big)\end{pmatrix}+B(y)\begin{pmatrix}\big(\sqrt{l_{e'}}\psi_{ee',x}(0,l_{e'}y)\big)\\ -\big(\sqrt{l_{e'}}\psi_{ee',x}(l_e,l_{e'}y)\big)\end{pmatrix}=0$$

for a.e. $y\in(0,1)$. Here, for a.e. $y\in(0,1)$ the $2E^2\times 2E^2$ matrices $A(y)$ and $B(y)$ satisfy

(i) $\operatorname{rank}\big(A(y),B(y)\big)=2E^2$,
(ii) $A(y)B^*(y)$ self-adjoint.

The operator is a lift from a one-particle operator to the two-particle Hilbert space, iff A and B are independent of y and have (at most) $2E\times 2E$ non-vanishing entries acting on the boundary values of ψ_{ee}.

Localised interactions on edges

So far two-particle interactions are localised at vertices (incorporated in boundary conditions).

One can also introduce singular interactions on the egdes, with an operator of the form

$$-\Delta_2 + \alpha\delta(x-y) \ ,$$

via self-adjoint extensions of a symmetric operator with domain characterised by $\Psi = (\psi_{ee'})$, where

$$\psi_{ee'} \in H^2([0,l_e]) \otimes H^2([0,l_{e'}]) \quad \text{and} \quad \psi_{ee}(x,x) = 0 \ .$$

As a result, in addition to boundary conditions at the vertices functions in the domain of the operator have to fulfil

$$\psi_{ee,x}(x_+,x) - \psi_{ee,x}(x_-,x) = \alpha\, \psi_{ee}(x,x) \ .$$

Lift to Fock space

In the same manner as a one-particle Laplacian $-\Delta_1$ can be second quantised to yield $d\Gamma(-\Delta_1)$, any of the two-particle operators $-\Delta_2 + \alpha\delta(x-y)$ can be lifted to the bosonic Fock space.

One chooses domains with appropriate boundary conditions to achieve self-adjoint realisations of

$$\sum_{j,k=1}^{n}\Big(-\frac{\partial^2\psi_{e_1,\dots,e_n}}{\partial x_{e_j}^2}-\frac{\partial^2\psi_{e_1,\dots,e_n}}{\partial x_{e_k}^2}+\alpha\delta(x_{e_j}-x_{e_k})\Big)$$

for all $n \geq 2$.

This type of two-particle interactions preserves the particle number.

Conclusions

Single-particle quantum graph models have been used successfully in many areas of mathematics and theoretical physics.

These models can be lifted to a many-particle level, and two-particle interactions can be included using self-adjoint extensions of symmetric operators. More specifically, the interactions are:

- Singular two-particle interactions in vertices
- Singular two-particle interactions on edges
- A combination of both

Outlook:

- Construction of specific two-particle models
- Spectrum, Weyl's law, trace formula
- Lift to Fock space, two-particle S-matrix
- Fermions
- Hartree-Fock approximation
- Bose-Einstein condensation