Some semiclassical and universal estimates of eigenvalues of quantum graphs

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"Universal" constraints on the spectrum

- H. Weyl, 1910, Laplace, $\lambda_n \sim n^{2/d}$
- W. Kuhn, F. Reiche, W. Thomas, W. Heisenberg, 1925, "sum rules" for atomic energies.
- L. Payne, G. Pólya, H. Weinberger, 1956: The gap is controlled by the average of the smaller eigenvalues:

$$\lambda_{n+1} - \lambda_n \leq \frac{4}{d}\frac{1}{n}\sum_{k \leq n} \lambda_k$$

"Universal" constraints on the spectrum with phase-space volume.

- Lieb -Thirring, 1977, for Schrödinger

$$\epsilon^{\mathbf{d/2}} \sum_{\lambda_{\mathbf{j}}(\epsilon)<\mathbf{0}} |\lambda_{\mathbf{j}}(\epsilon)|^{\rho} \leq \mathbf{L}_{\rho,\mathbf{d}} \int_{\mathbf{R^d}} (\mathbf{V}_{-}(\mathbf{x}))^{\rho+\mathbf{d/2}}\, \mathbf{dx}$$

- Li - Yau, 1983 (Berezin 1973), for Laplace

$$\sum_{j=1}^{k} \lambda_j \geq \frac{d}{d+2} \frac{4\pi^2 k^{1+2/d}}{(C_d|\Omega|)^{2/d}}$$

“Universal” constraints on the spectrum

- Ashbaugh-Benguria 1991, isoperimetric conjecture of PPW proved.
- H. Yang 1991, unpublished, formulae like PPW, respecting Weyl asymptotics for the first time.
- Harrell 1993-present, commutator approach; with Michel, Stubbe, El Soufi and Ilias, Hermi, Yildirim.
- Ashbaugh-Hermi, Levitin-Parnovsky, Cheng-Yang, Cheng-Chen, some others.

Riesz means

- The counting function,

  $N(z) := \#(\lambda_k \leq z)$

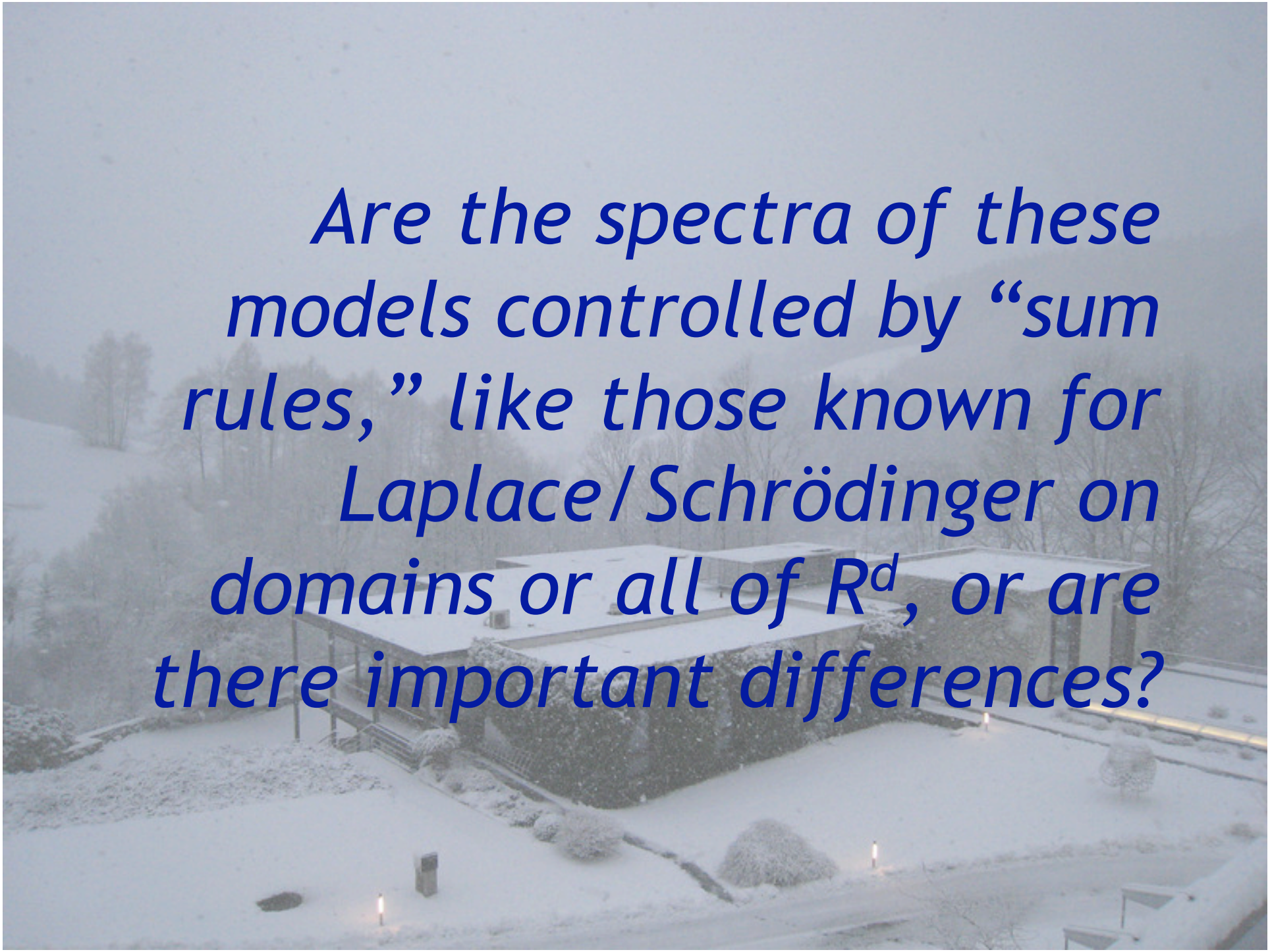
- Integrals of the counting function, known as *Riesz means* (Safarov, Laptev, Weidl, etc.):

$$R_\rho(z) := \sum_j (z - \lambda_j)_+^\rho$$

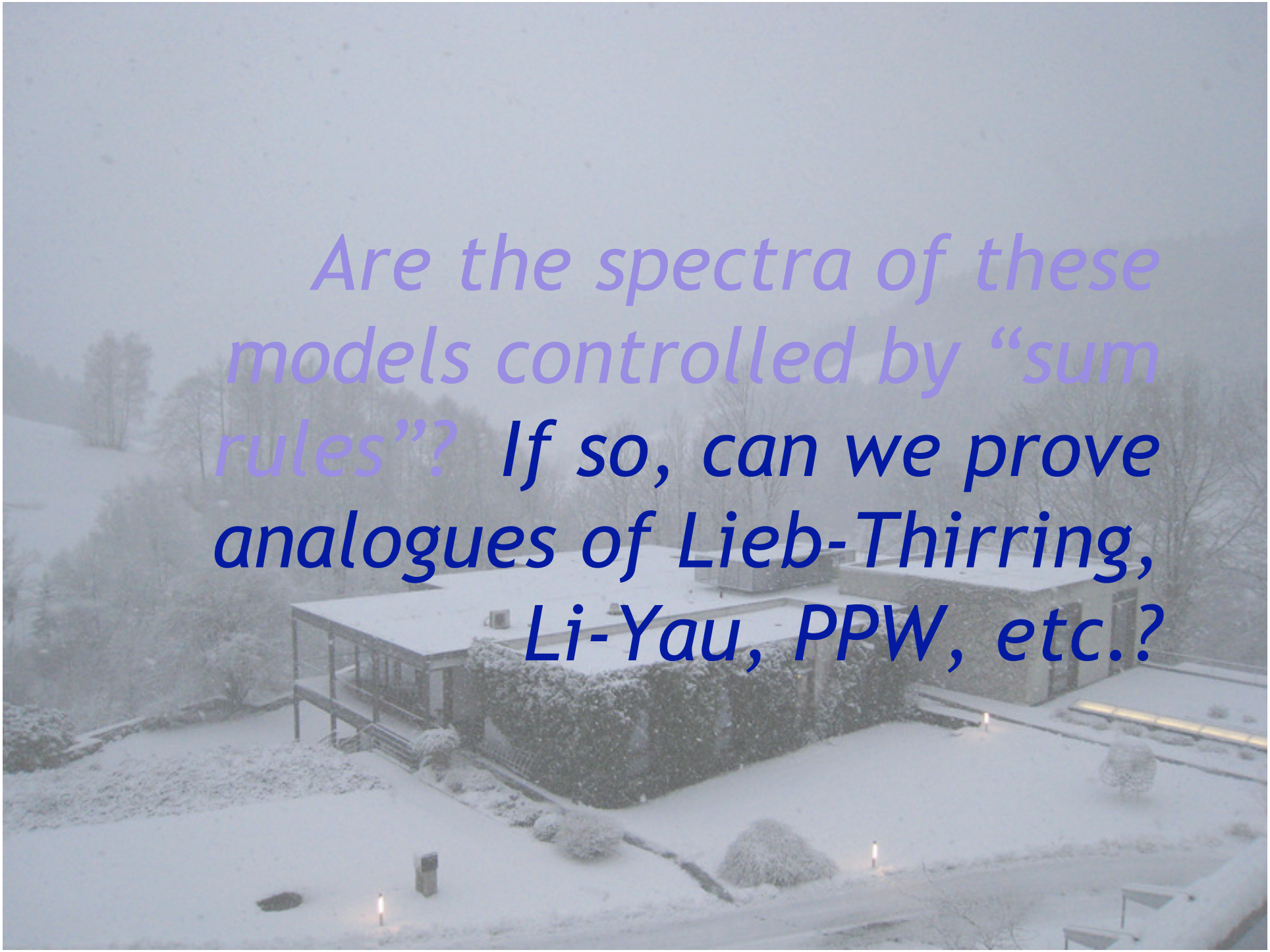
- Chandrasekharan and Minakshisundaram, 1952

Some models in nanophysics:

1. Schrödinger operators on curves and surfaces embedded in space. *Quantum wires and waveguides*.
2. Periodic Schrödinger operators. *Electrons in crystals*.
3. Quantum graphs. *Nanoscale circuits*
4. Relativistic Hamiltonians on curved surfaces. *Graphene*.



Are the spectra of these models controlled by "sum rules," like those known for Laplace/Schrödinger on domains or all of R^d, or are there important differences?



Are the spectra of these models controlled by "sum rules"? If so, can we prove analogues of Lieb-Thirring, Li-Yau, PPW, etc.?

Commutators of operators

- [G, [H, G]] = 2 GHG - G^2H - HG^2
- Etc., etc. Typical consequence:

$$\langle \phi_{\mathbf{j}}, [\mathbf{G}, [\mathbf{H}, \mathbf{G}]] \phi_{\mathbf{j}} \rangle = \sum_{\mathbf{k}:\lambda_{\mathbf{k}} \neq \lambda_{\mathbf{j}}} (\lambda_{\mathbf{k}} - \lambda_{\mathbf{j}}) |\mathbf{G}_{\mathbf{kj}}|^{\mathbf{2}}$$

(Abstract version of Bethe's sum rule)

A "sum rule" identity for $H=H^*$, $G=G^*$, If $J = \{\lambda_1, \ldots, \lambda_k\} \leq z \leq J^c$:

$$\frac{1}{2}\sum_{\lambda_j \in J}(z-\lambda_j)^2 \langle [G,[H,G]]\phi_j, \phi_j\rangle - \sum_{\lambda_j \in J}(z-\lambda_j)\|[H,G]\phi_j\|^2$$

$$=$$

$$\sum_{\lambda_j \in J}\sum_{\lambda_k \in J^c}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)|\langle G\phi_j, \phi_k\rangle|^2$$

Harrell-Stubbe TAMS 1997

For $J = \{\lambda_1 \ldots \lambda_n\}$, the right side ≤ 0!

Basic ideas of the strategy

1. There is an exact identity involving traces including [G, [H, G]] and [H,G]*[H,G].

2. For the lower part of the spectrum it implies an inequality of the form:

$$\sum (z - \lambda_k)^2 (\ldots) \quad \leq \quad \sum (z - \lambda_k) (\ldots)$$

Basic ideas of the strategy

1. A good choice of G for the Laplacian is a coordinate function, because
   a) $[H,G] = -2\,\partial/\partial x_k$, and
   b) $[G, [H, G]] = 2$

2. For Schrödinger, sum rules conect eigenvalues with the kinetic energy.

3. Spectral information can be extracted from Riesz means with classical transforms.

Dirichlet problem:

Trace identities imply differential inequalities

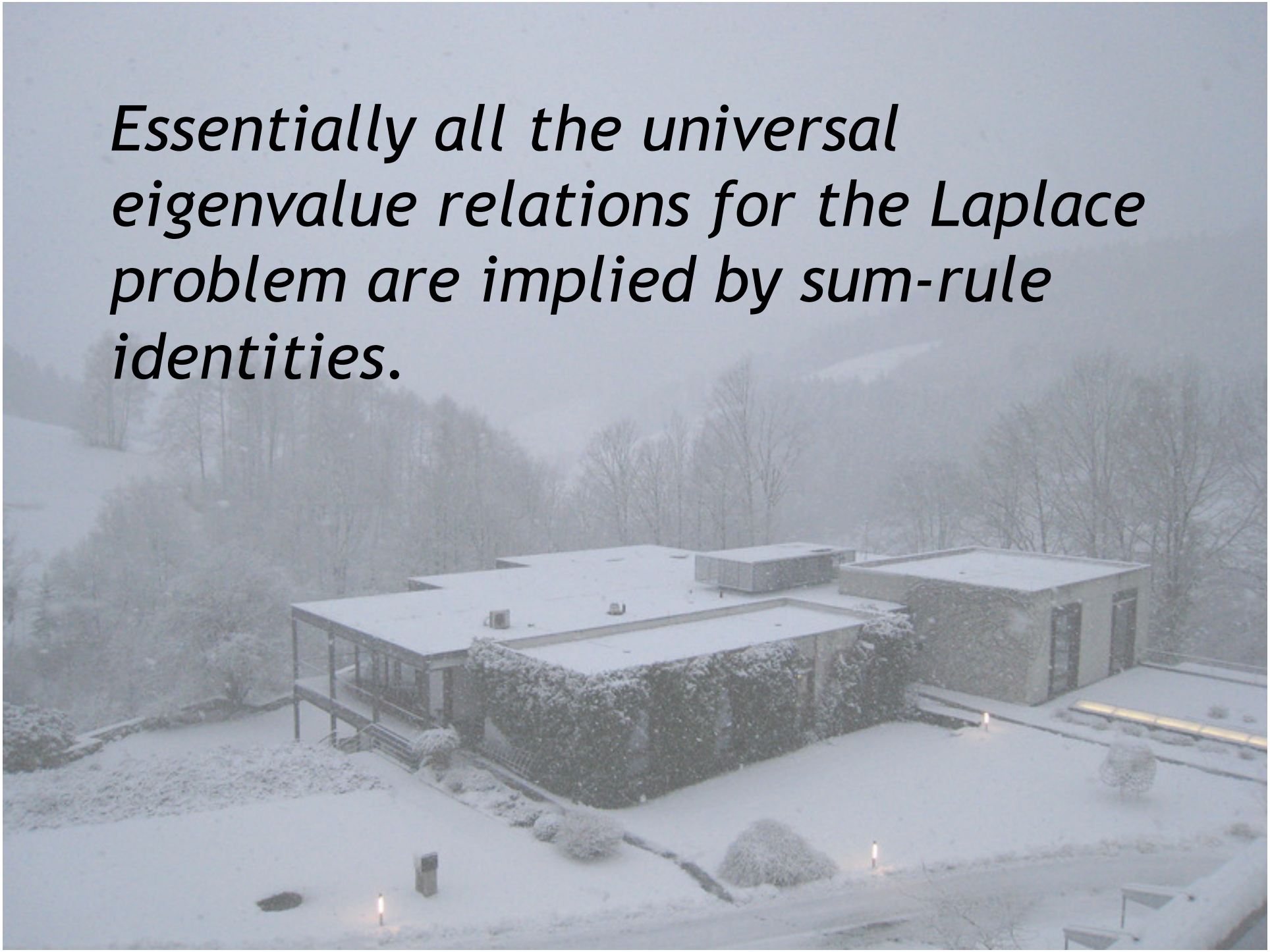
$$R_2(z) \leq \frac{4}{d} \sum_k (z - \lambda_k) T_k$$

Harrell-Hermi JFA 08: Laplacian

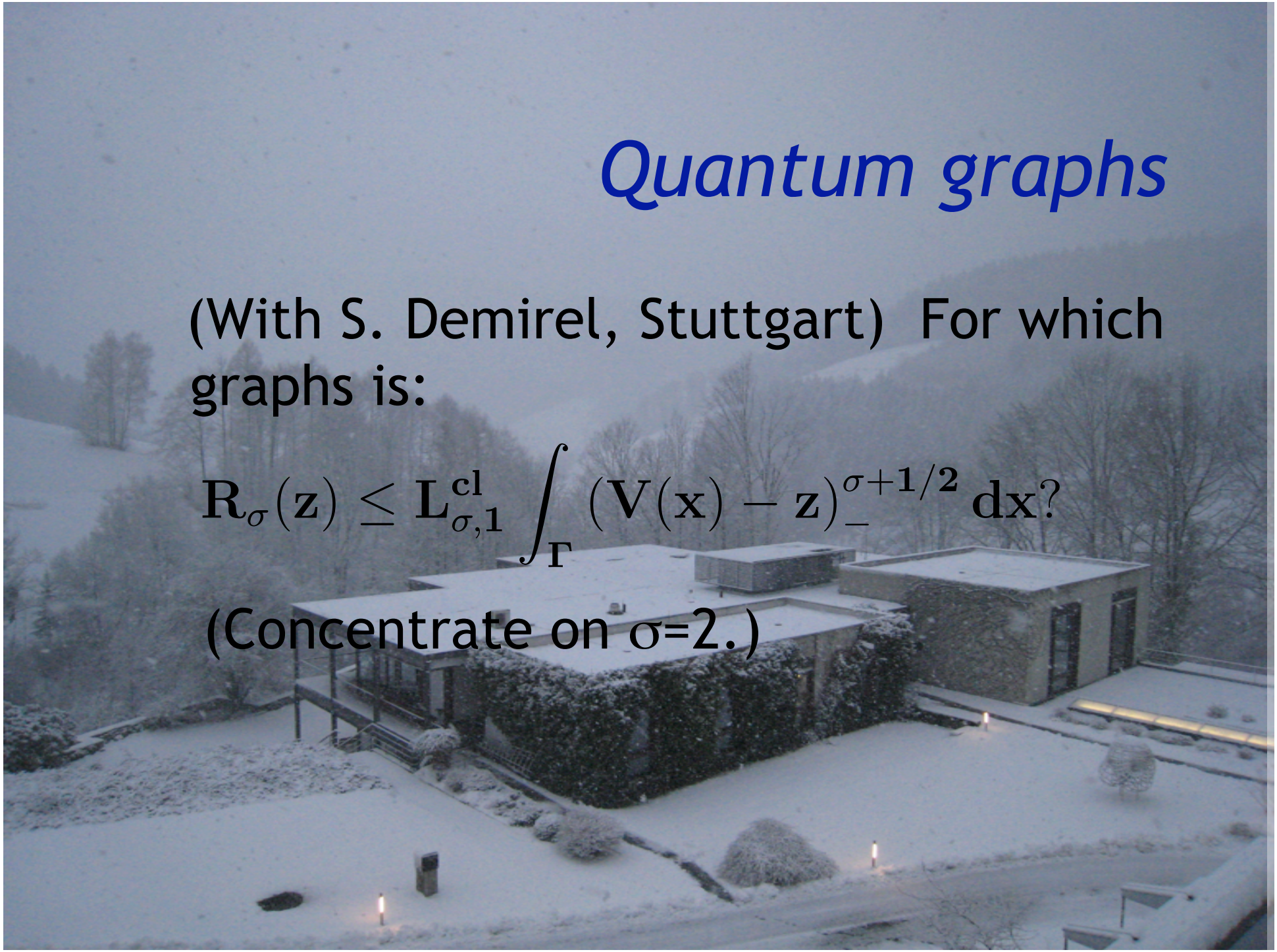
$$\left(1 + \frac{4}{d}\right) R_2(z) - \frac{2z}{d} R_2'(z) \leq 0.$$

Consequences – universal bound for k >j:

$$\frac{\overline{\lambda_k}}{\overline{\lambda_j}} \leq \frac{4+d}{2+d} \left(\frac{k}{j}\right)^{2/d}$$



Essentially all the universal eigenvalue relations for the Laplace problem are implied by sum-rule identities.



Quantum graphs

(With S. Demirel, Stuttgart) For which graphs is:

$$\mathbf{R}_\sigma(\mathbf{z}) \leq \mathbf{L}^{\mathbf{cl}}_{\sigma,\mathbf{1}} \int_{\mathbf{\Gamma}} (\mathbf{V}(\mathbf{x}) - \mathbf{z})_-^{\sigma+\mathbf{1/2}}\, \mathbf{dx}?$$

(Concentrate on σ=2.)

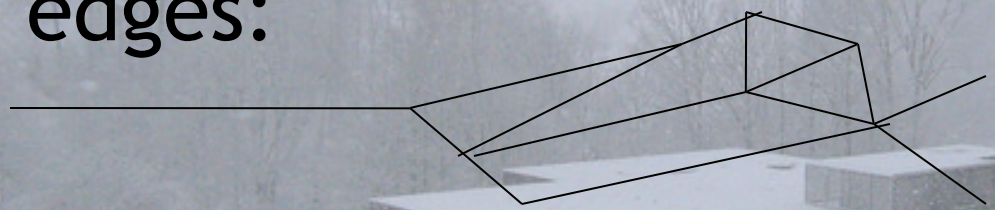
ON SEMICLASSICAL AND UNIVERSAL INEQUALITIES FOR EIGENVALUES OF QUANTUM GRAPHS

SEMRA DEMIREL AND EVANS M. HARRELL II

Abstract. We study the spectra of quantum graphs with the method of trace identities (sum rules), which are used to derive inequalities of Lieb-Thirring, Payne-Pólya-Weinberger, and Yang types, among others. We show that the sharp constants of these inequalities and even their forms depend on the topology of the graph. Conditions are identified under which the sharp constants are the same as for the classical inequalities; in particular, this is true in the case of trees. We also provide some counterexamples where the classical form of the inequalities is false.

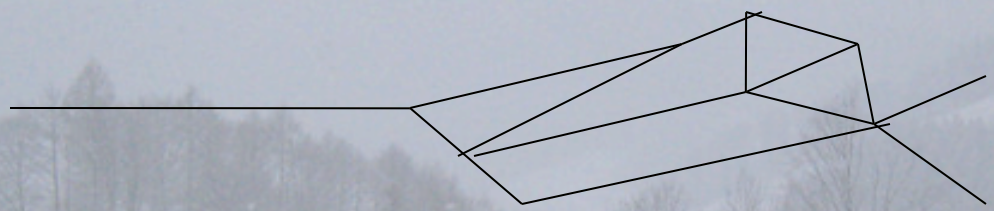
Quantum graphs

1. A graph (in the sense of network) with a 1-D Schrödinger operator on the edges:



connected by “Kirchhoff conditions” at vertices. Sum of outgoing derivatives vanishes.

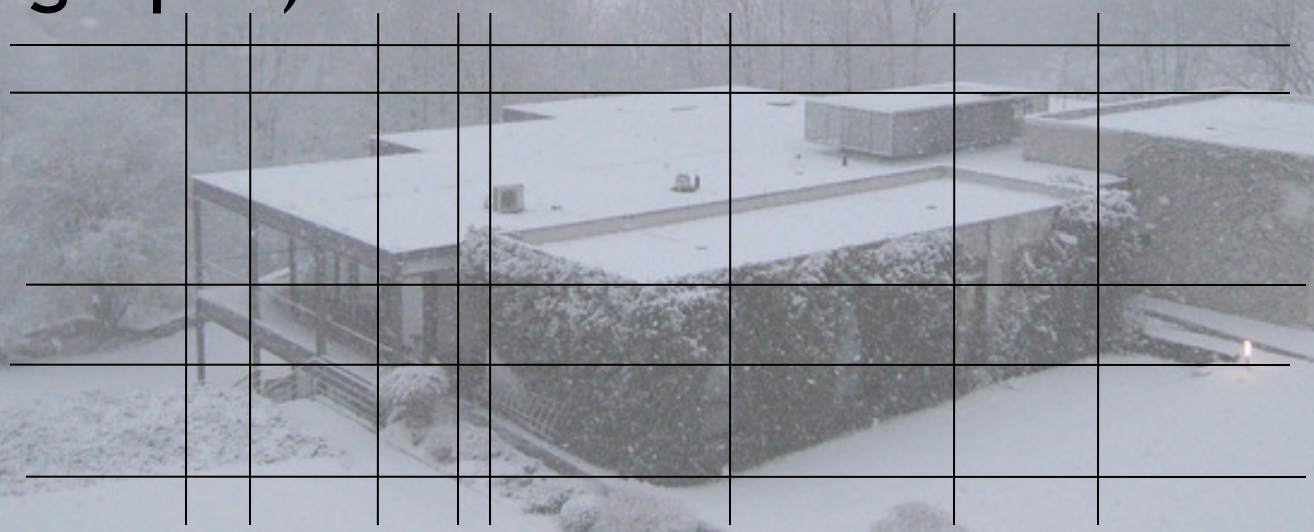
Quantum graphs



Is this one-dimensional or not? Does the topology matter?

Quantum graphs are L-T one-dimensional for:

1. Trees.
2. Scottish tartans (infinite rectangular graphs):

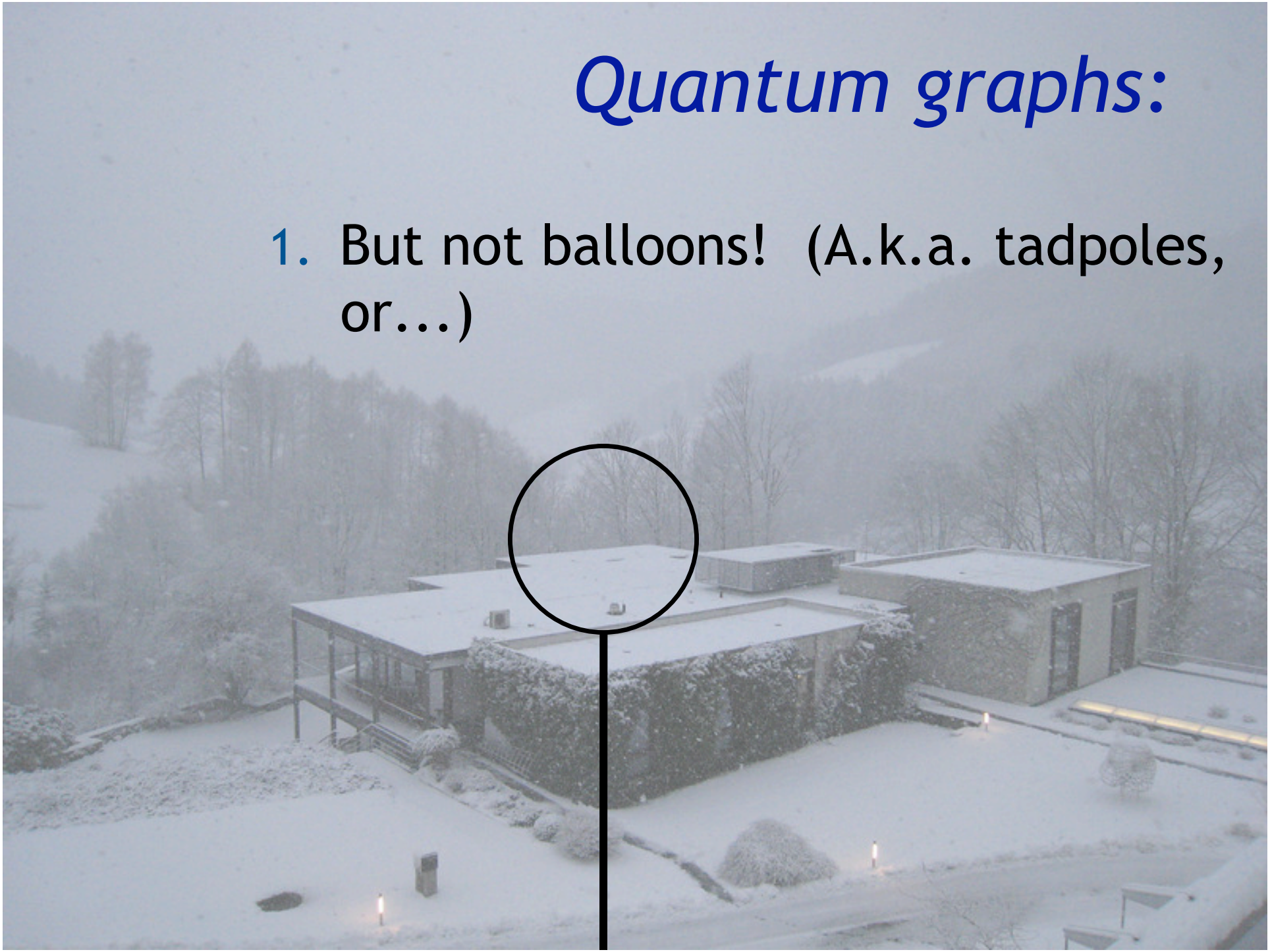


Quantum graphs are L-T one-dimensional for:

1. Trees.
2. Infinite rectangular graphs.
3. Bathroom tiles, a.k.a. honeycombs, etc.:

Quantum graphs:

1. But not balloons! (A.k.a. tadpoles, or...)



Quantum graphs:

1. But not balloons! (A.k.a. tadpoles, or...)

Put a soliton potential on the loop:

$$V = \frac{-2a^2}{\cosh^2(ax)}\chi_{\text{loop}}$$

$$\phi = \frac{\cosh(aL)}{\cosh(ax)} \quad \text{resp.} \quad e^{-ax}$$

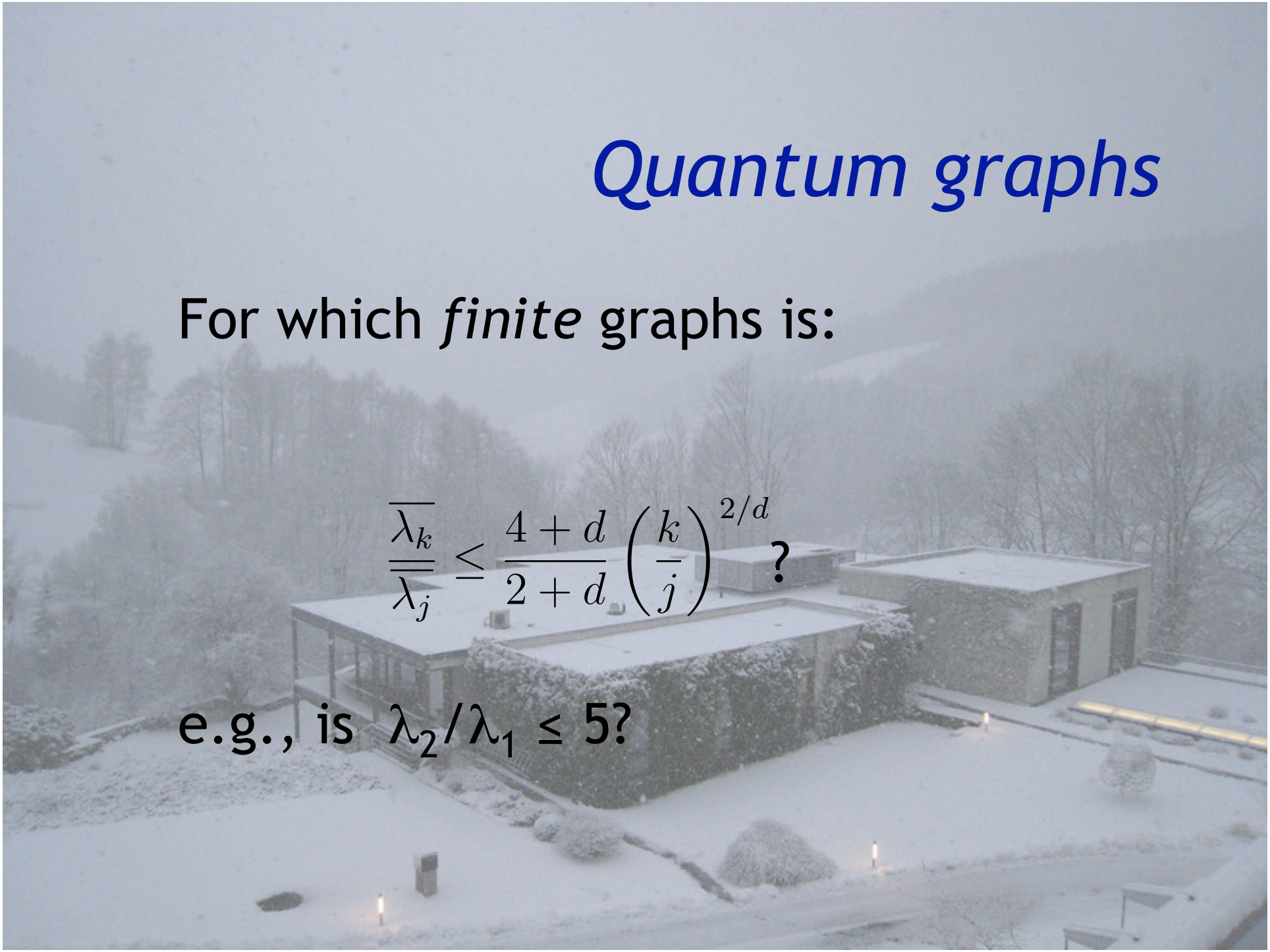
$\lambda_1 = -a^2$ solves a transcendental equation, but $\frac{|\lambda_1|^\sigma}{\int |V|^{\sigma+1/2}}$ is exactly determined!

Quantum graphs

1. But not balloons! (A.k.a. tadpoles, or...)

$\rho = 3/2$: ratio is 3/11 vs. $L^{cl} = 3/16$.

$\rho = 2$: ratio is messy expression 0.20092...
vs. $L^{cl} = 8/(15\,\pi) = 0.169765...$



Quantum graphs

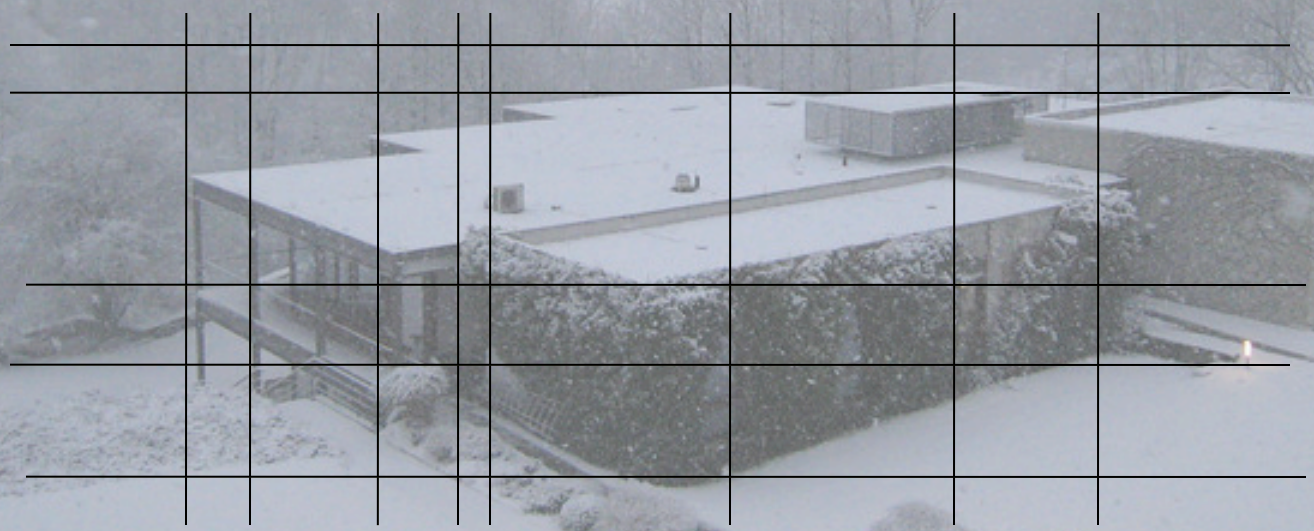
For which *finite* graphs is:

$$\frac{\overline{\lambda_k}}{\overline{\lambda_j}} \leq \frac{4+d}{2+d}\left(\frac{k}{j}\right)^{2/d} \; ?$$

e.g., is $\lambda_2/\lambda_1 \leq 5$?

Quantum graphs

1. Trees.
2. Rectangular graphs/bathroom tiles with external edges:



Quantum graphs

- But not balloons!

$$\frac{\lambda_2}{\lambda_1} = \left(\frac{\pi - \arctan(1/\sqrt{(2)})}{\arctan(1/\sqrt{(2)})} \right) \doteq 16.8$$

Quantum graphs

- Fancy balloons can have arbitrarily large λ_2/λ_1.

Why?

If we can establish the analogue of the trace inequality,

$$\mathbf{R}_\rho(\mathbf{z}) - \alpha \frac{\mathbf{2}\rho}{\mathbf{d}} \sum (\mathbf{z} - \lambda_\mathbf{k})_+^{\rho-\mathbf{1}} \|\nabla \phi_\mathbf{k}\|^\mathbf{2} \leq \mathbf{0},$$

then all the rest of the inequalities follow (LT, PPW, ratios, statistics, etc.), sometimes with modifications.

Calculate commutators with a good G.

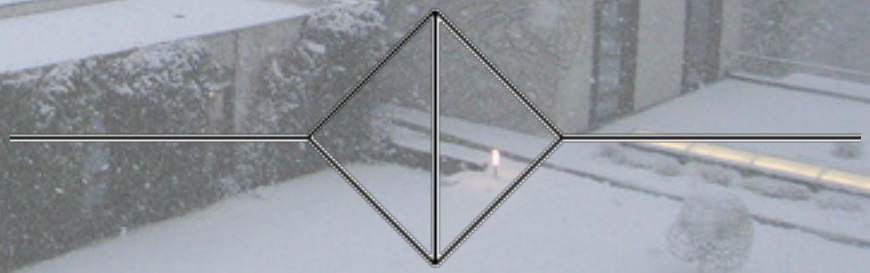
When does a quadratic inequality hold?

- If the graph can be covered by a family of transits where on each edge G' = cst, and for each edge there is some G where this constant is not 0, then

$$\sum_j (z-\lambda_j)_+ - 4\epsilon \frac{a_{max}}{a_{min}} (z-\lambda_j)_+ \|\phi_j'\|^2 \leq 0.$$

When does a quadratic inequality hold?

- Conjecture: This is possible unless the graph can be disconnected from all leaves by removal of one point, or contains a “Wheatstone bridge”



Some take-away messages

1. On quantum graphs, sum rules reflect the topology.

2. The QG is spectrally one-dimensional if the graph can be covered uniformly by a family of functions that resemble coordinate functions as much as possible.

3. This is not always possible: Connected with a question of classical circuit theory.

4. Full understanding of role of topology is open.

Articles related to this seminar

- S. Demirel and E.M. Harrell, Rev.Math. Physics, to appear.
- E.M. Harrell and J. Stubbe, On Trace Identities and Universal Eigenvalue Estimates for Some Partial Differential Operators, Trans. Amer. Math. Soc. 349(1997)1797-1809.
- E.M. Harrell, Commutators, eigenvalue gaps, and mean curvature in the theory of Schrödinger operators, Communications PDE, 2007
- A. El Soufi, E.M. Harrell, and S. Ilias, Universal inequalities for the eigenvalues of Laplace and Schrödinger operators on submanifolds, Trans AMS,2009.
- E.M. Harrell and L. Hermi, Differential inequalities for Riesz means and Weyl-type bounds for eigenvalues, J. Funct. Analysis 2008.
- E.M. Harrell and L. Hermi, On Riesz Means of Eigenvalues, preprint 2008.
- E.M. Harrell and J. Stubbe, Universal bounds and semiclassical estimates for eigenvalues of abstract Schrödinger operators, preprint 2008.
- E.M. Harrell and S. Yildirim Yolcu, Eigenvalue inequalities for Klein-Gordon Operators, J. Funct. Analysis 2009.
- E.M. Harrell and J. Stubbe, Trace identities for eigenvalues, with applications to periodic Schrödinger operators and to the geometry of numbers, Trans. AMS, to appear.


THE END