Sum rules and semiclassical limits for quantum Hamiltonians on surfaces, periodic structures, and graphs

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GT MATH

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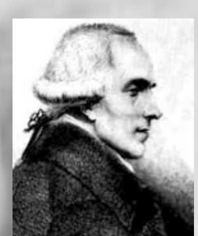
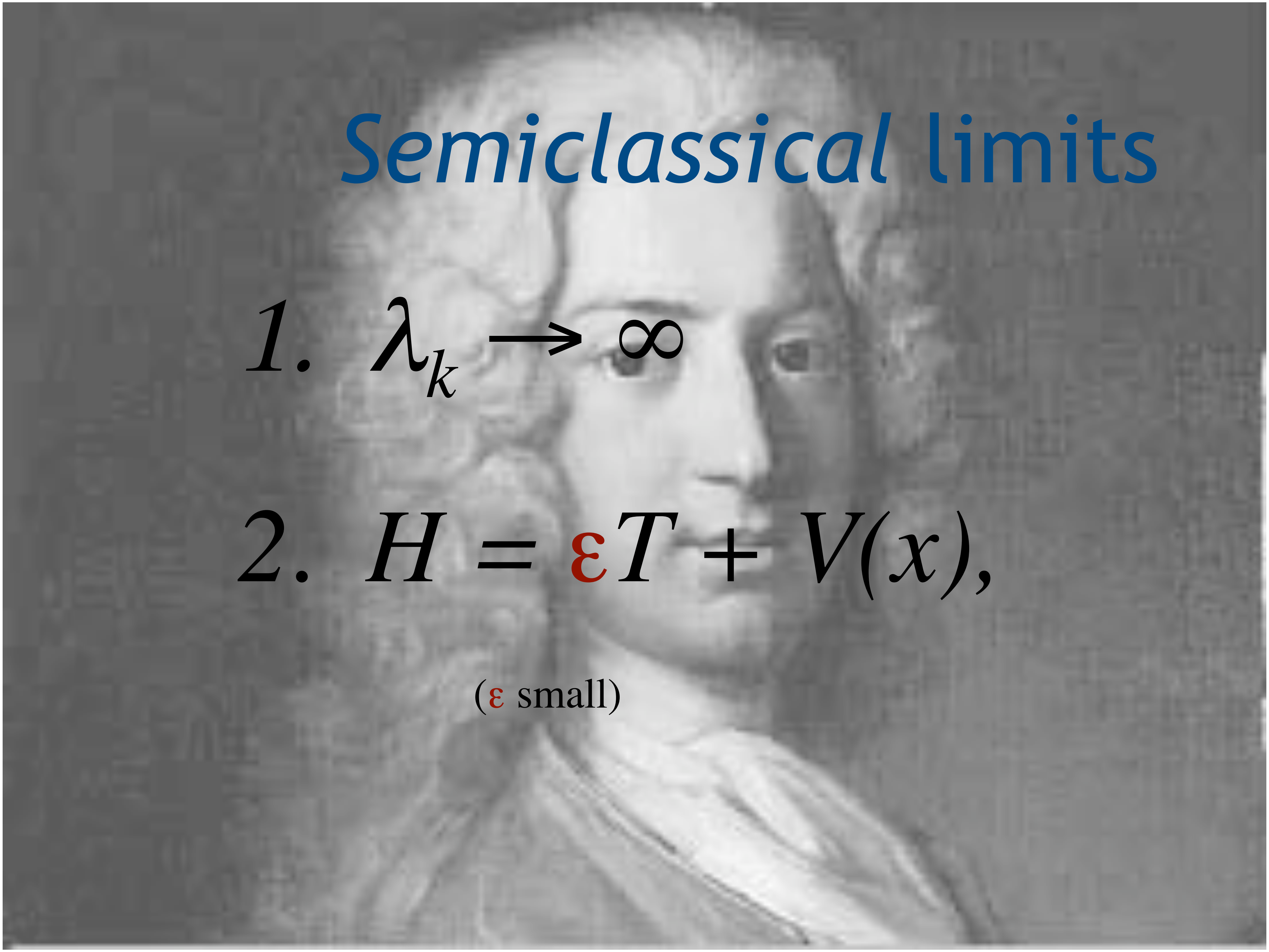


Discrete spectra of Laplace and Schrödinger operators.

$$H = -\frac{\hbar^2}{2m}\Delta + V(\mathbf{x})$$

$$H\,\phi_k = \lambda_k\,\phi_k$$



Semiclassical limits

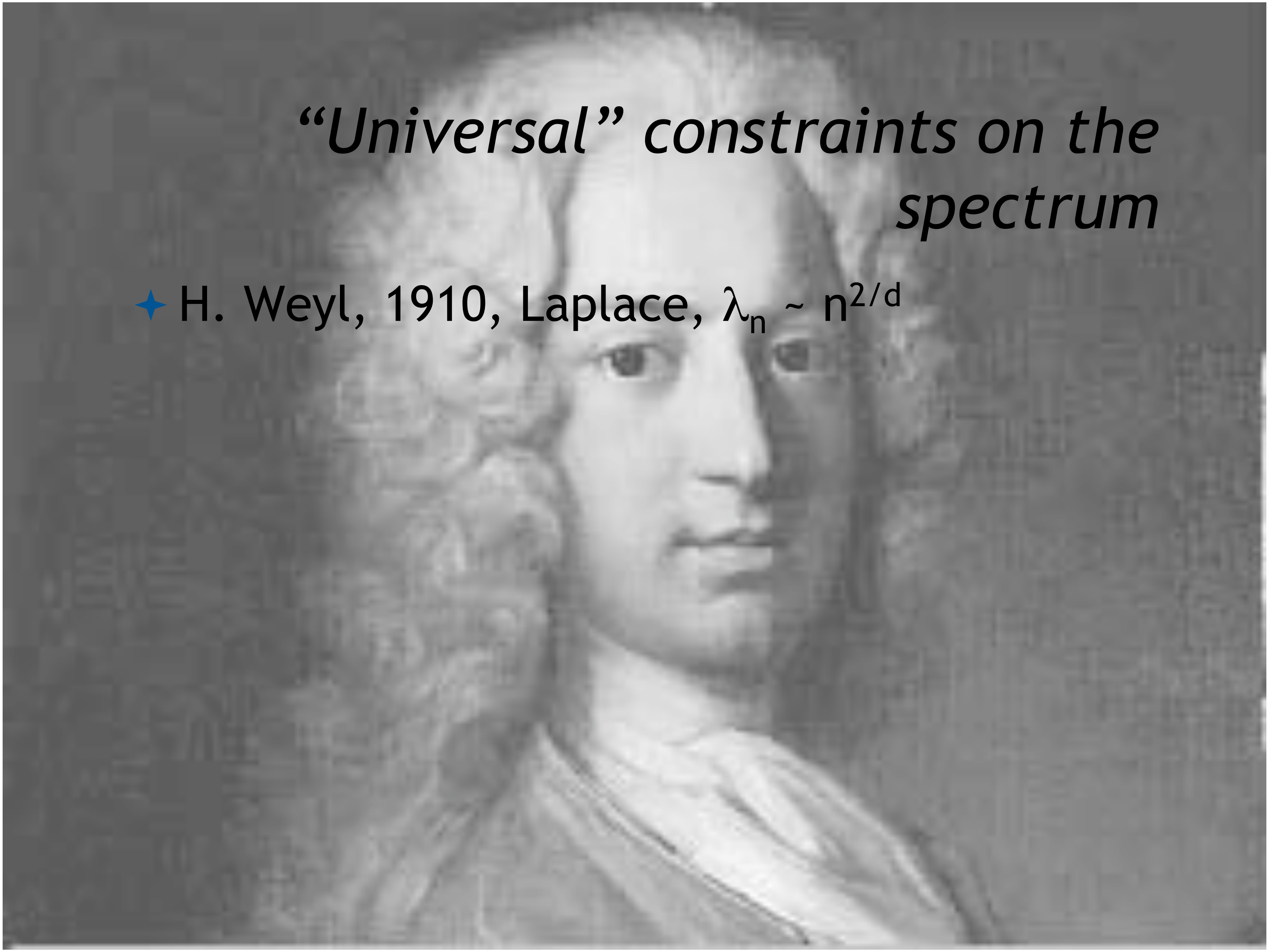
1. $\lambda_k \to \infty$

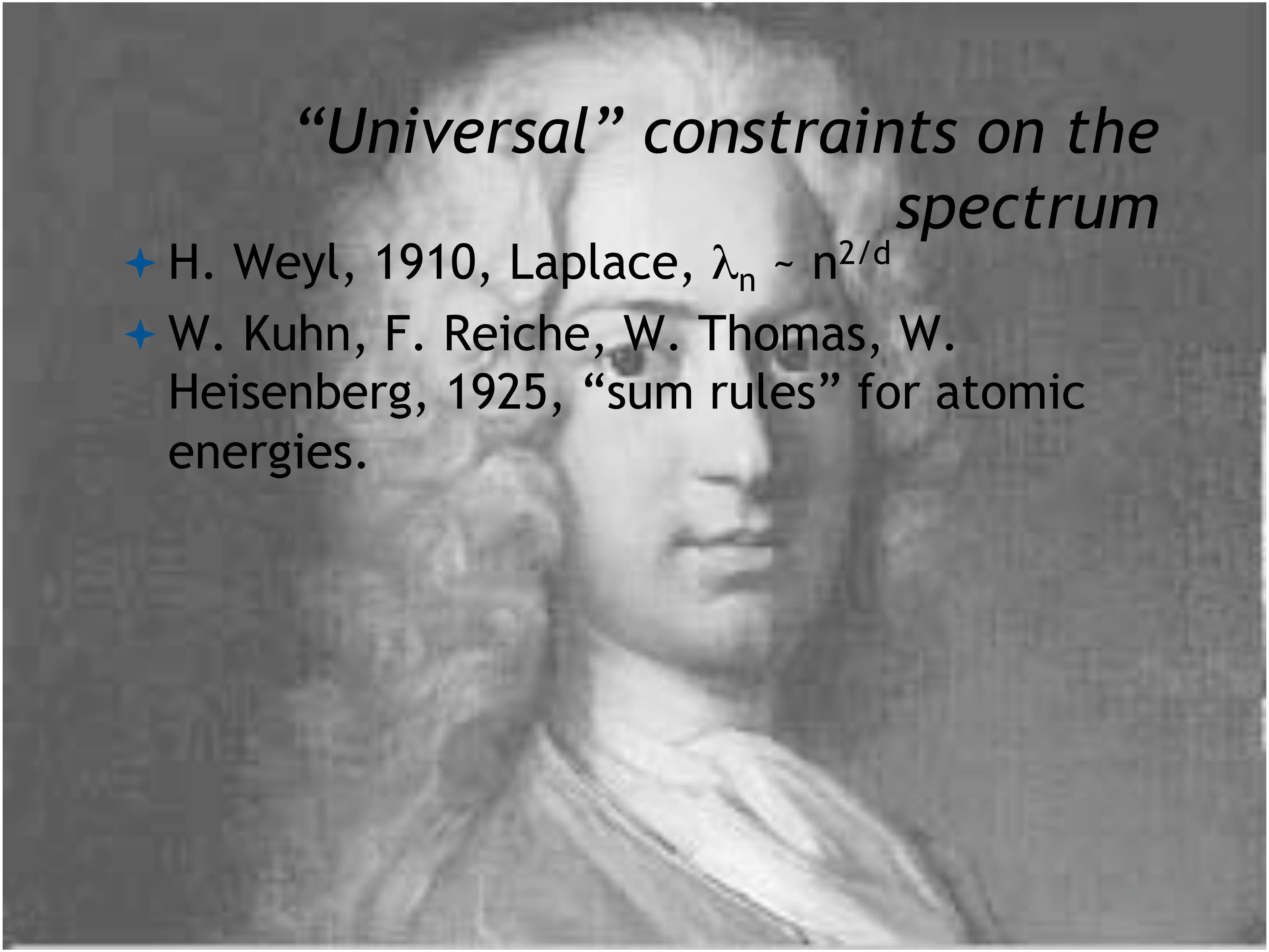
2. $H = \varepsilon T + V(x),$

(ε small)

“Universal” constraints on the spectrum

- H. Weyl, 1910, Laplace, $\lambda_n \sim n^{2/d}$





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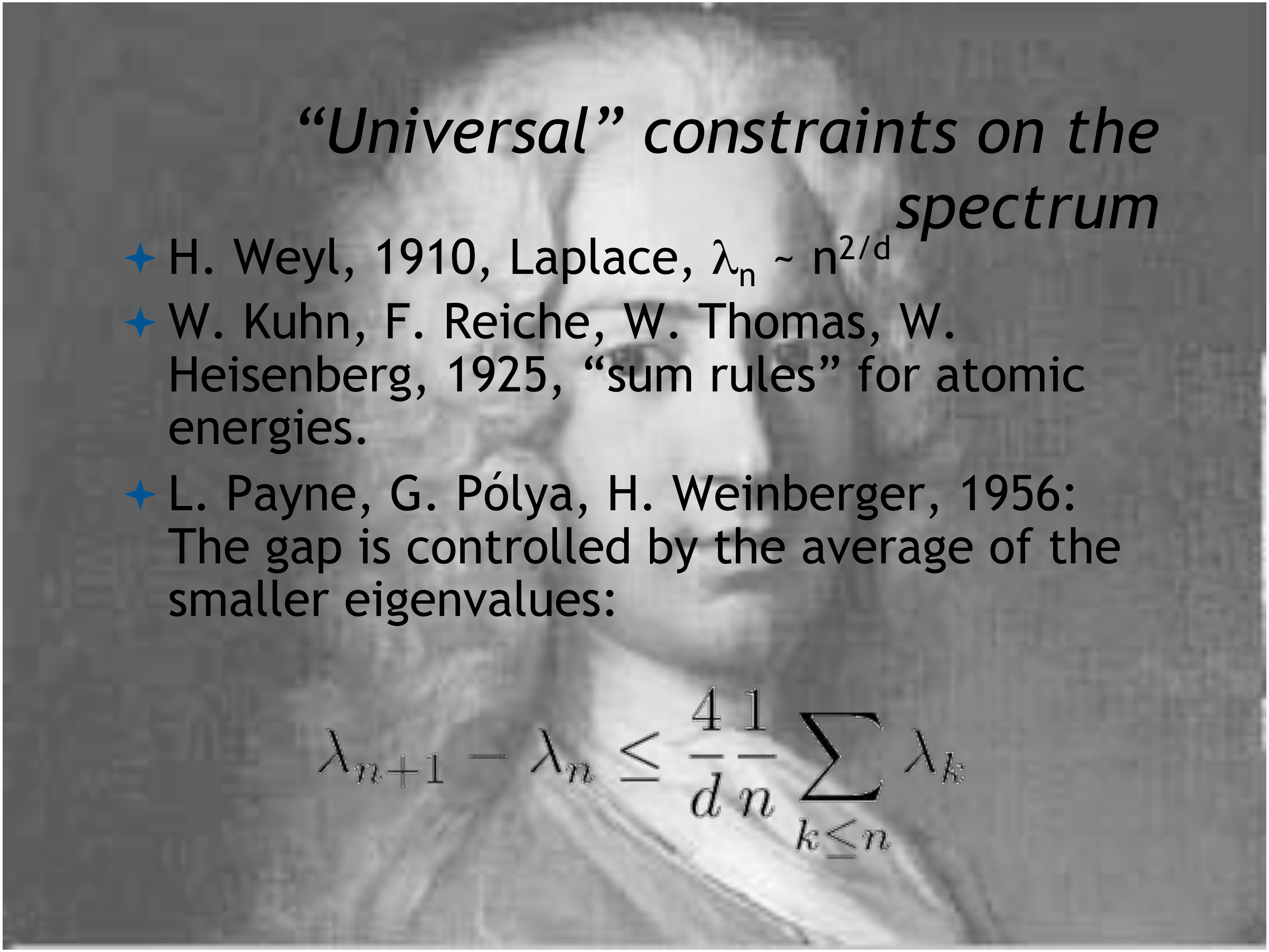
- W. Kuhn, F. Reiche, W. Thomas, W. Heisenberg, 1925, "sum rules" for atomic energies.



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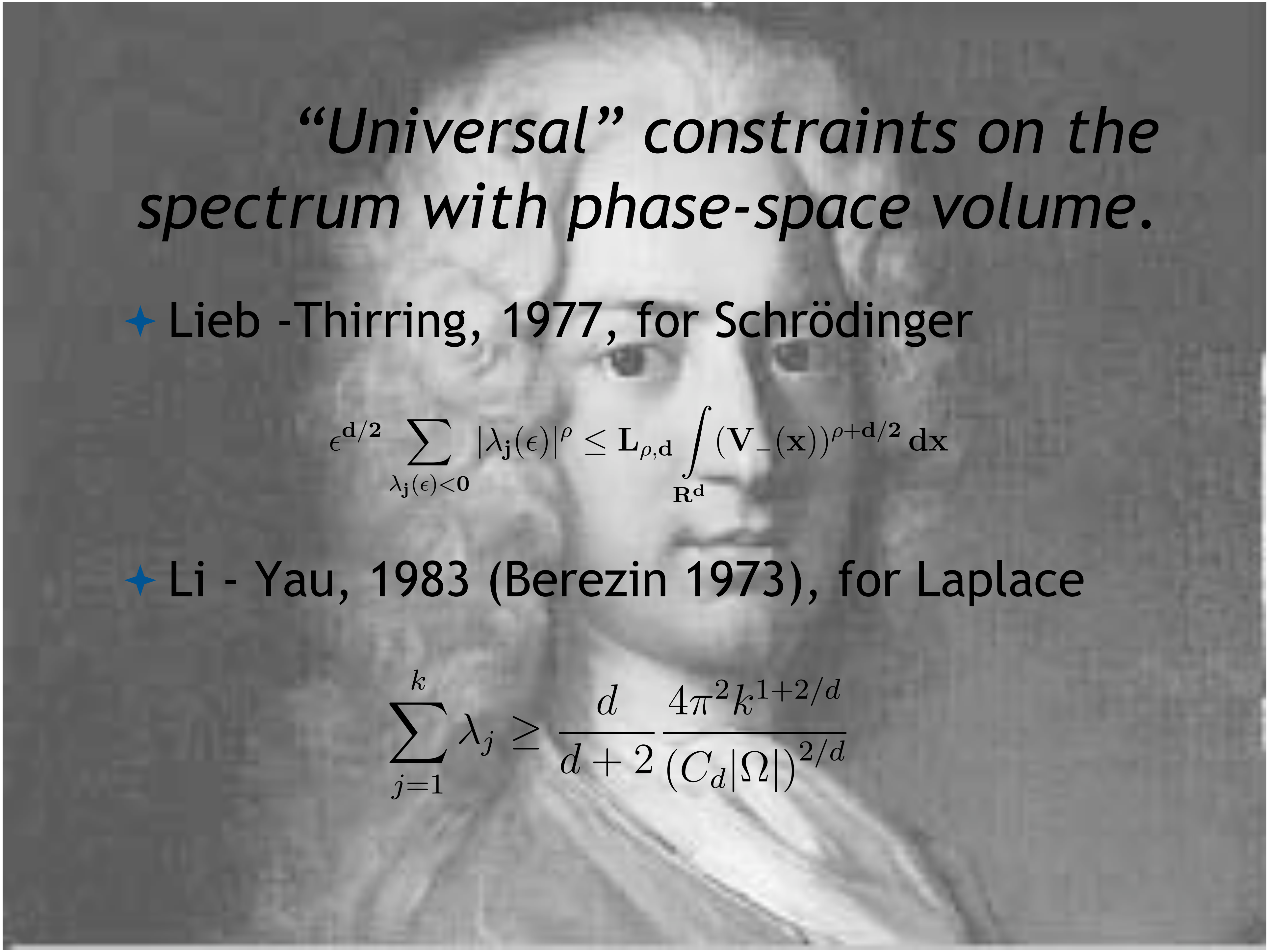
- W. Kuhn, F. Reiche, W. Thomas, W. Heisenberg, 1925, "sum rules" for atomic energies.
- L. Payne, G. Pólya, H. Weinberger, 1956: The gap is controlled by the average of the smaller eigenvalues:

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

"Universal" constraints on the spectrum

- 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- H. Yang 1991, unpublished, formulae like PPW, respecting Weyl asymptotics for the first time.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.



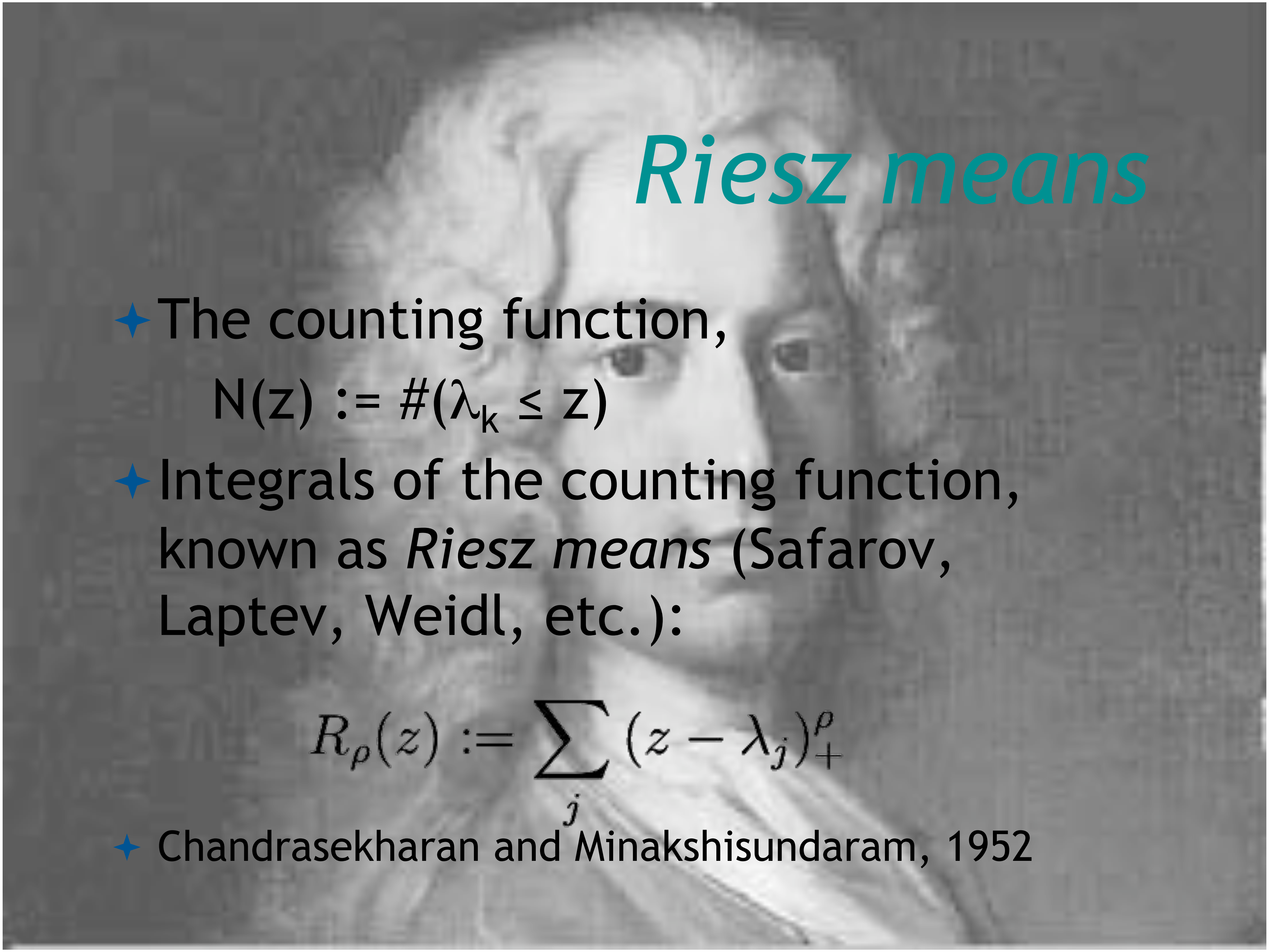
"Universal" constraints on the spectrum with phase-space volume.

- Lieb -Thirring, 1977, for Schrödinger

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

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

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



Riesz means

- The counting function,

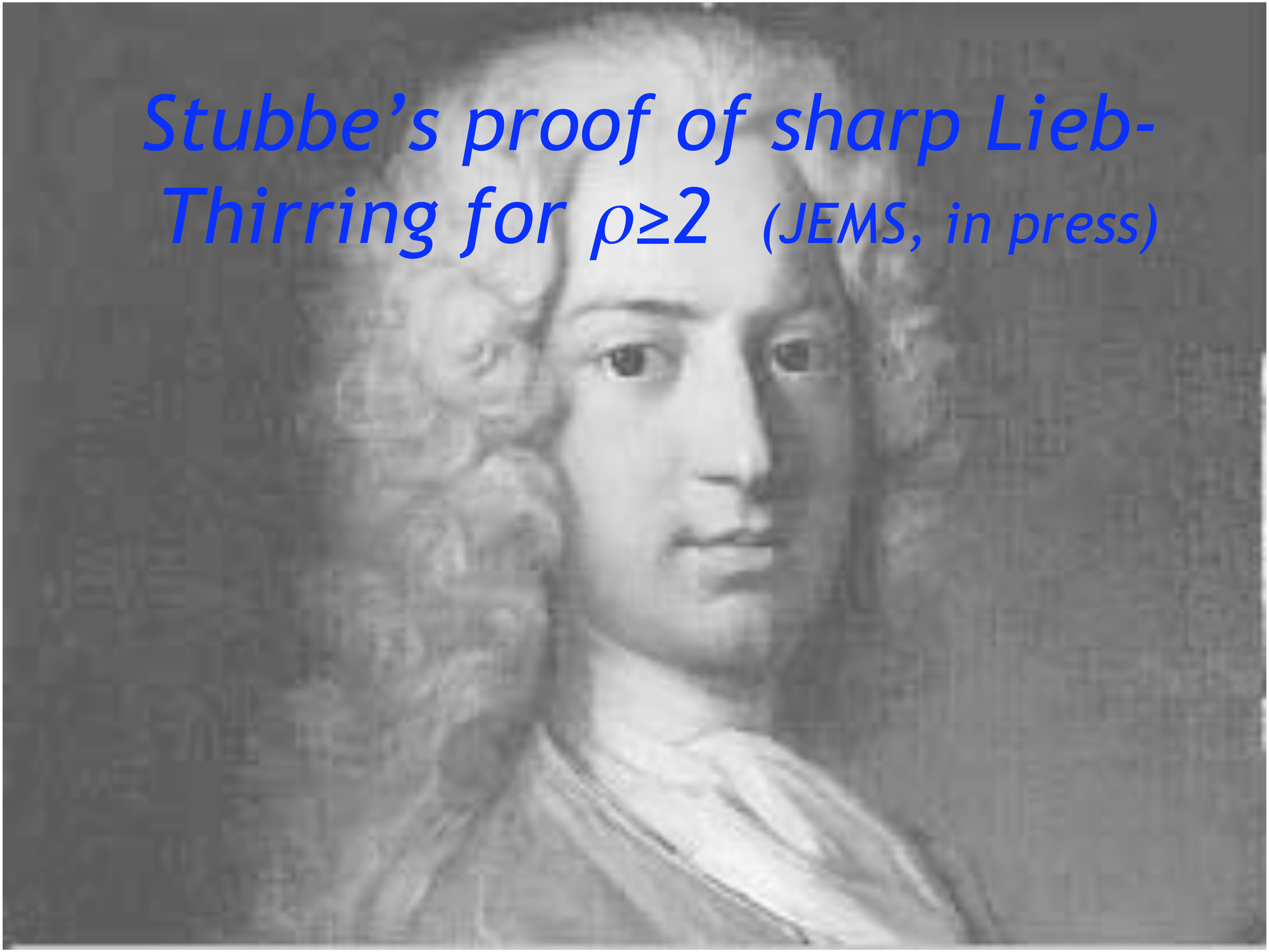
  $N(z) := \#(\lambda_k \leq z)$

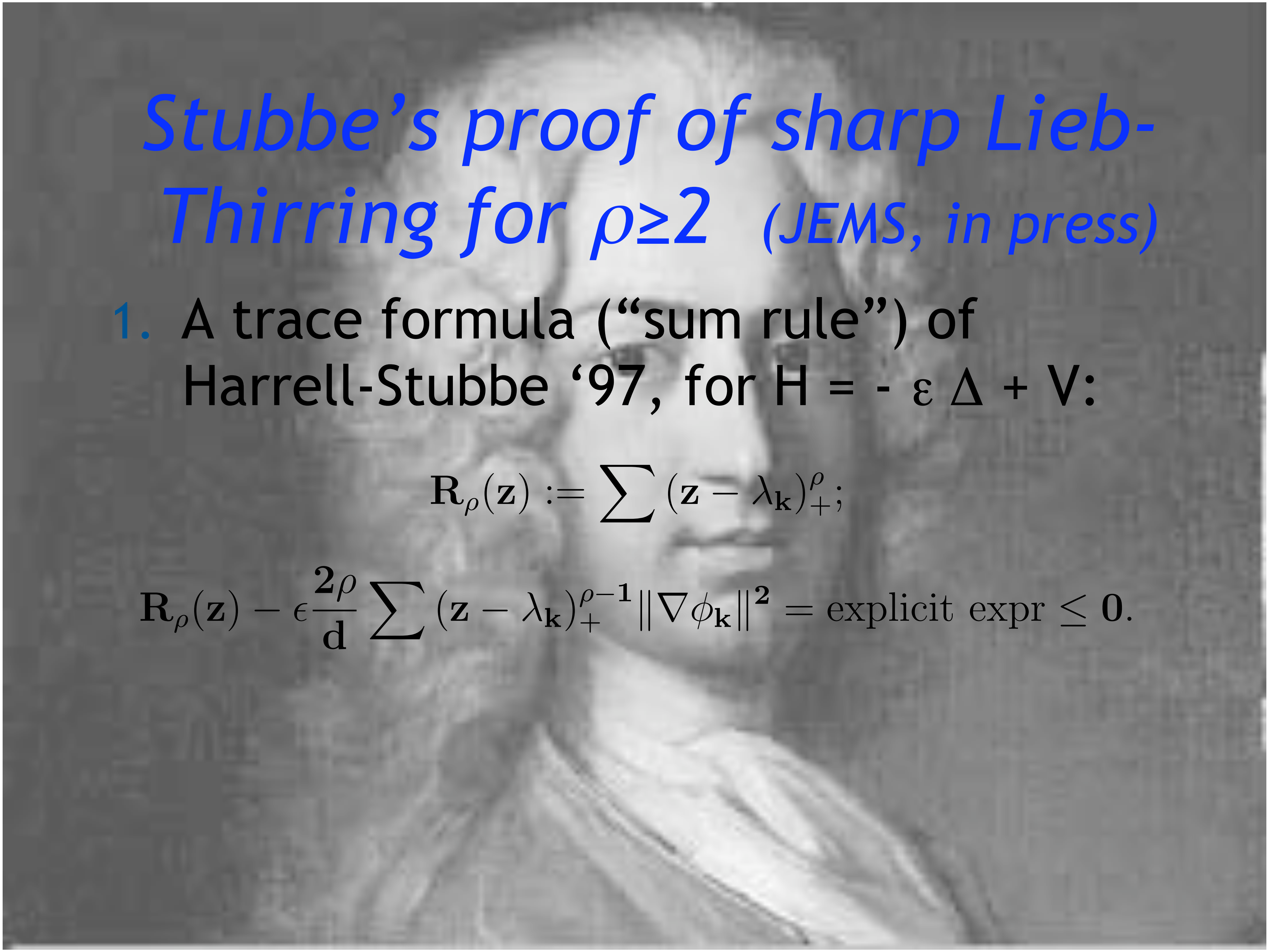
- Integrals of the counting function, known as *Riesz means* (Safarov, Laptev, Weidl, etc.):

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

- Chandrasekharan and Minakshisundaram, 1952

Stubbe's proof of sharp Lieb-Thirring for $\rho \geq 2$ (JEMS, in press)



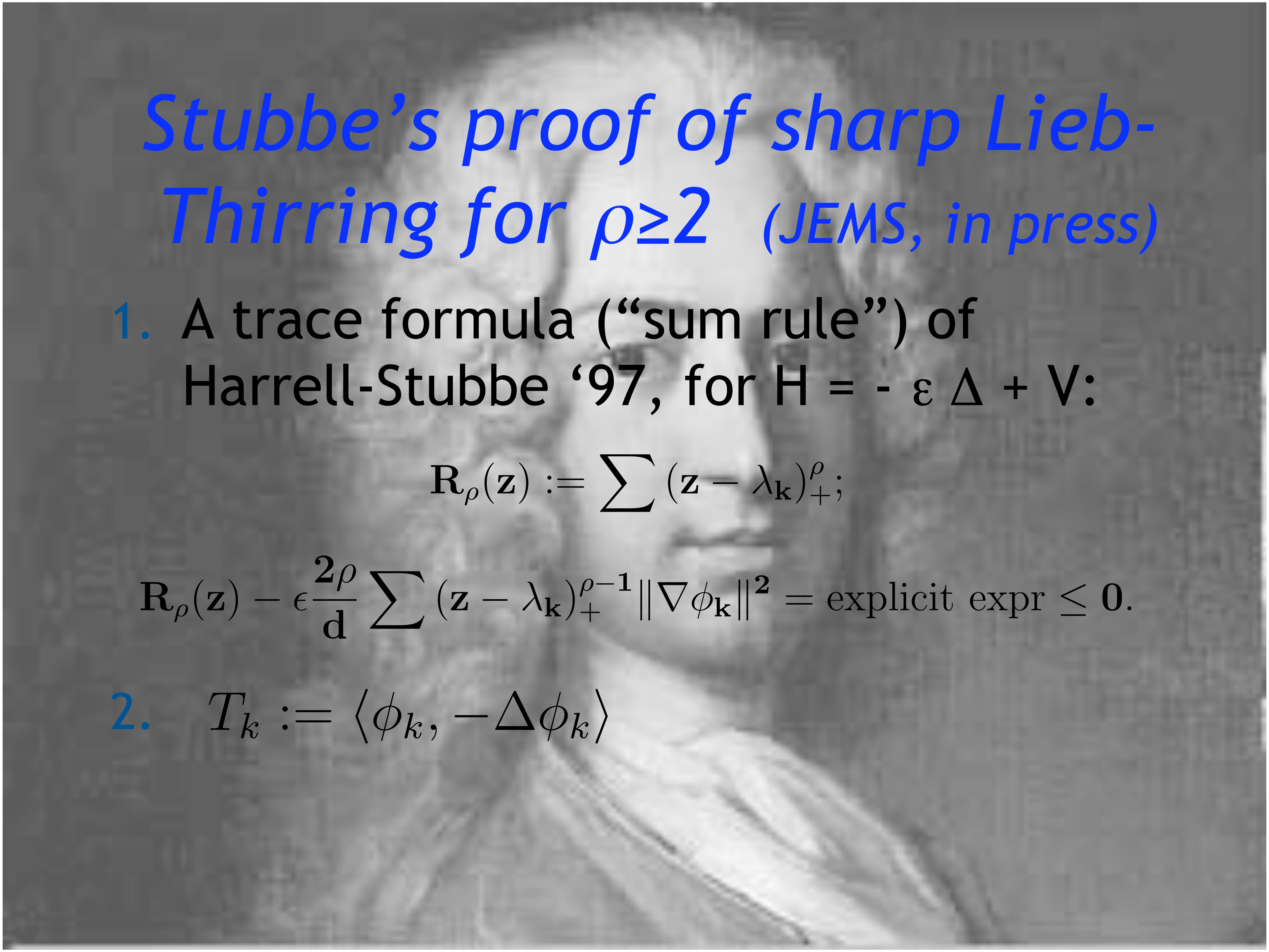


Stubbe's proof of sharp Lieb-Thirring for ρ≥2 (JEMS, in press)

1. A trace formula ("sum rule") of Harrell-Stubbe '97, for H = - ε Δ + V:

$$\mathbf{R}_\rho(\mathbf{z}) := \sum (\mathbf{z} - \lambda_\mathbf{k})_+^\rho;$$

$$\mathbf{R}_\rho(\mathbf{z}) - \epsilon \frac{\mathbf{2}\rho}{\mathbf{d}} \sum (\mathbf{z} - \lambda_\mathbf{k})_+^{\rho - \mathbf{1}} \|\nabla \phi_\mathbf{k}\|^\mathbf{2} = \text{explicit expr} \leq \mathbf{0}.$$



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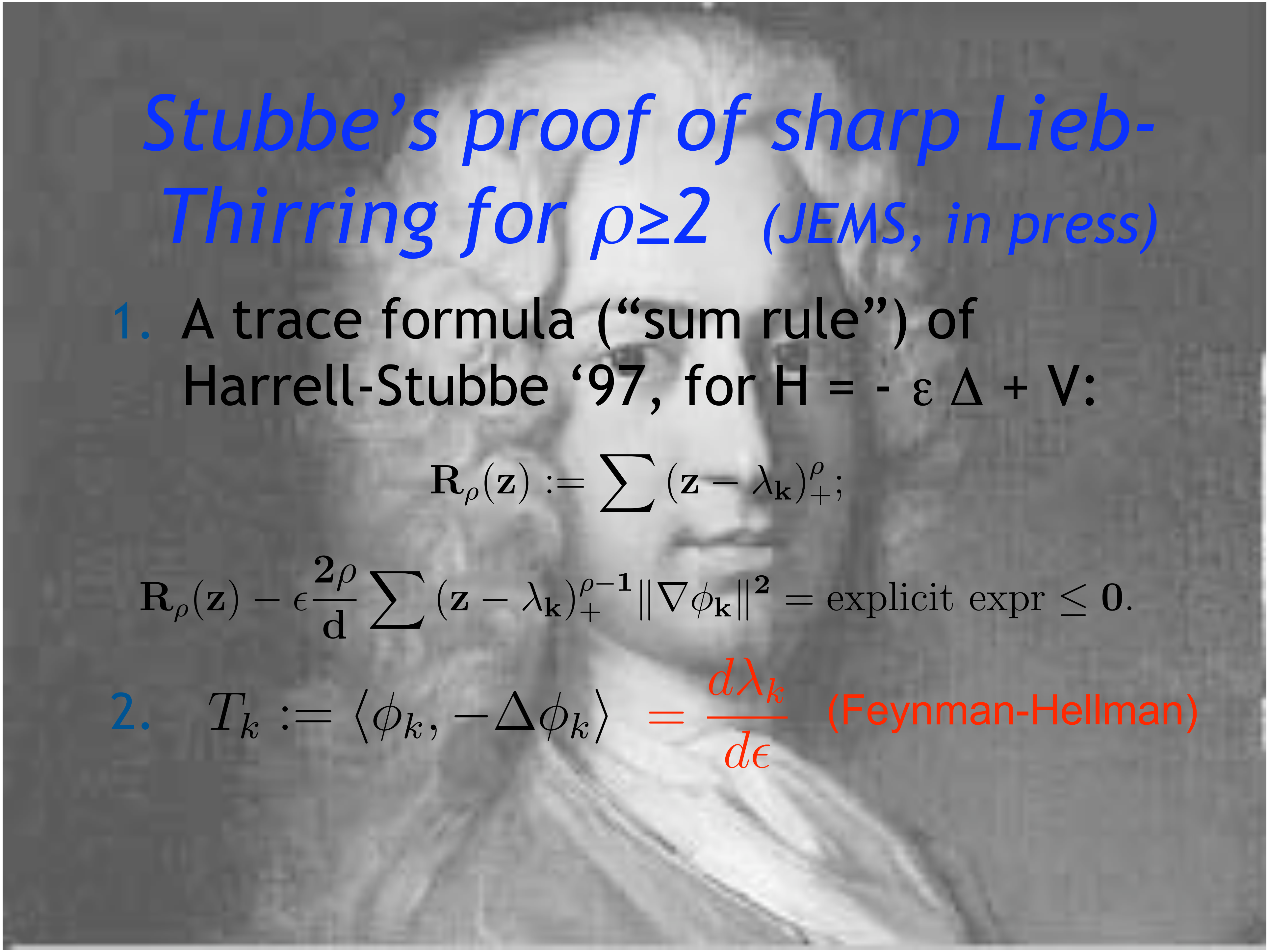
2. $T_k := \langle \phi_k, -\Delta \phi_k \rangle$



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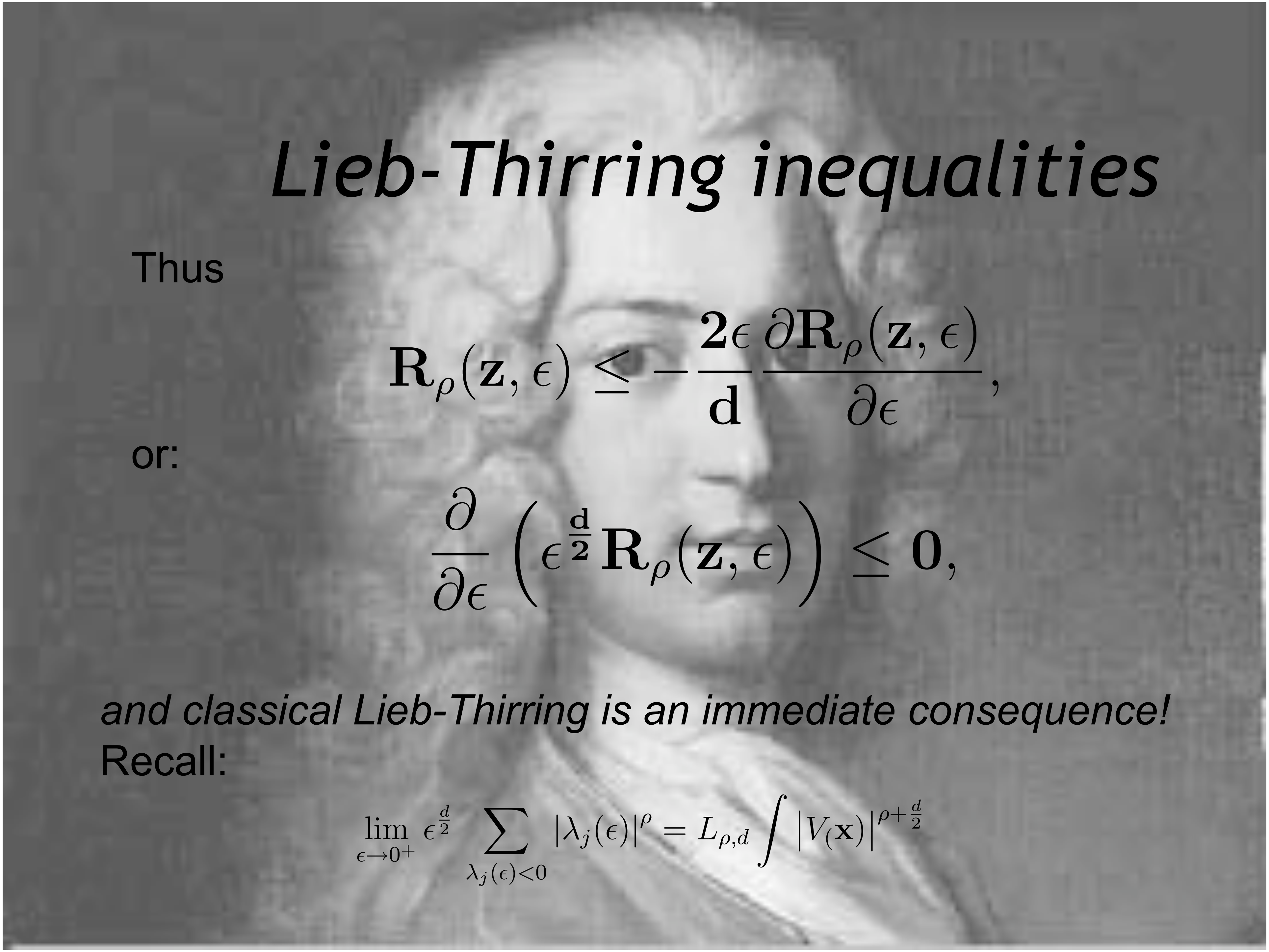
2. $T_k := \langle \phi_k, -\Delta \phi_k \rangle = \dfrac{d\lambda_k}{d\epsilon}$ (Feynman-Hellman)



Lieb-Thirring inequalities

Thus

$$\mathbf{R}_\rho(\mathbf{z},\epsilon) \le -\frac{\mathbf{2}\epsilon}{\mathbf{d}}\frac{\partial \mathbf{R}_\rho(\mathbf{z},\epsilon)}{\partial\epsilon},$$

or:

$$\frac{\partial}{\partial\epsilon}\left(\epsilon^{\frac{\mathbf{d}}{\mathbf{2}}}\mathbf{R}_\rho(\mathbf{z},\epsilon)\right) \le \mathbf{0},$$

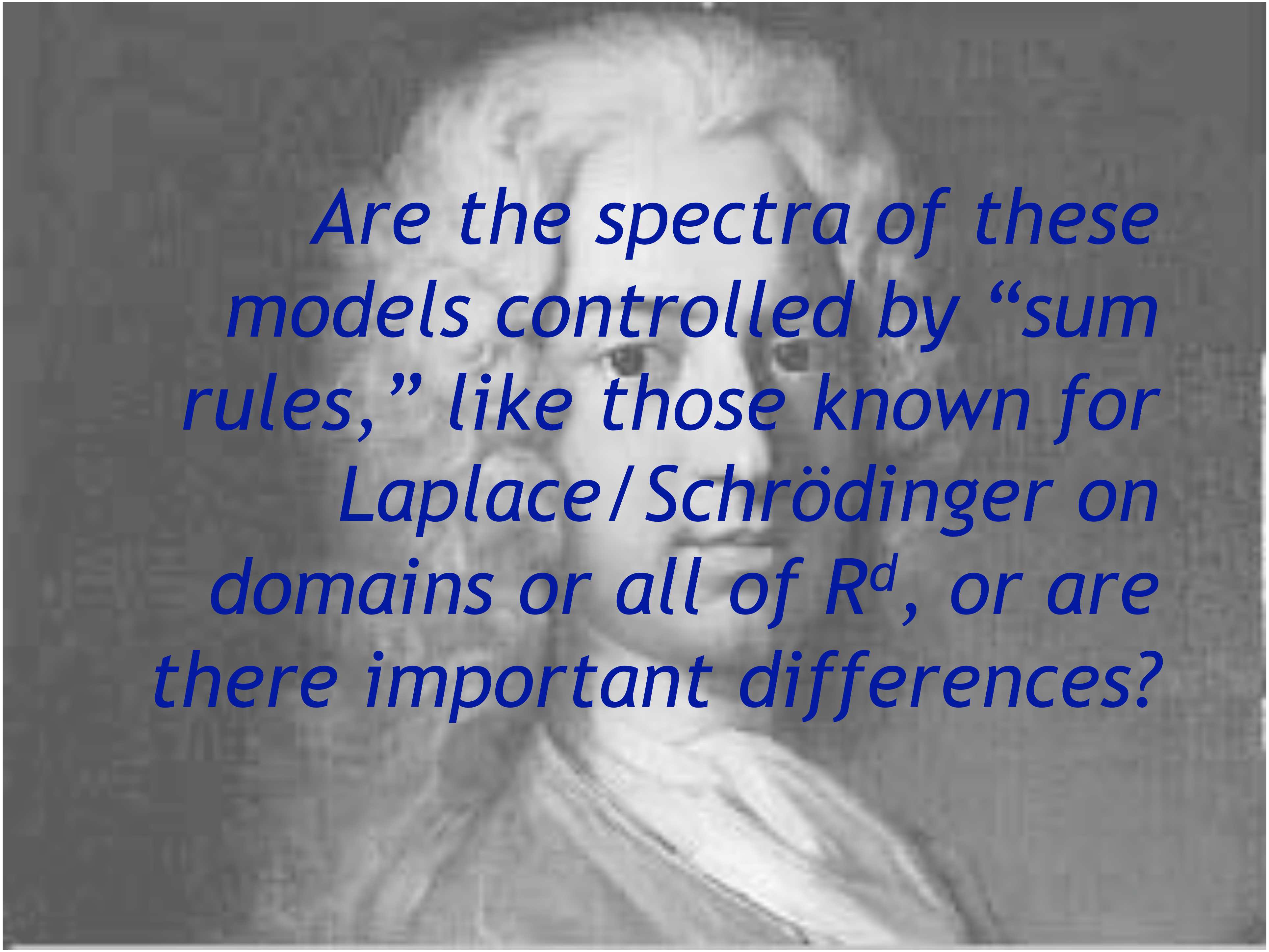
and classical Lieb-Thirring is an immediate consequence!

Recall:

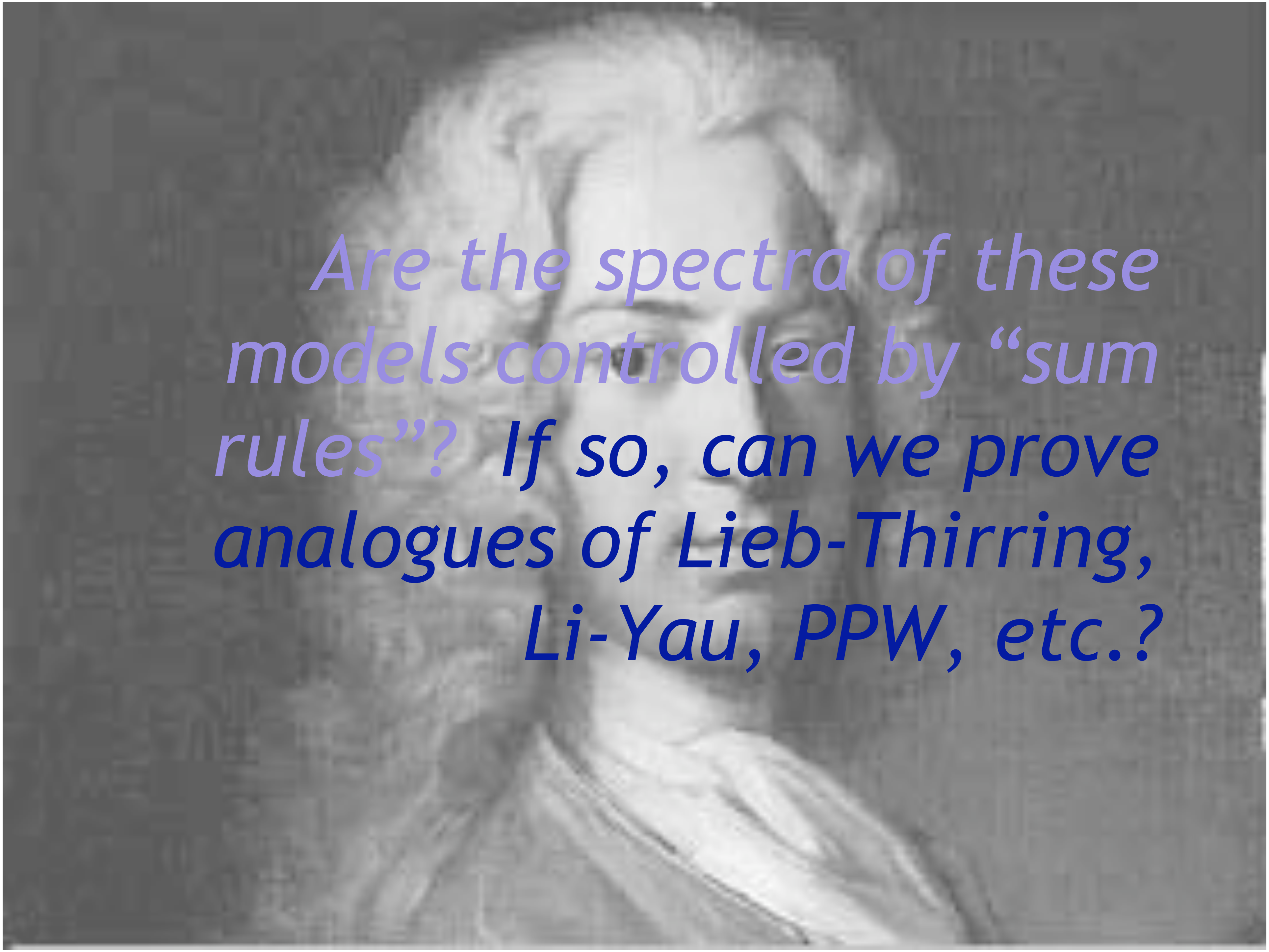
$$\lim_{\epsilon\to 0^+} \epsilon^{\frac{d}{2}} \sum_{\lambda_j(\epsilon)<0} |\lambda_j(\epsilon)|^\rho = L_{\rho,d}\int \left|V_{(}\mathbf{x})\right|^{\rho+\frac{d}{2}}$$

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*.

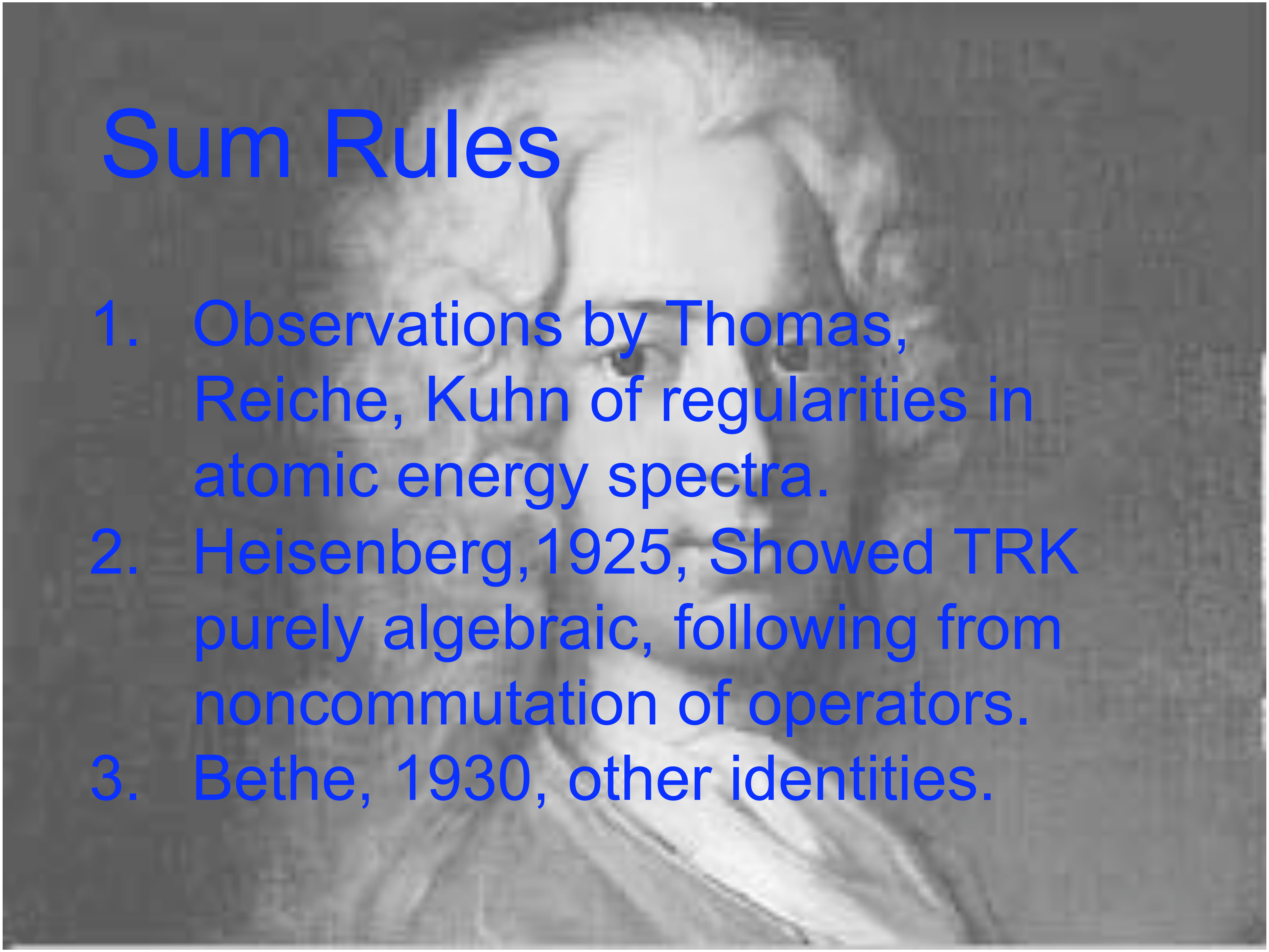


Are the spectra of these models controlled by “sum rules,” like those known for Laplace/Schrödinger on domains or all of R^d, or are there important differences?


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

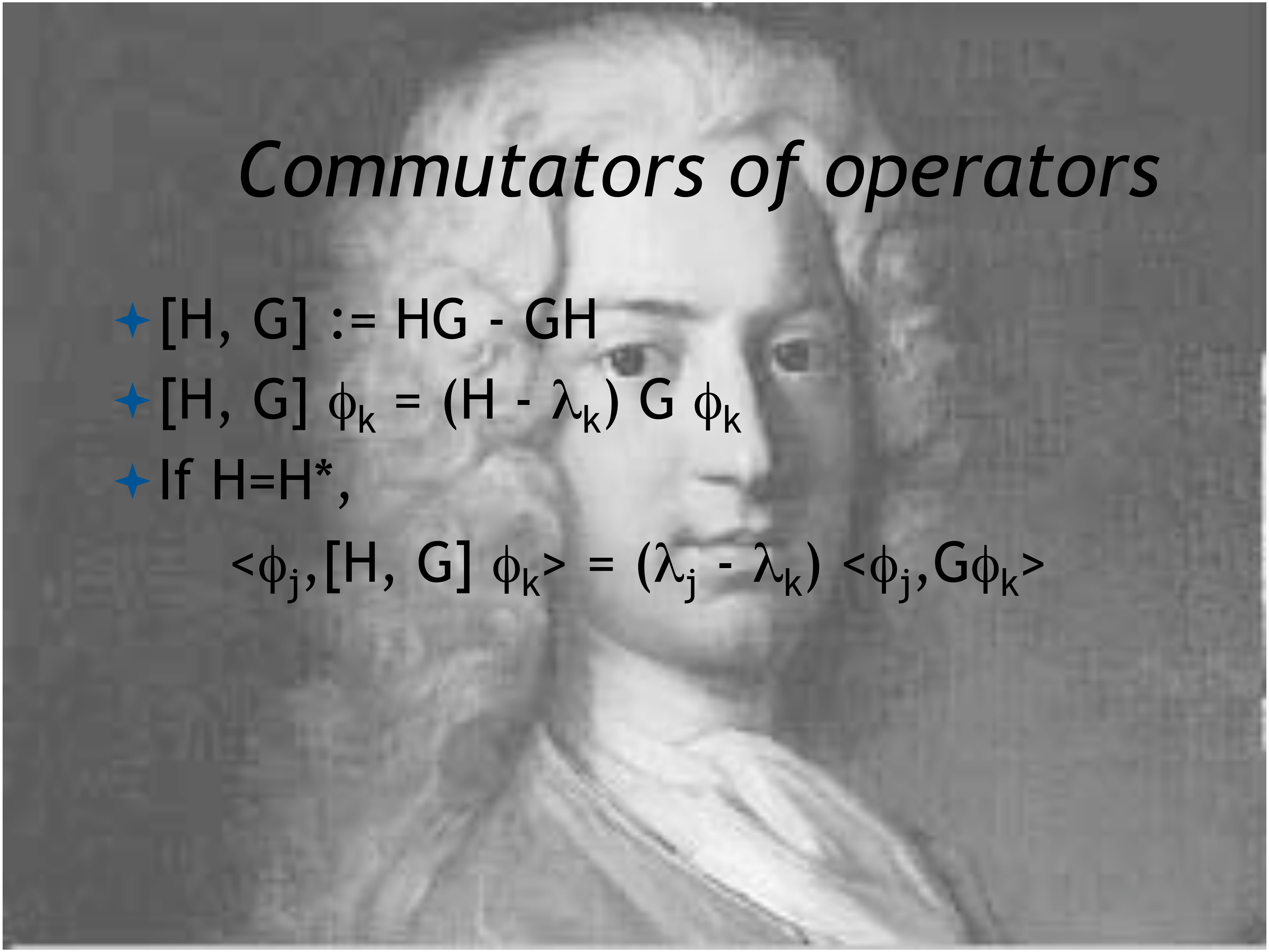
Sum Rules

1. Used by Heisenberg in 1925 to explain regularities in atomic energy spectra



Sum Rules

1. Observations by Thomas, Reiche, Kuhn of regularities in atomic energy spectra.
2. Heisenberg,1925, Showed TRK purely algebraic, following from noncommutation of operators.
3. Bethe, 1930, other identities.



Commutators of operators

- $[H, G] := HG - GH$
- $[H, G]\, \phi_k = (H - \lambda_k)\, G\, \phi_k$
- If $H=H^*$,

$$\langle \phi_j, [H, G]\, \phi_k \rangle = (\lambda_j - \lambda_k)\, \langle \phi_j, G\phi_k \rangle$$

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)

1^{st} and 2^{nd} commutators

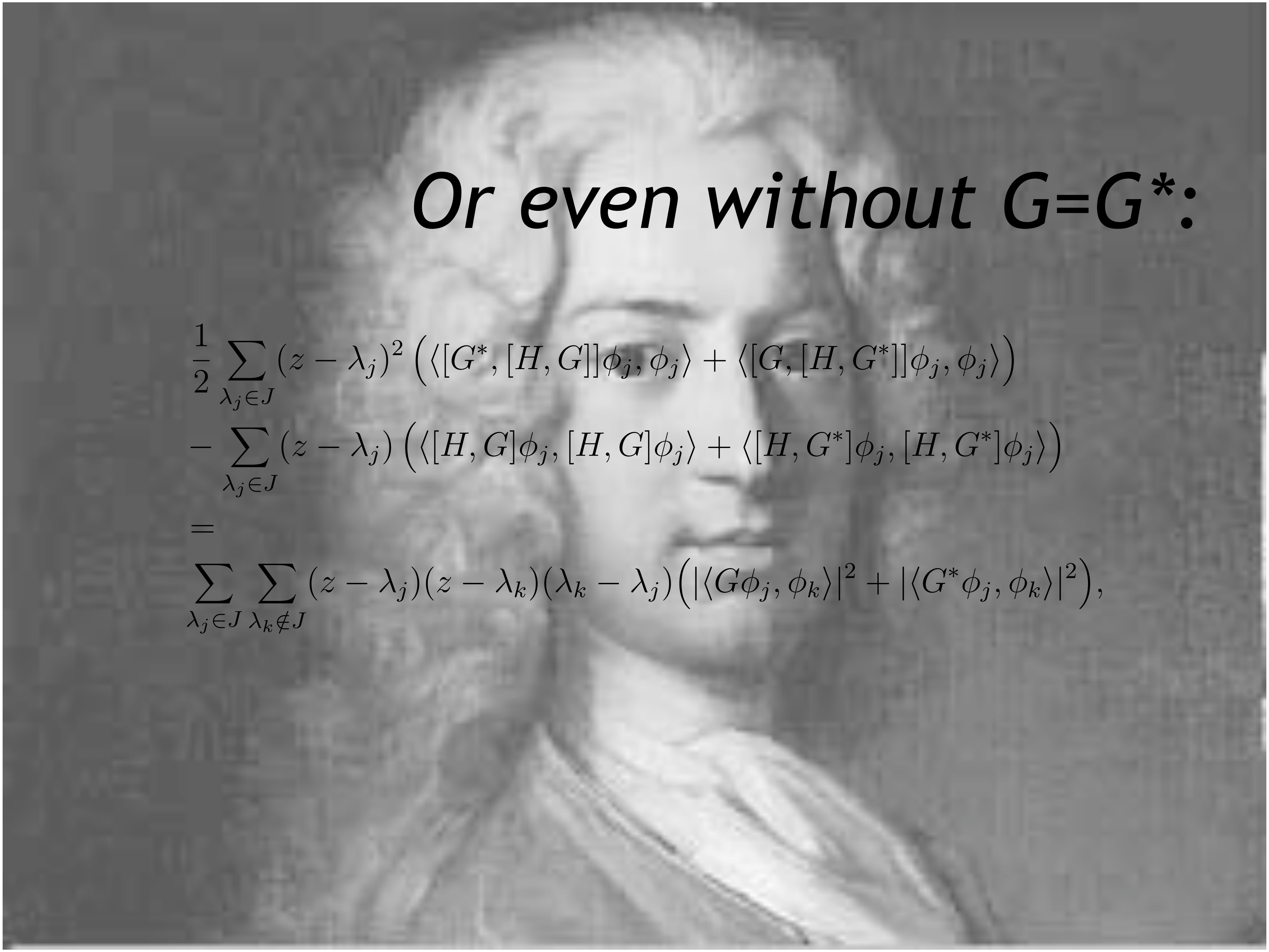
$$\frac{1}{2}\sum_{\lambda_j \in J}(z-\lambda_j)^2\,\langle [G,[H,G]]\phi_j,\phi_j\rangle - \sum_{\lambda_j \in J}(z-\lambda_j)\|[H,G]\phi_j\|^2$$

$$=$$

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

Harrell-Stubbe TAMS 1997

The only assumptions are that H and G are self-adjoint, and that the eigenfunctions are a complete orthonormal sequence. (If continuous spectrum, need a spectral integral on right.)



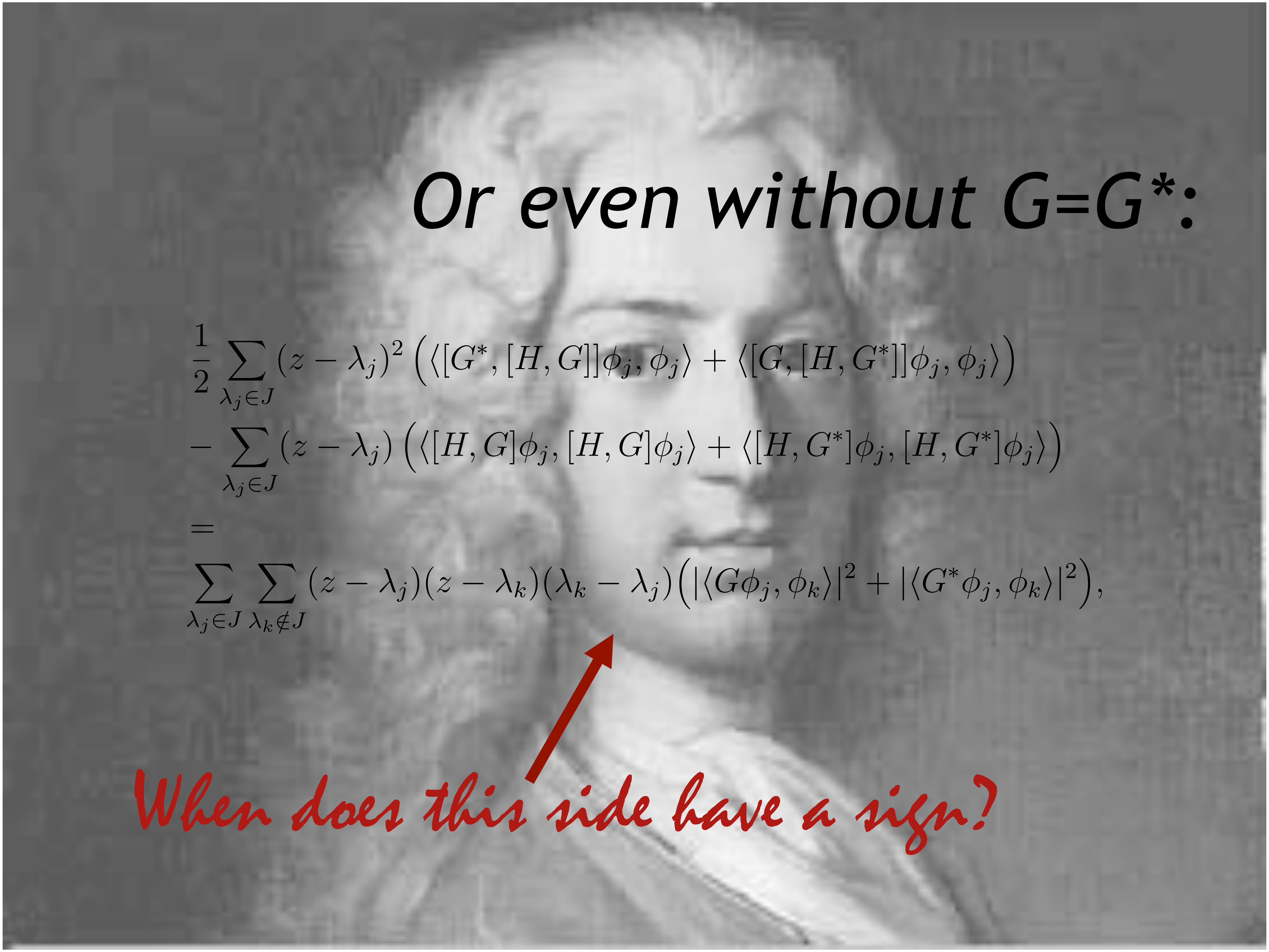
Or even without G=G:*

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

$$
-\sum_{\lambda_j\in J}(z-\lambda_j)\Big(\langle[H,G]\phi_j,[H,G]\phi_j\rangle+\langle[H,G^*]\phi_j,[H,G^*]\phi_j\rangle\Big)
$$

$$
=
$$

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



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\begin{aligned}
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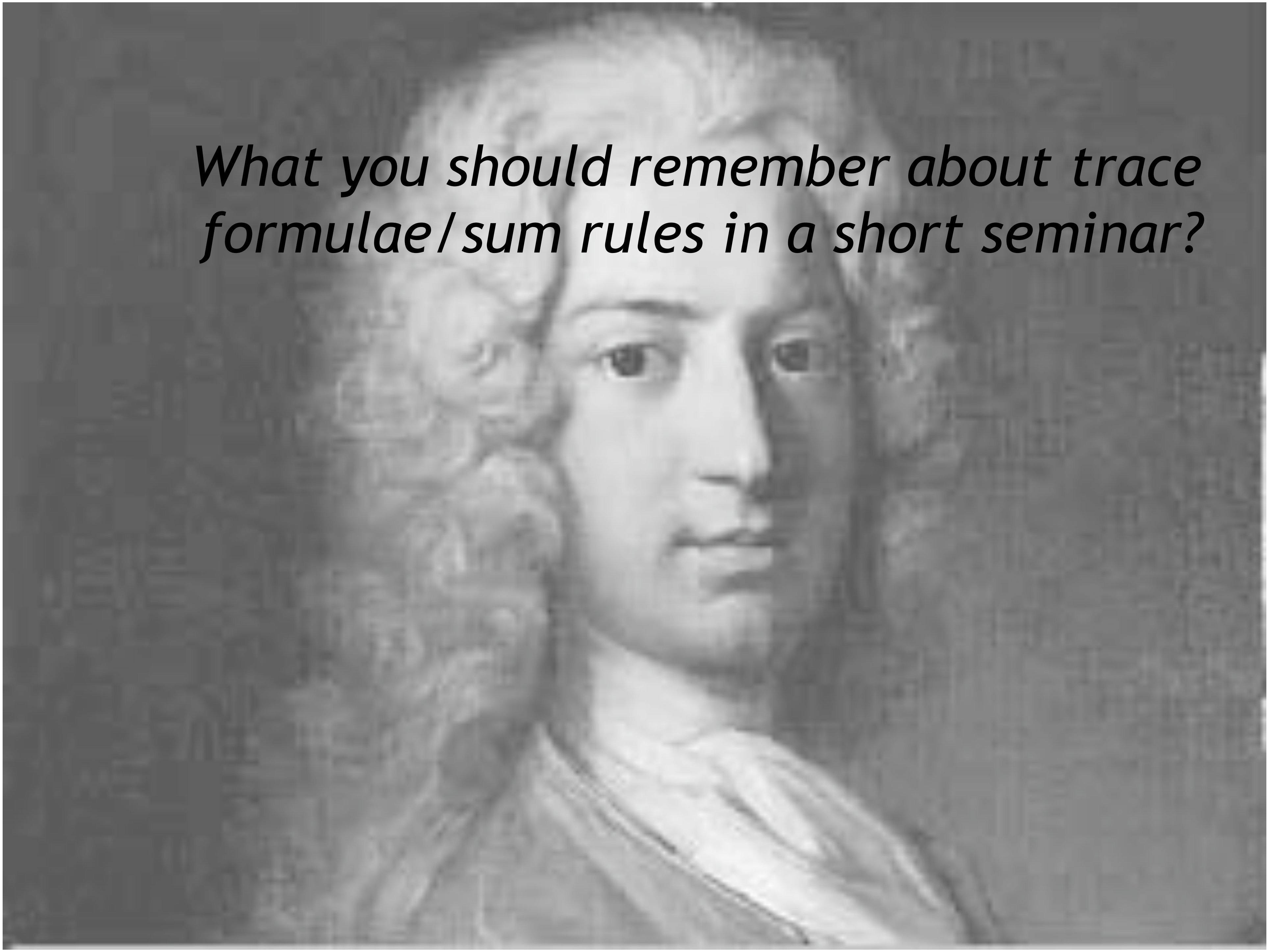
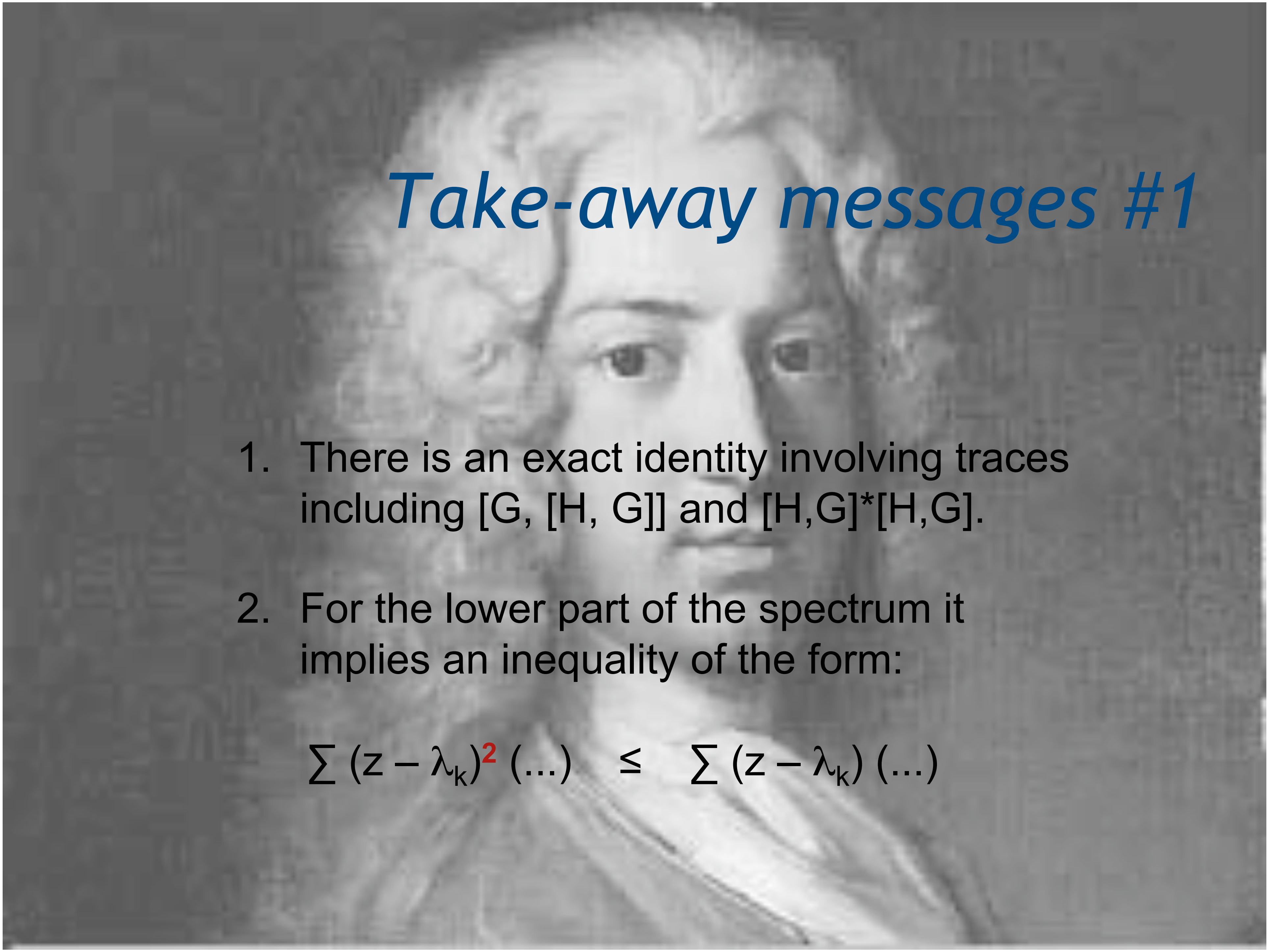
&-\sum_{\lambda_j\in J}(z-\lambda_j)\Big(\langle[H,G]\phi_j,[H,G]\phi_j\rangle+\langle[H,G^*]\phi_j,[H,G^*]\phi_j\rangle\Big)\\
&=\\
&\sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\Big(|\langle G\phi_j,\phi_k\rangle|^2+|\langle G^*\phi_j,\phi_k\rangle|^2\Big),
\end{aligned}
$$

When does this side have a sign?



What you should remember about trace formulae/sum rules in a short seminar?

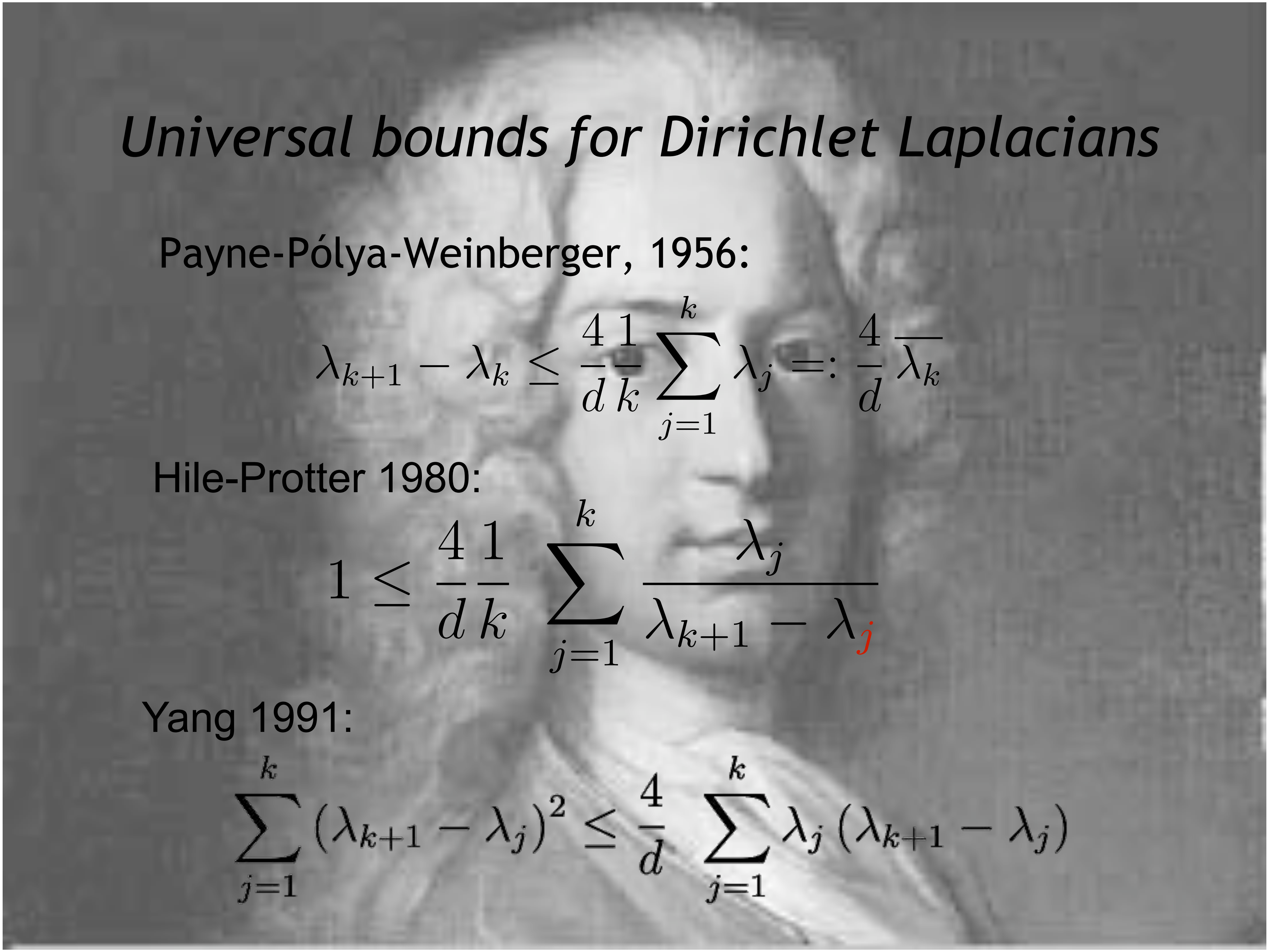


Take-away messages #1

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:

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



Universal bounds for Dirichlet Laplacians

Payne-Pólya-Weinberger, 1956:

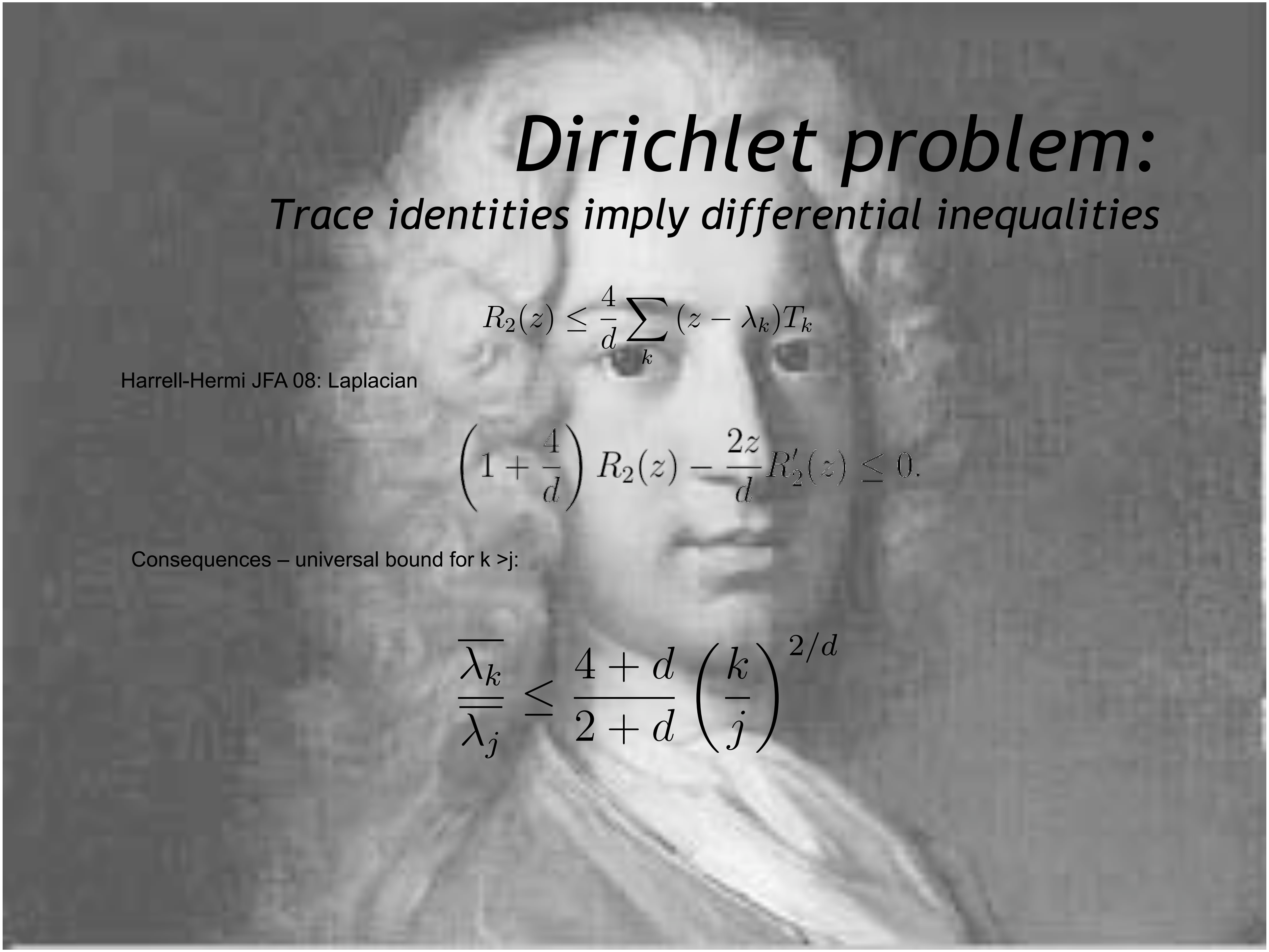
$$\lambda_{k+1} - \lambda_k \leq \frac{4}{d}\frac{1}{k}\sum_{j=1}^{k} \lambda_j =: \frac{4}{d}\,\overline{\lambda_k}$$

Hile-Protter 1980:

$$1 \leq \frac{4}{d}\frac{1}{k} \sum_{j=1}^{k} \frac{\lambda_j}{\lambda_{k+1} - \lambda_j}$$

Yang 1991:

$$\sum_{j=1}^{k} (\lambda_{k+1} - \lambda_j)^2 \leq \frac{4}{d} \sum_{j=1}^{k} \lambda_j \,(\lambda_{k+1} - \lambda_j)$$



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:

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

Dirichlet problem:

Trace identities imply differential inequalities

$$R_2(z) \le \frac{4}{d}\sum_k (z-\lambda_k)\cancel{T_k}\,(\lambda_k - z + z)$$

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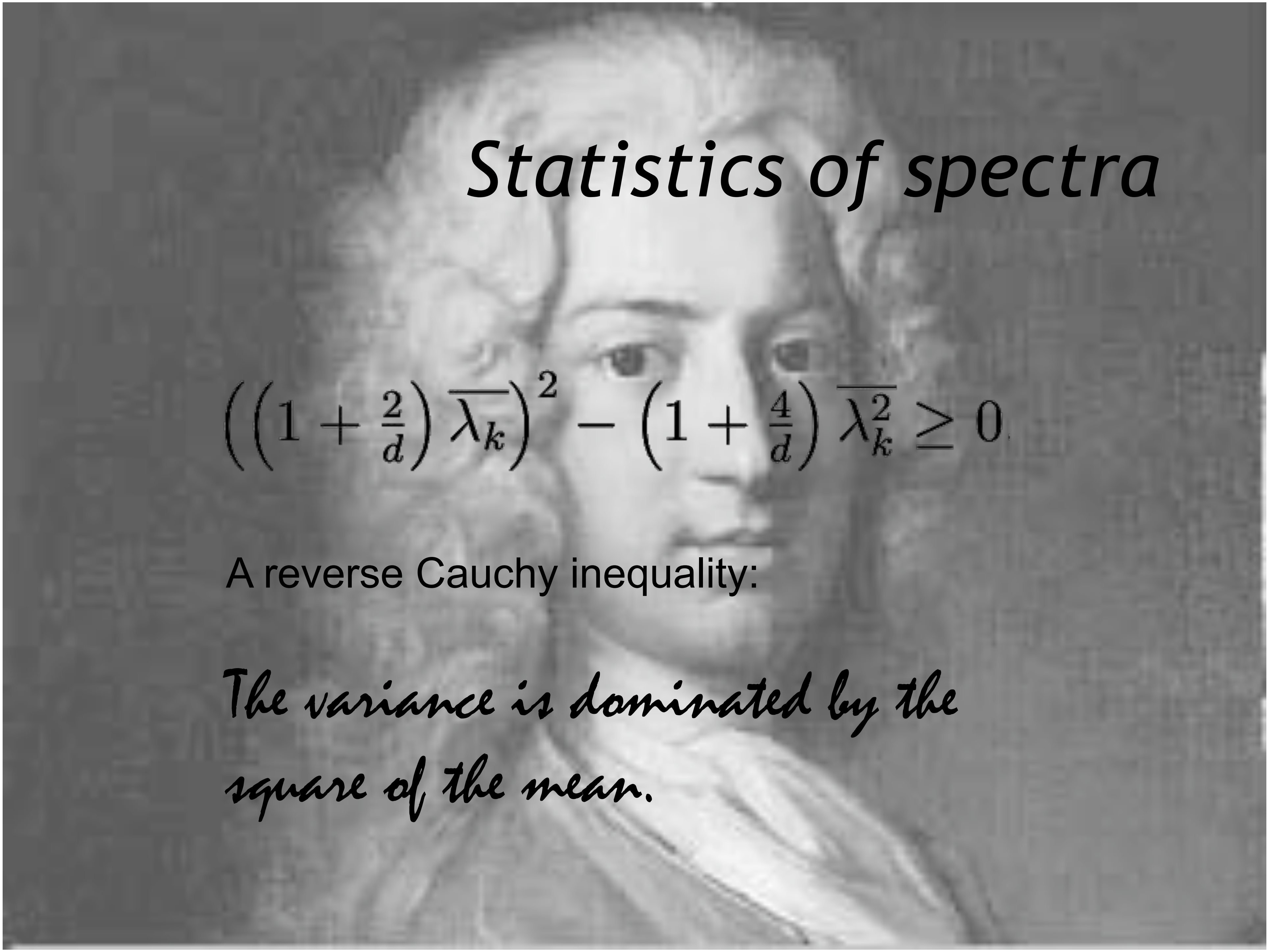
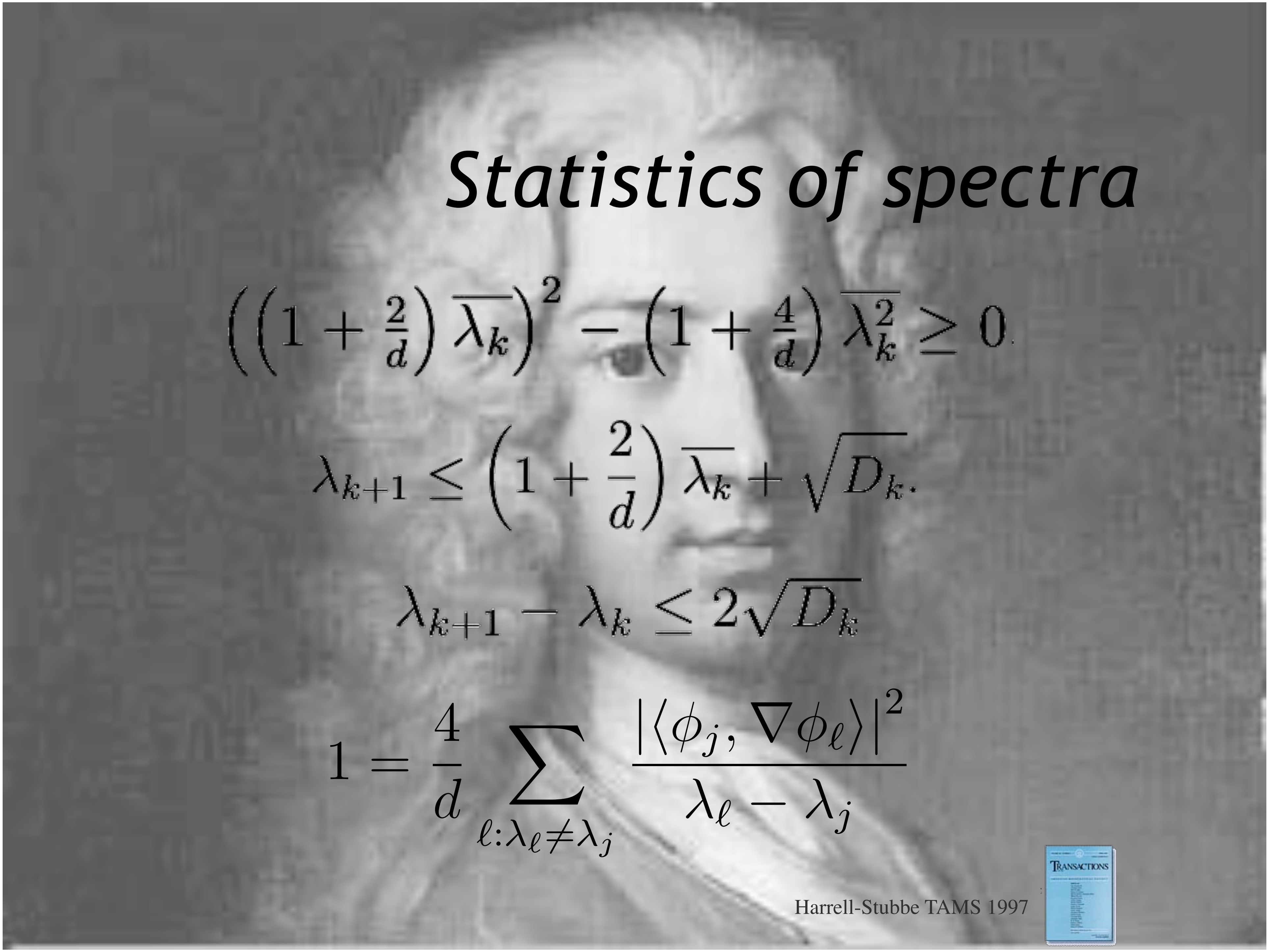


Statistics of spectra

$$\left(\left(1+\frac{2}{d}\right)\overline{\lambda_k}\right)^2-\left(1+\frac{4}{d}\right)\overline{\lambda_k^2}\geq 0$$

A reverse Cauchy inequality:

The variance is dominated by the square of the mean.



Statistics of spectra

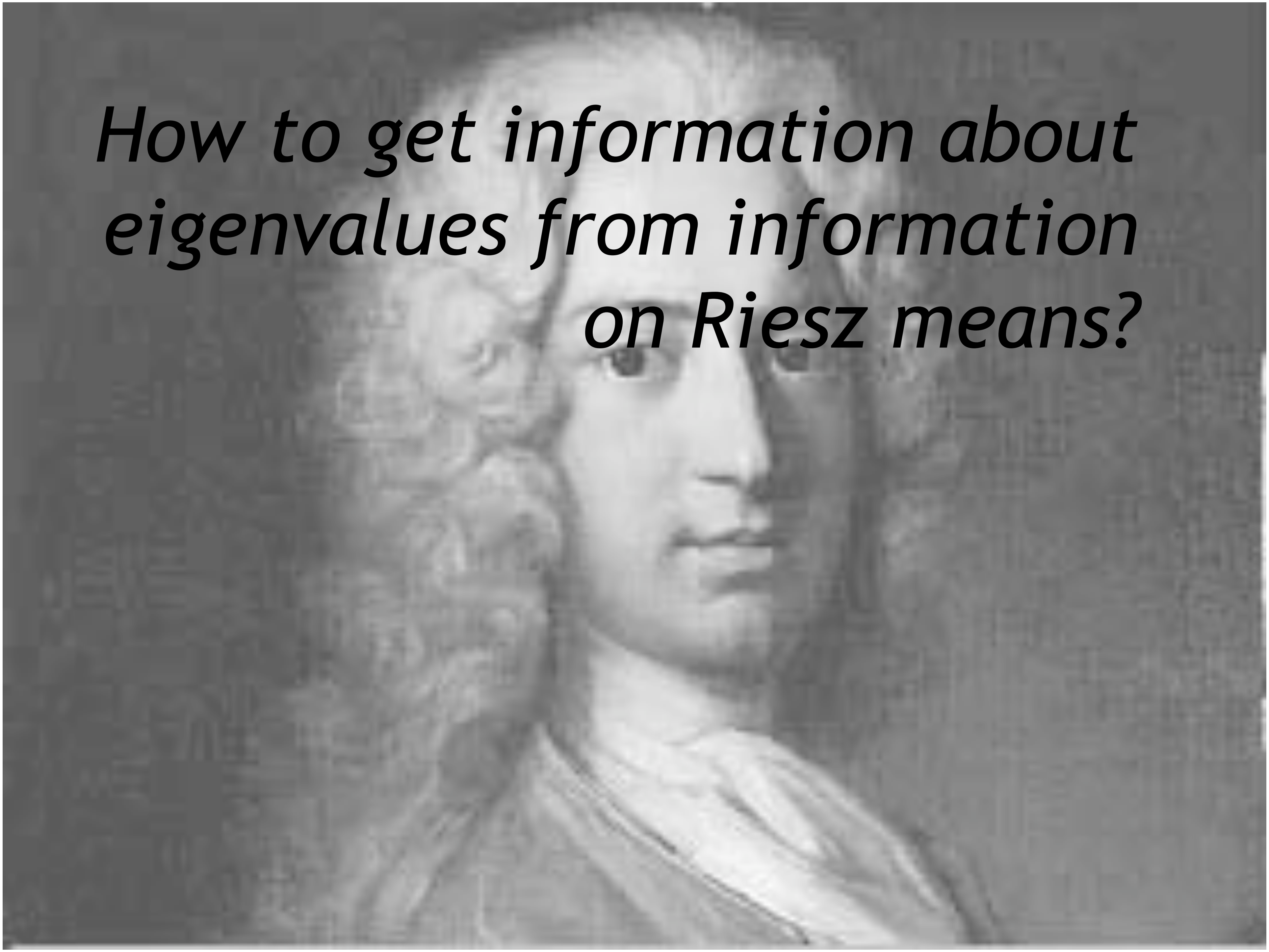
$$\left(\left(1+\frac{2}{d}\right)\overline{\lambda_k}\right)^2-\left(1+\frac{4}{d}\right)\overline{\lambda_k^2}\geq 0.$$

$$\lambda_{k+1}\leq\left(1+\frac{2}{d}\right)\overline{\lambda_k}+\sqrt{D_k}.$$

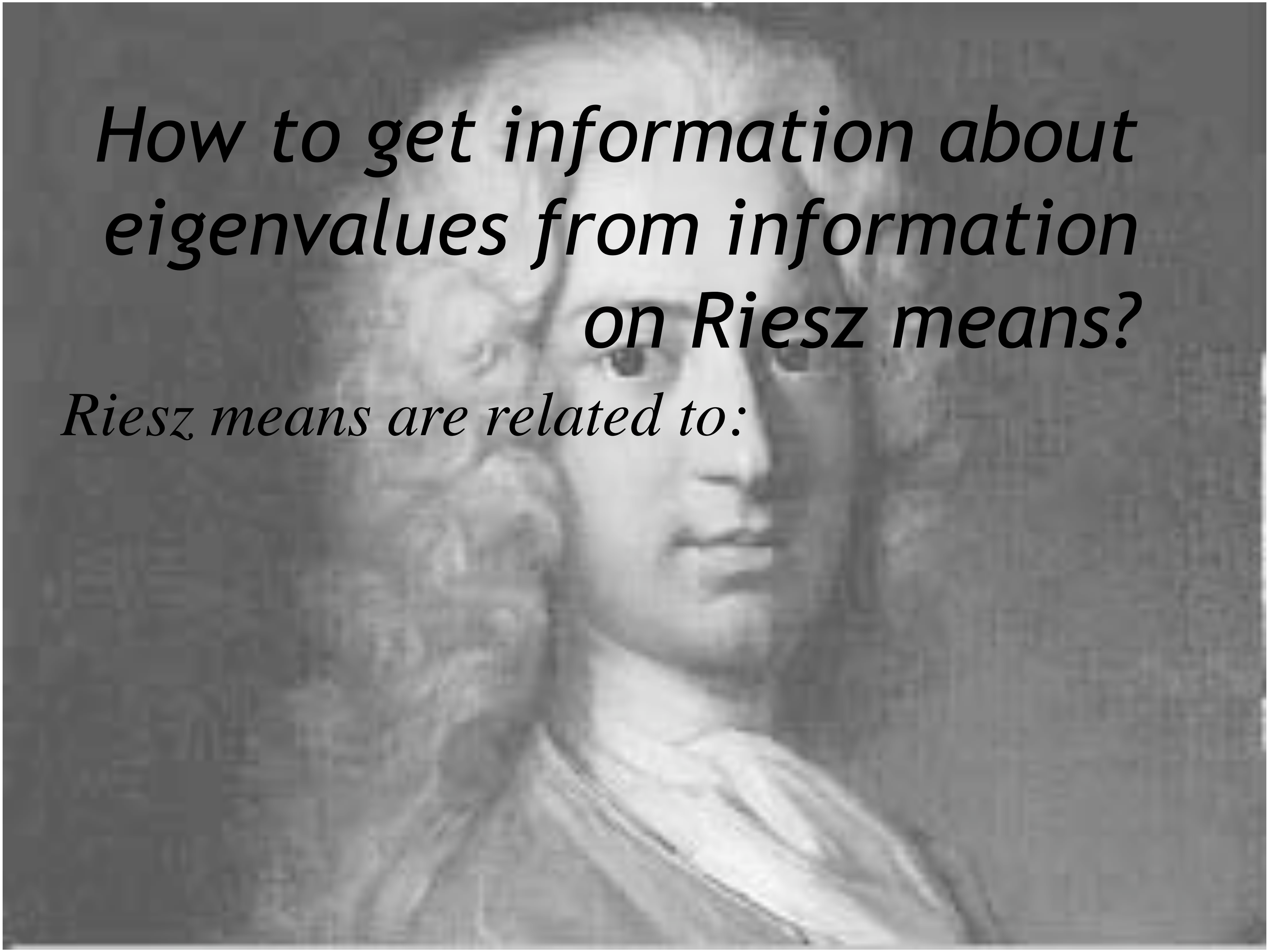
$$\lambda_{k+1}-\lambda_k\leq 2\sqrt{D_k}$$

$$1=\frac{4}{d}\sum_{\ell:\lambda_\ell\neq\lambda_j}\frac{\left|\langle\phi_j,\nabla\phi_\ell\rangle\right|^2}{\lambda_\ell-\lambda_j}$$

Harrell-Stubbe TAMS 1997

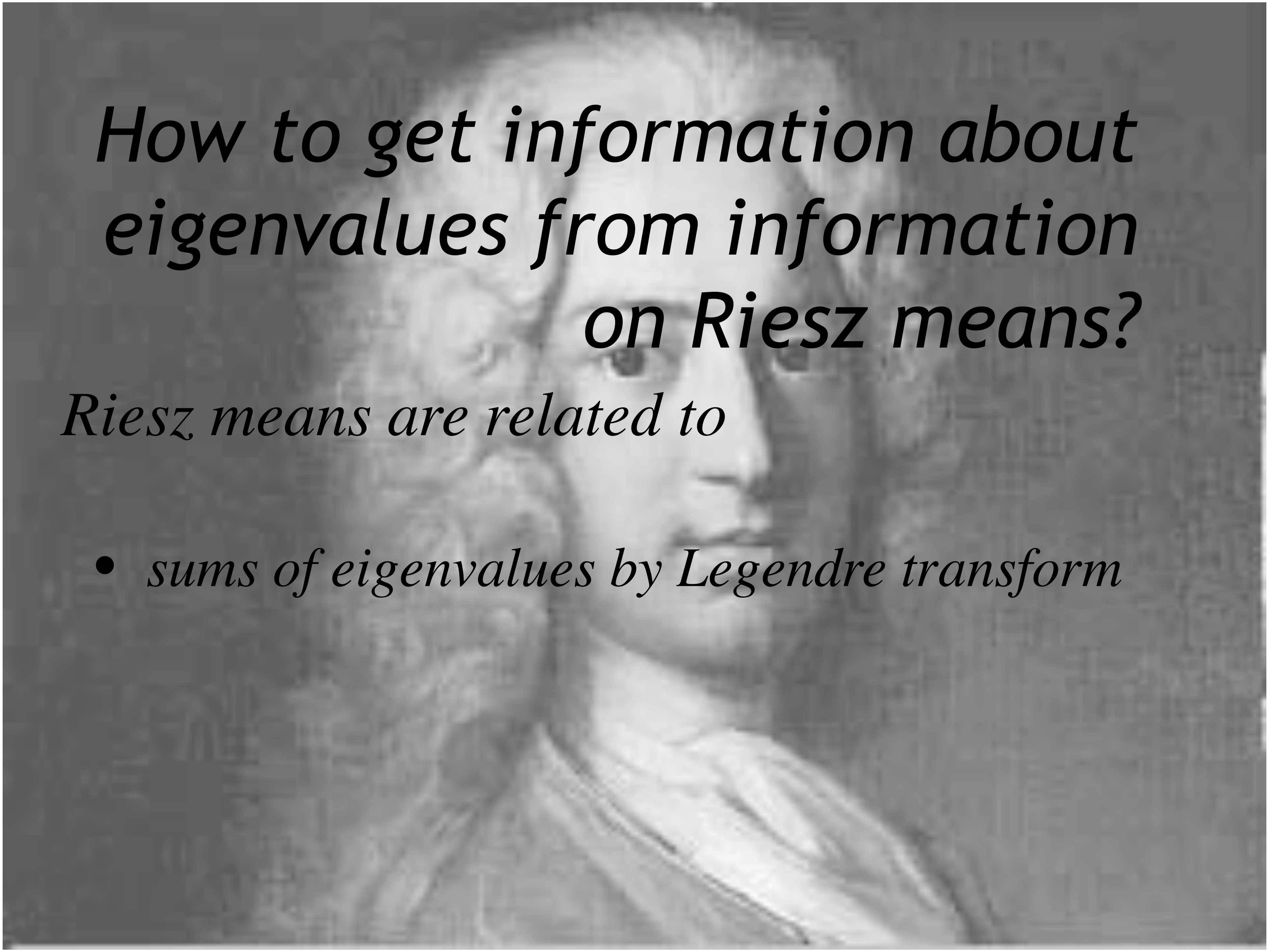


How to get information about eigenvalues from information on Riesz means?



How to get information about eigenvalues from information on Riesz means?

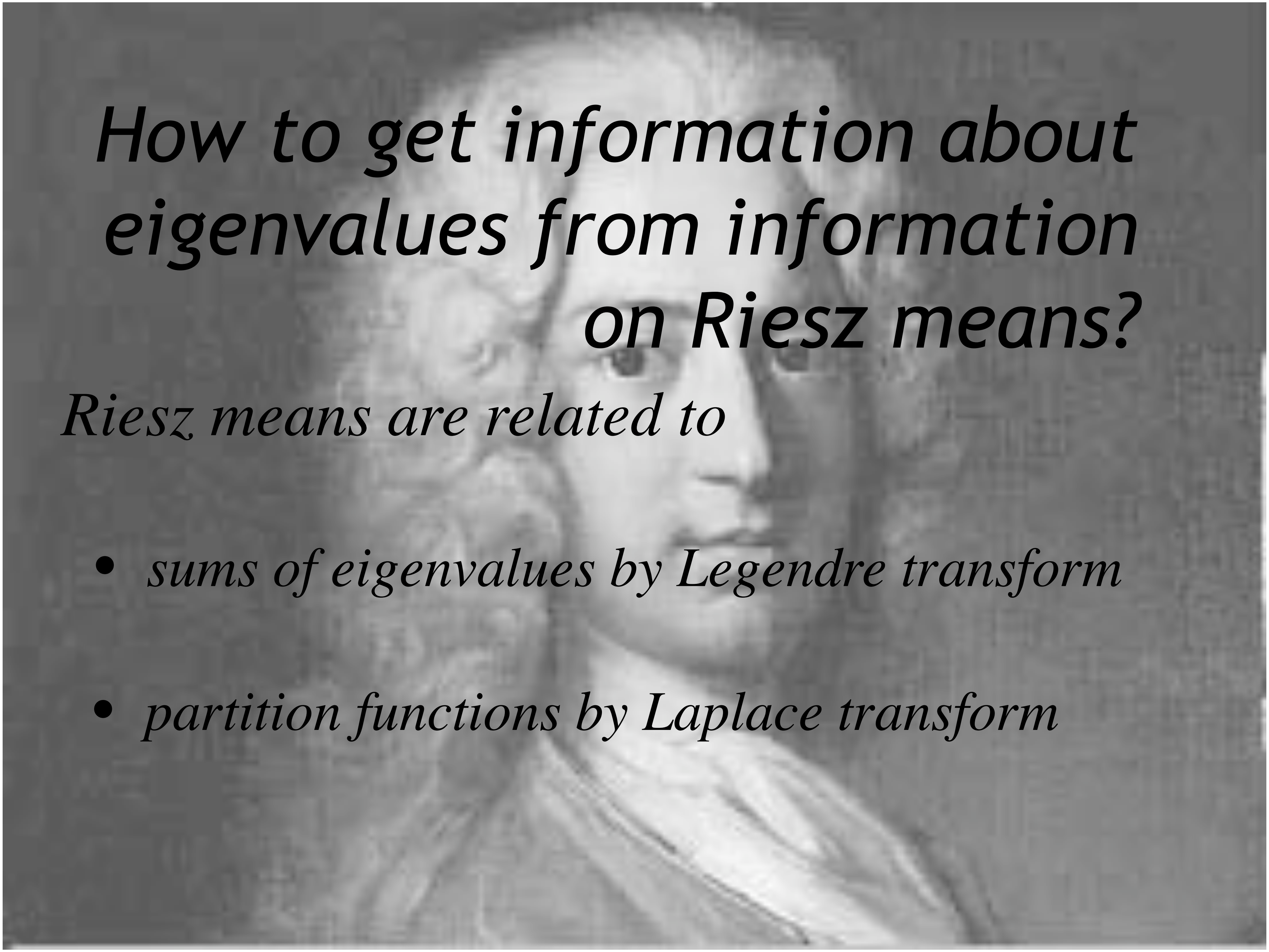
Riesz means are related to:



How to get information about eigenvalues from information on Riesz means?

Riesz means are related to

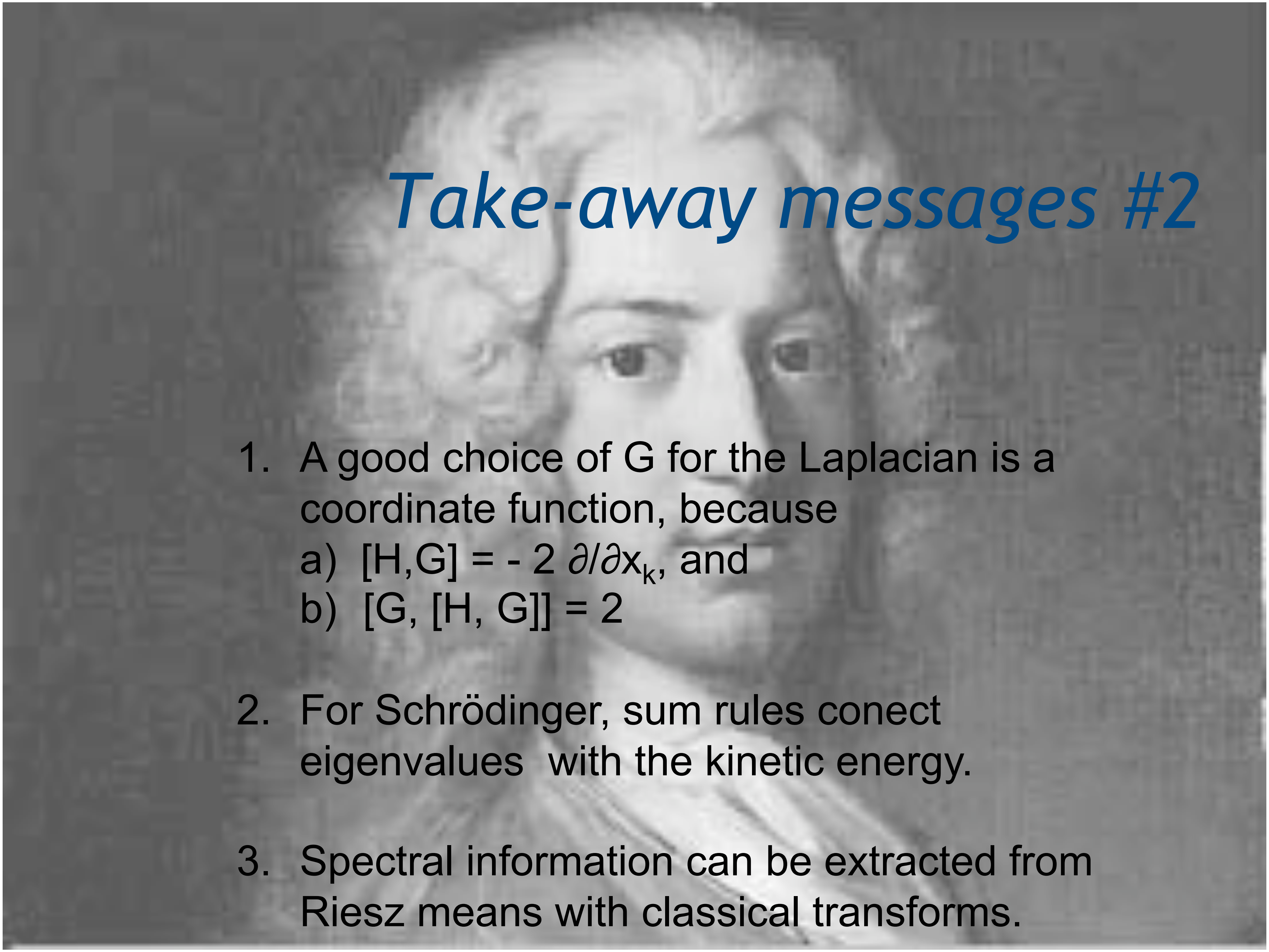
- *sums of eigenvalues by Legendre transform*



How to get information about eigenvalues from information on Riesz means?

Riesz means are related to

- *sums of eigenvalues by Legendre transform*
- *partition functions by Laplace transform*



Take-away messages #2

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.

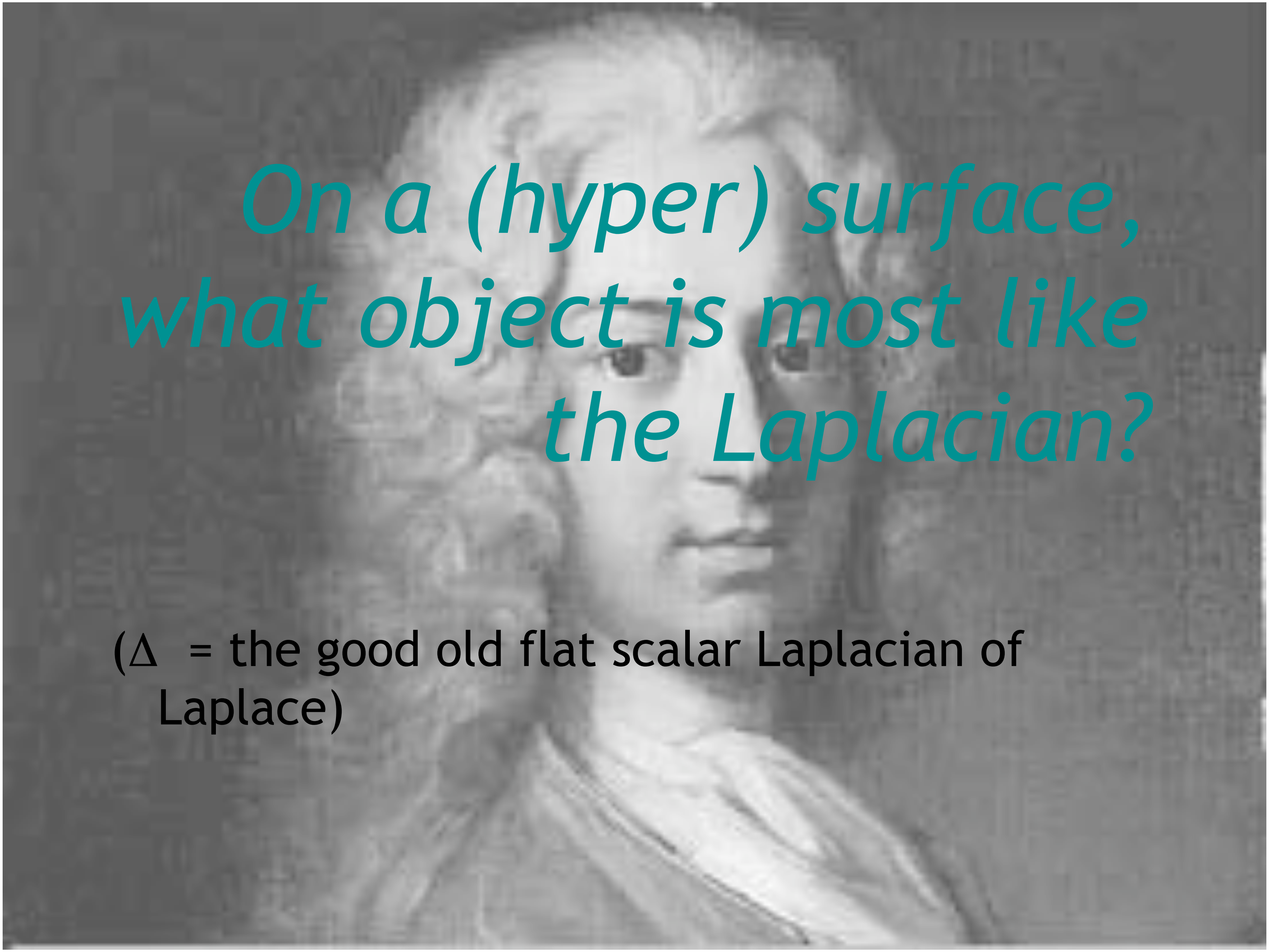
3. Spectral information can be extracted from Riesz means with classical transforms.

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*.

In each of the four models there are new features in the trace inequality.

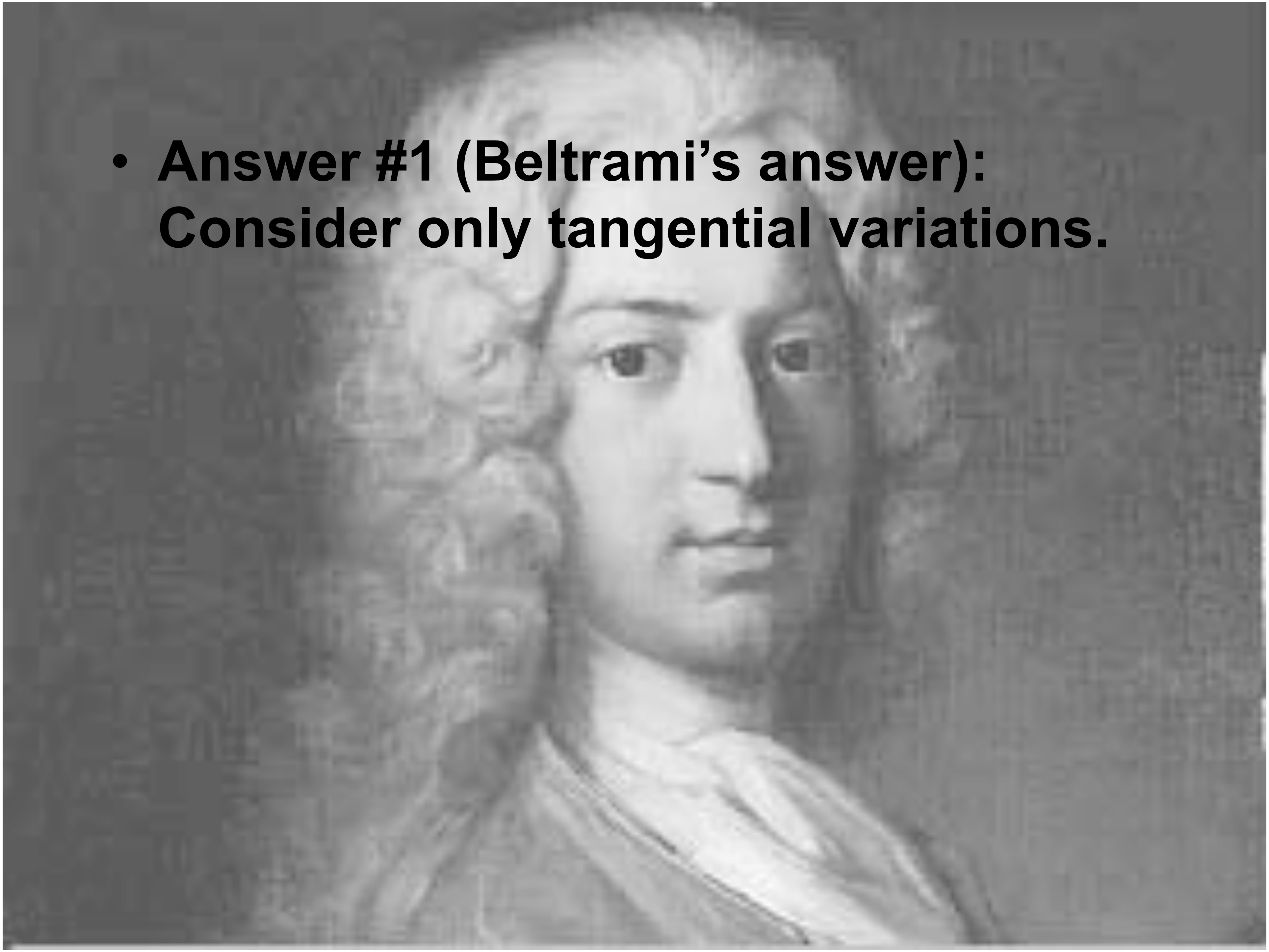
1. Schrödinger operators on curves and surfaces. *Explicit curvature terms.*
2. Periodic Schrödinger operators. *Geometry of the dual lattice.*
3. Quantum graphs. *Topology*
4. Relativistic Hamiltonians. *First-order ΨDO rather than second-order.*



On a (hyper) surface, what object is most like the Laplacian?

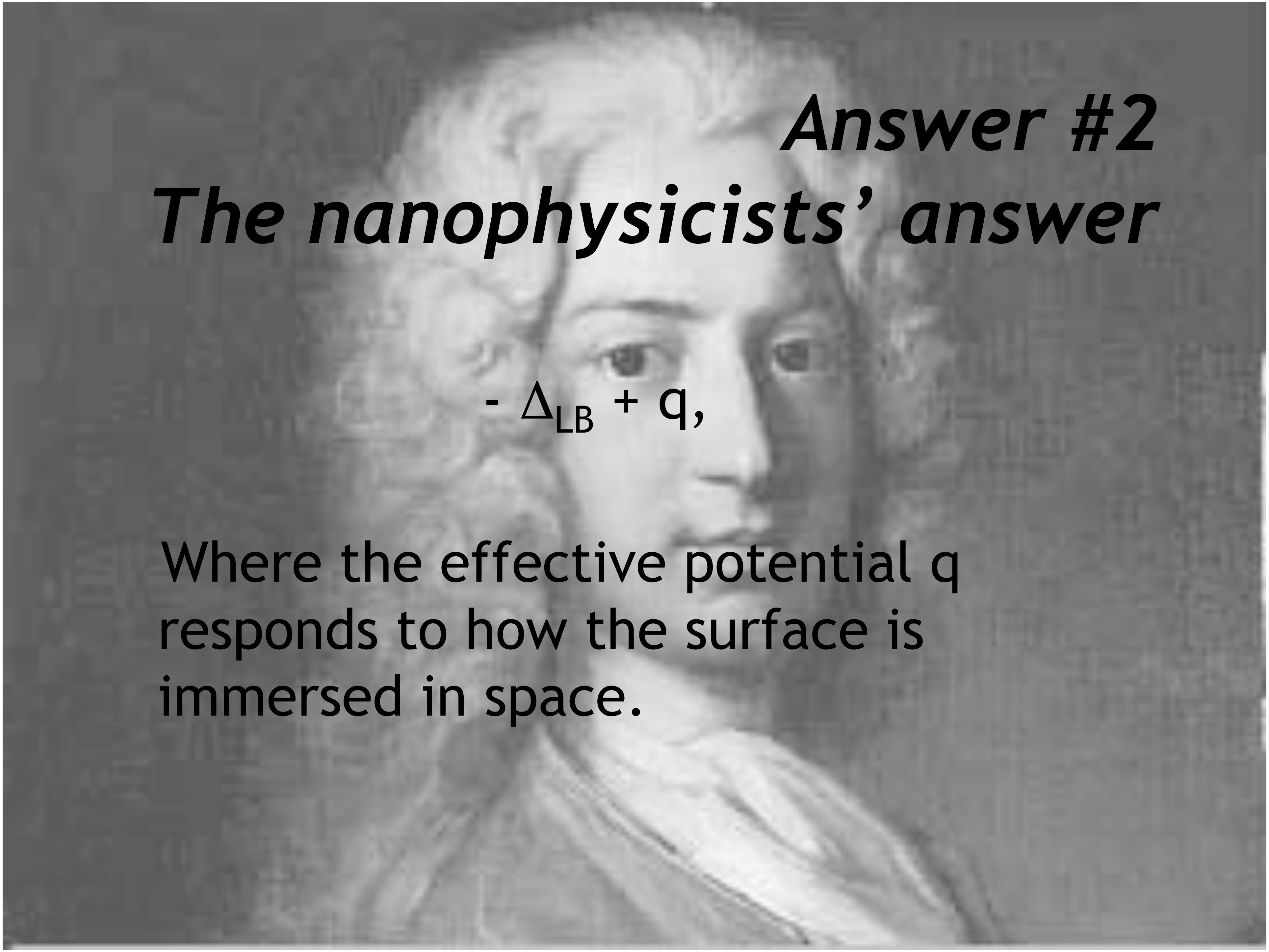
(Δ = the good old flat scalar Laplacian of Laplace)

- **Answer #1 (Beltrami’s answer): Consider only tangential variations.**



Difficulty:

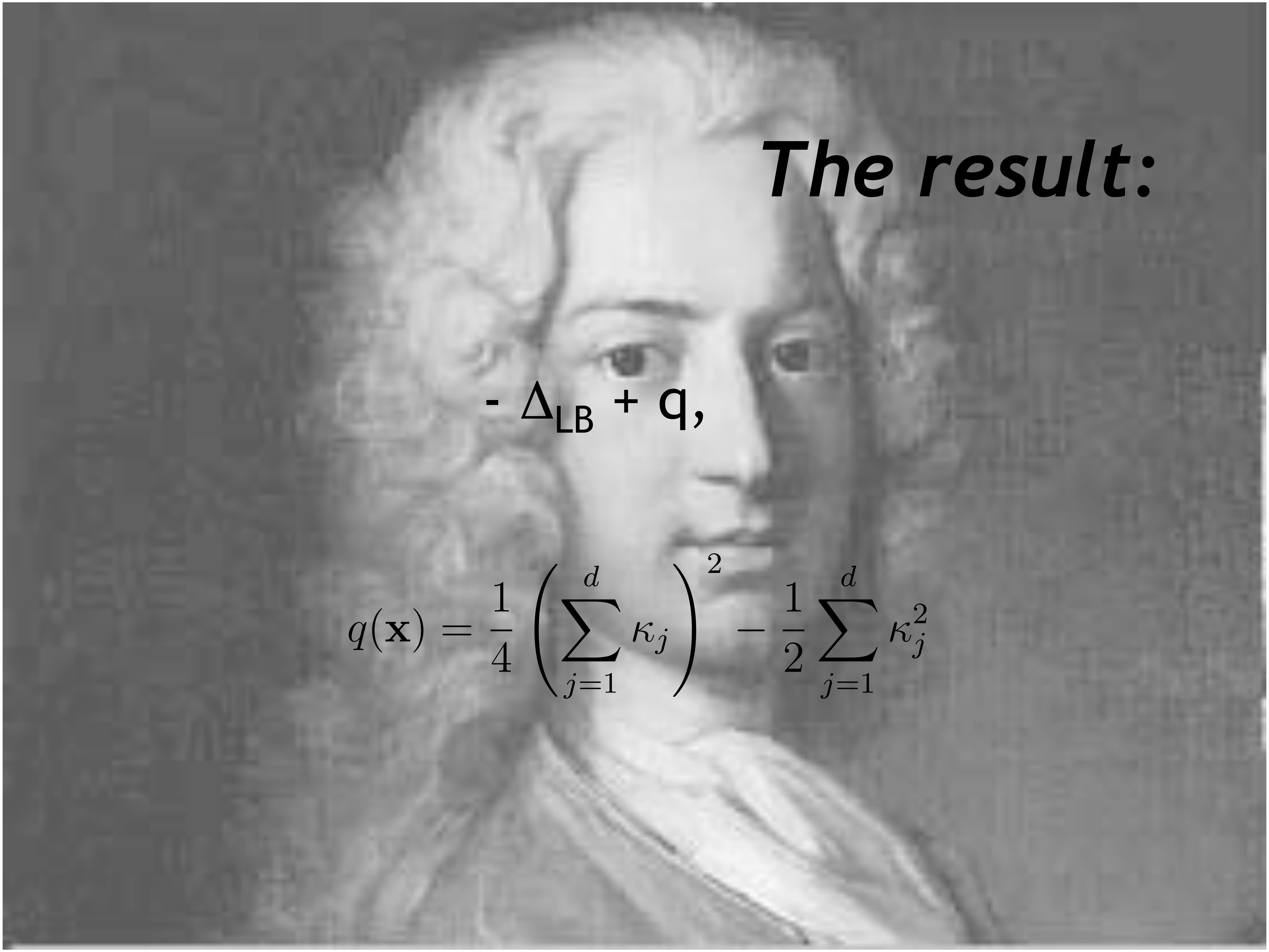
- **The Laplace-Beltrami operator is an intrinsic object, and as such is unaware that the surface is immersed!**



Answer #2
The nanophysicists' answer

$$- \Delta_{LB} + q,$$

Where the effective potential q responds to how the surface is immersed in space.



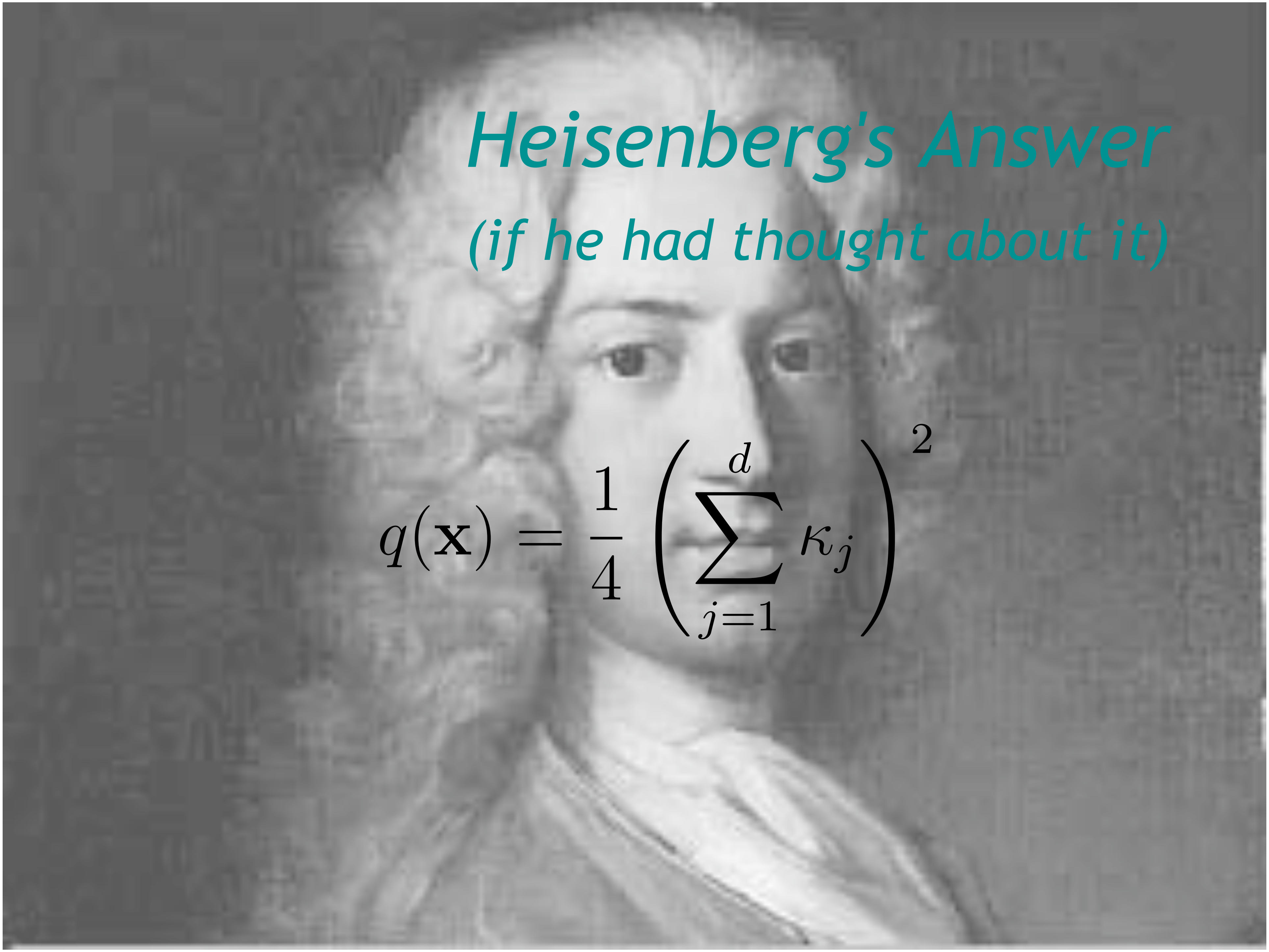
The result:

$-\Delta_{LB} + q,$

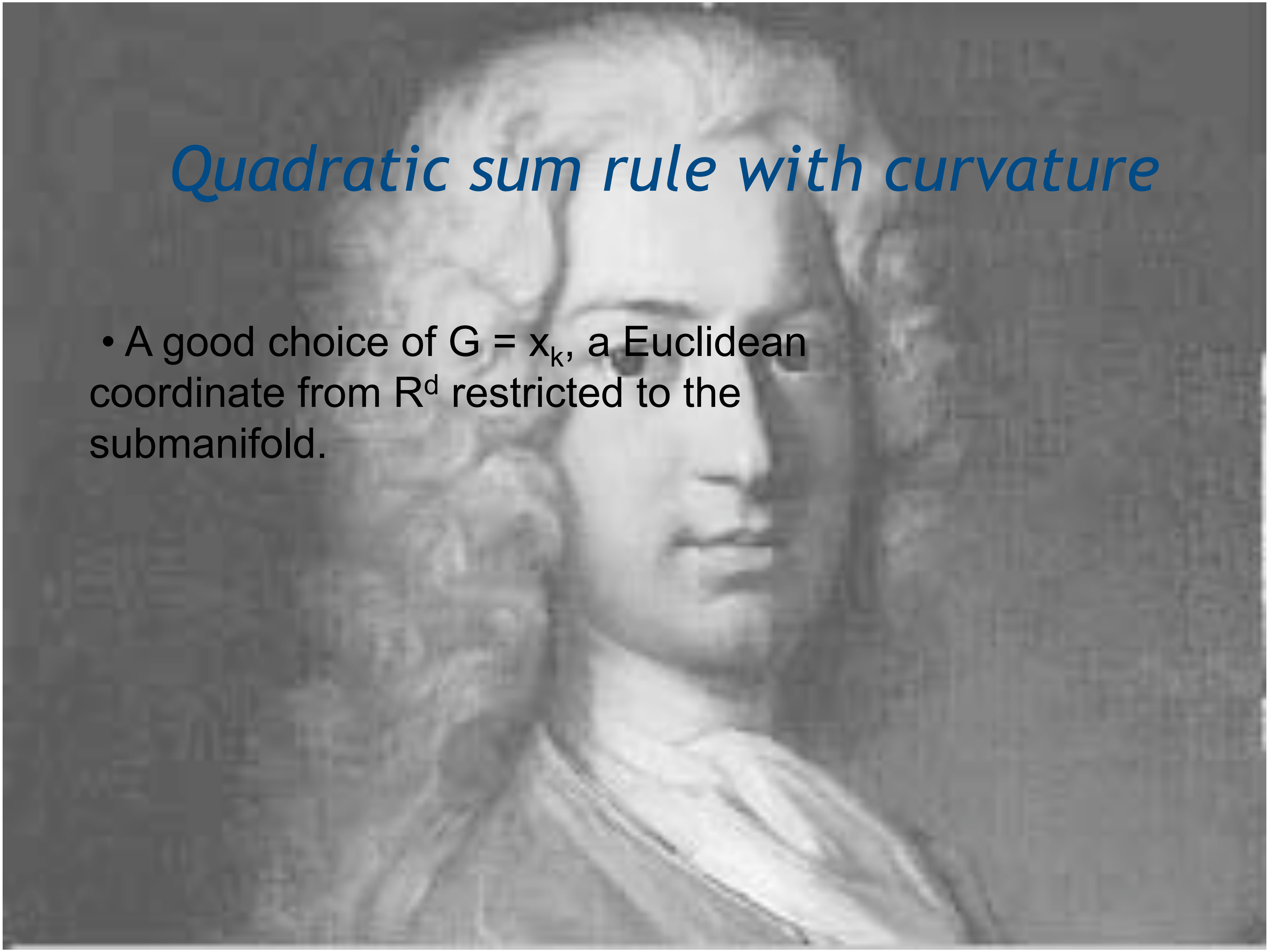
$$q(\mathbf{x}) = \frac{1}{4}\left(\sum_{j=1}^{d} \kappa_j\right)^2 - \frac{1}{2}\sum_{j=1}^{d} \kappa_j^2$$

Heisenberg's Answer

(if he had thought about it)



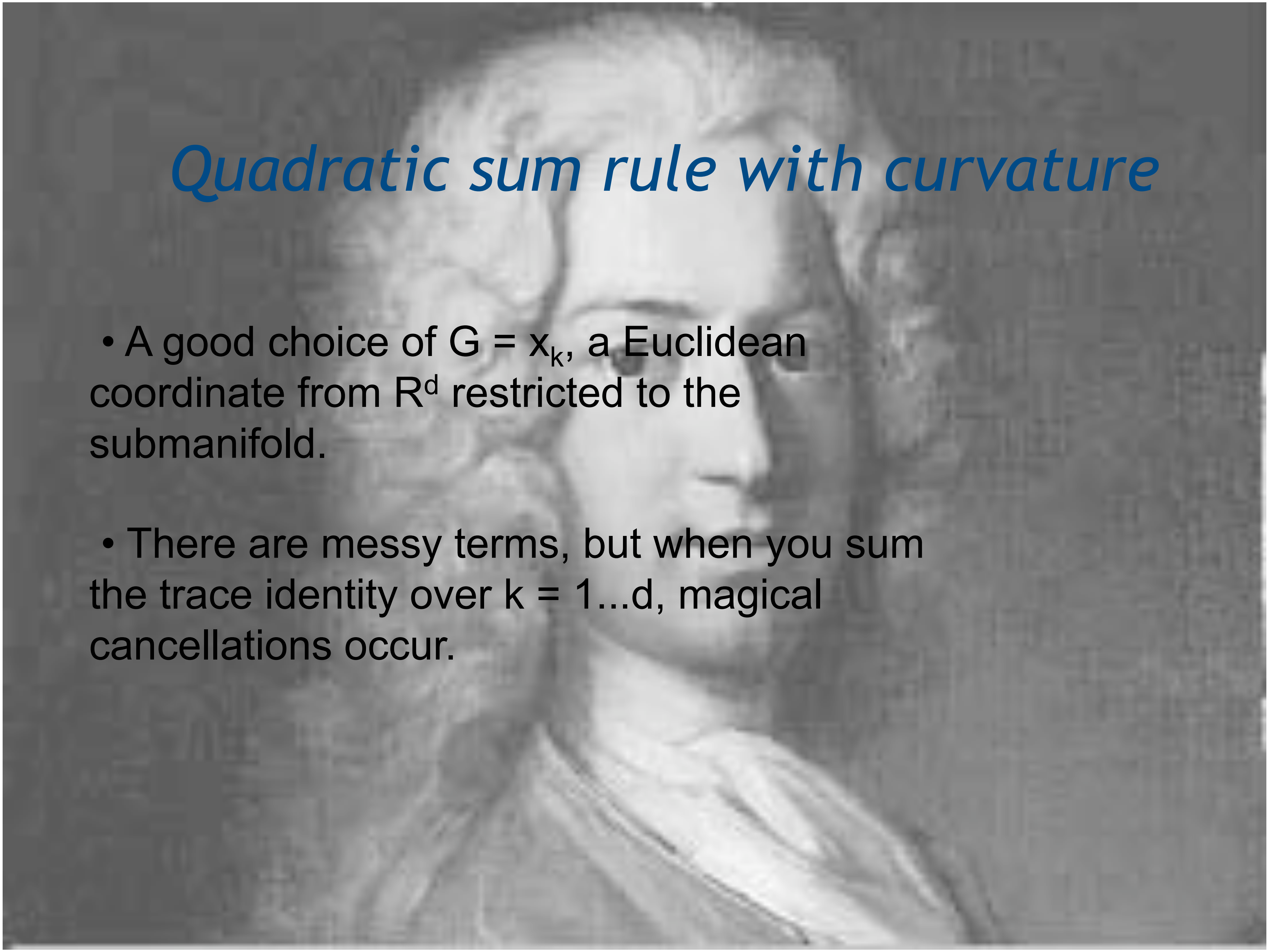
$$q(\mathbf{x}) = \frac{1}{4}\left(\sum_{j=1}^{d} \kappa_j\right)^2$$



Quadratic sum rule with curvature

- A good choice of $G = x_k$, a Euclidean coordinate from R^d restricted to the submanifold.

Quadratic sum rule with curvature



- A good choice of $G = x_k$, a Euclidean coordinate from R^d restricted to the submanifold.

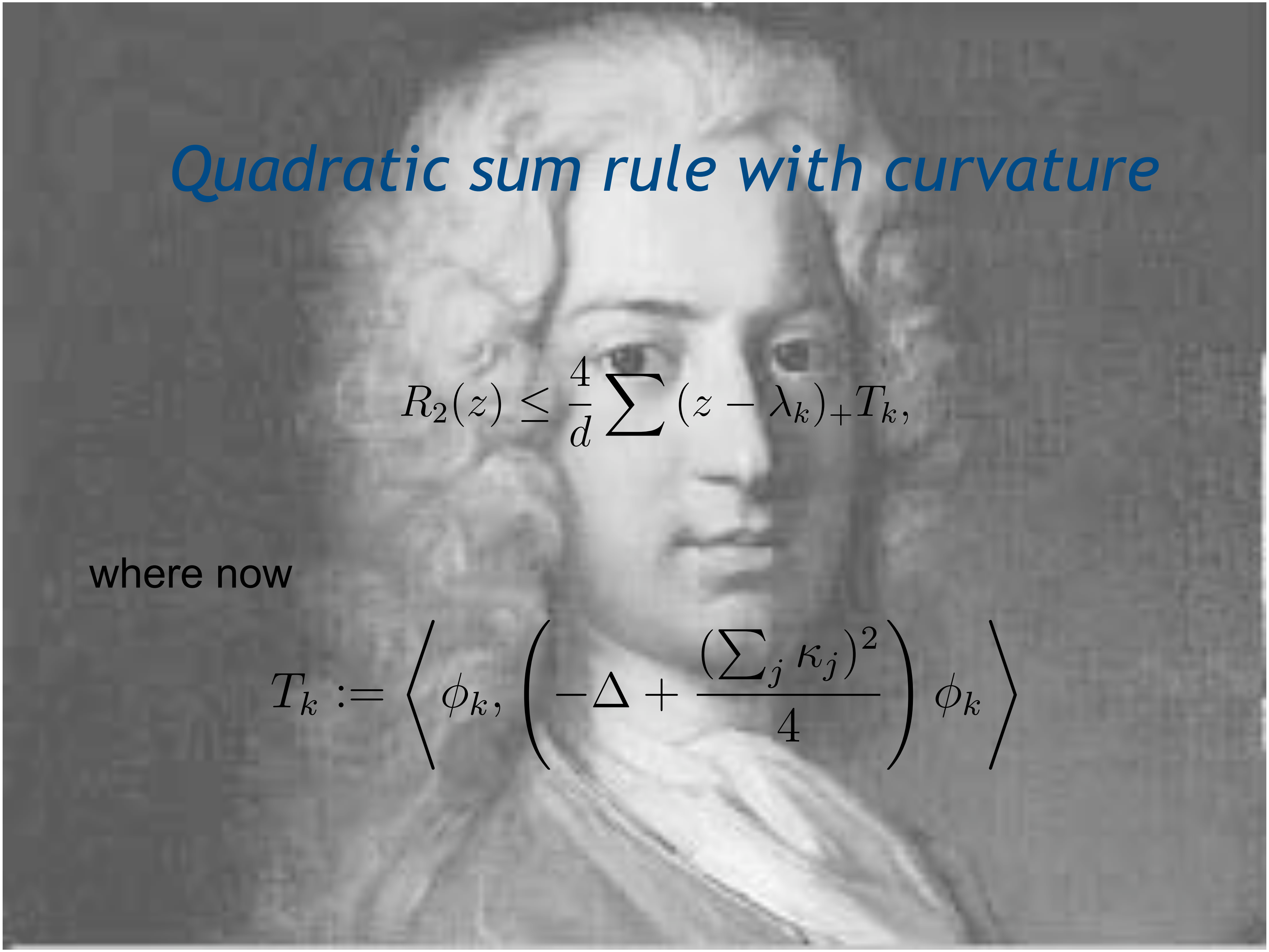
- There are messy terms, but when you sum the trace identity over $k = 1...d$, magical cancellations occur.

Quadratic sum rule with curvature

- A good choice of $G = x_k$, a Euclidean coordinate from R^d restricted to the submanifold.

- There are messy terms, but when you sum the trace identity over $k = 1...d$, magical cancellations occur.

- Since there are second derivatives of x_k, there is a curvature contribution that doesn't go away.

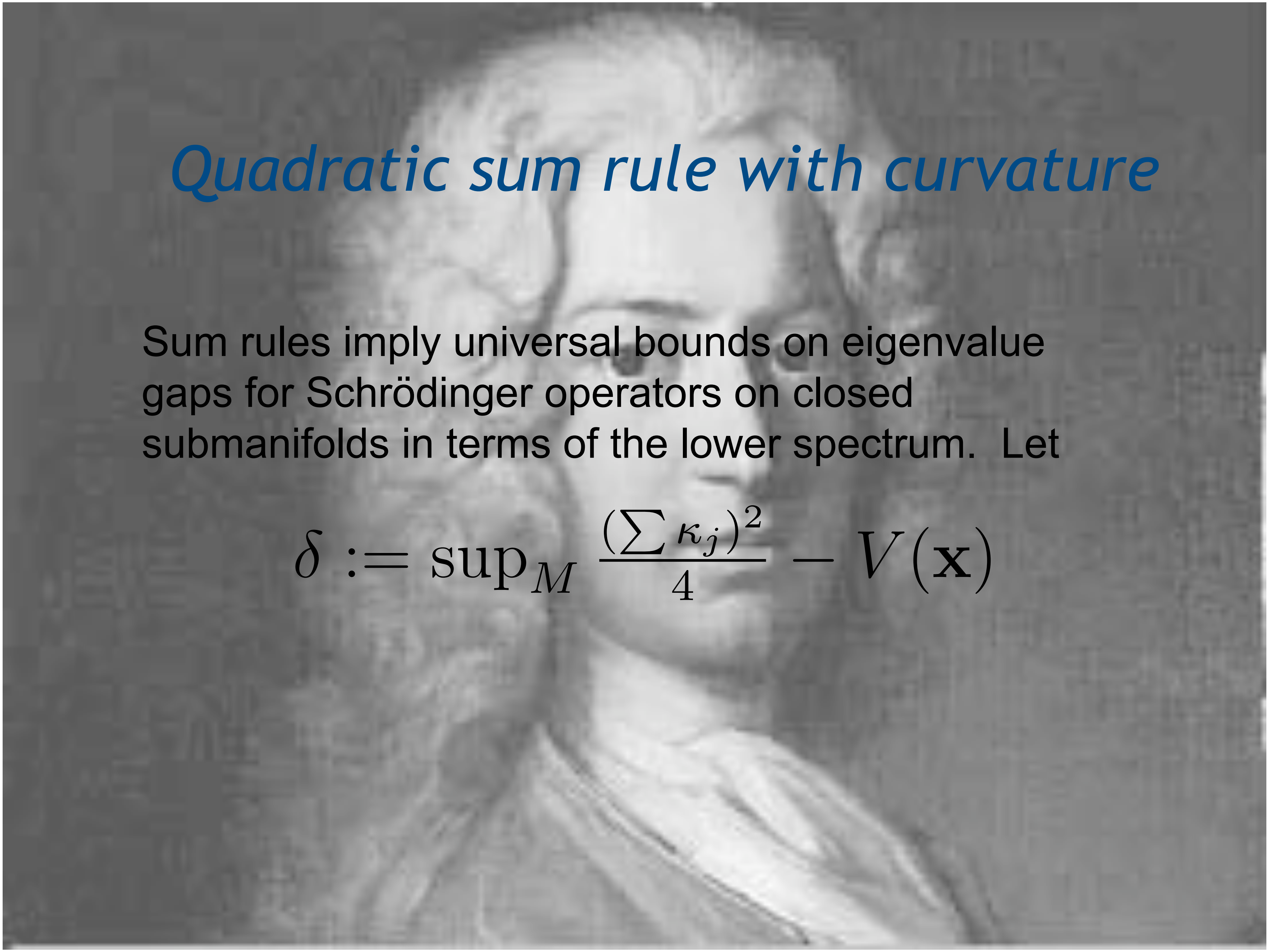


Quadratic sum rule with curvature

$$R_2(z) \leq \frac{4}{d} \sum (z - \lambda_k)_+ T_k,$$

where now

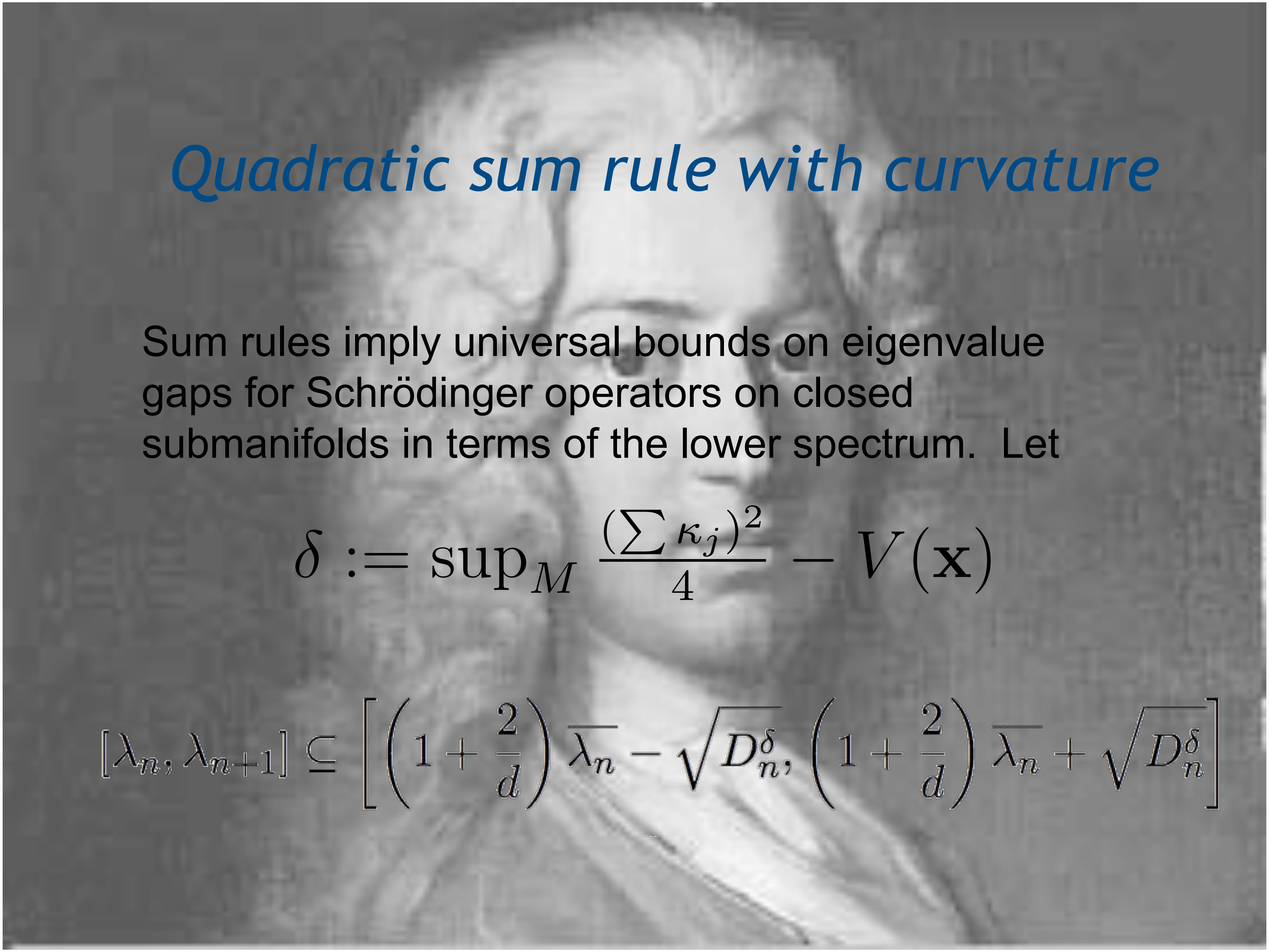
$$T_k := \left\langle \phi_k, \left(-\Delta + \frac{(\sum_j \kappa_j)^2}{4} \right) \phi_k \right\rangle$$



Quadratic sum rule with curvature

Sum rules imply universal bounds on eigenvalue gaps for Schrödinger operators on closed submanifolds in terms of the lower spectrum. Let

$$\delta := \sup_M \frac{(\sum \kappa_j)^2}{4} - V(\mathbf{x})$$

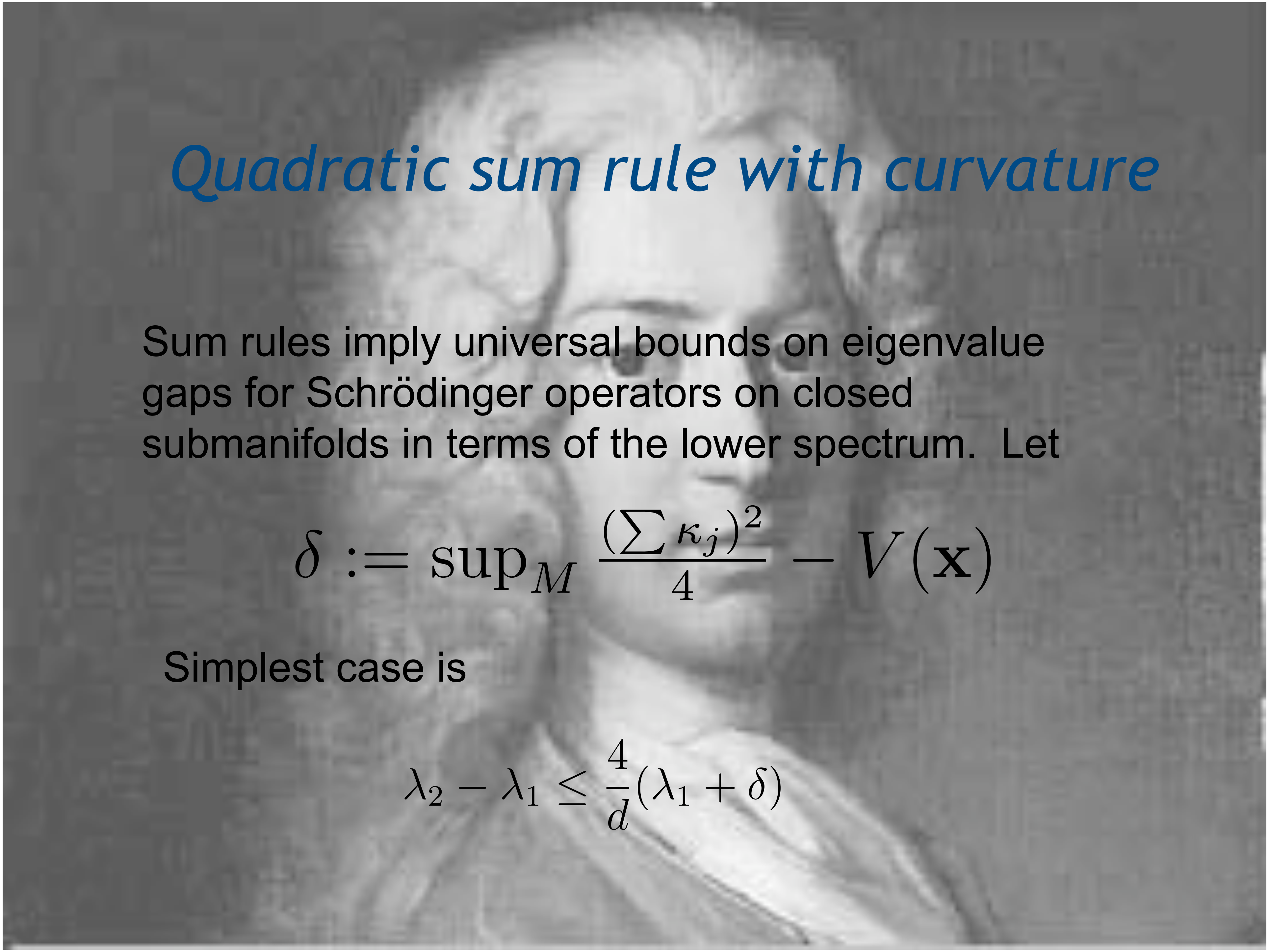


Quadratic sum rule with curvature

Sum rules imply universal bounds on eigenvalue gaps for Schrödinger operators on closed submanifolds in terms of the lower spectrum. Let

$$\delta := \sup_M \frac{(\sum \kappa_j)^2}{4} - V(\mathbf{x})$$

$$[\lambda_n, \lambda_{n+1}] \subseteq \left[\left(1+\frac{2}{d}\right)\overline{\lambda_n} - \sqrt{D_n^\delta}, \left(1+\frac{2}{d}\right)\overline{\lambda_n} + \sqrt{D_n^\delta}\right]$$



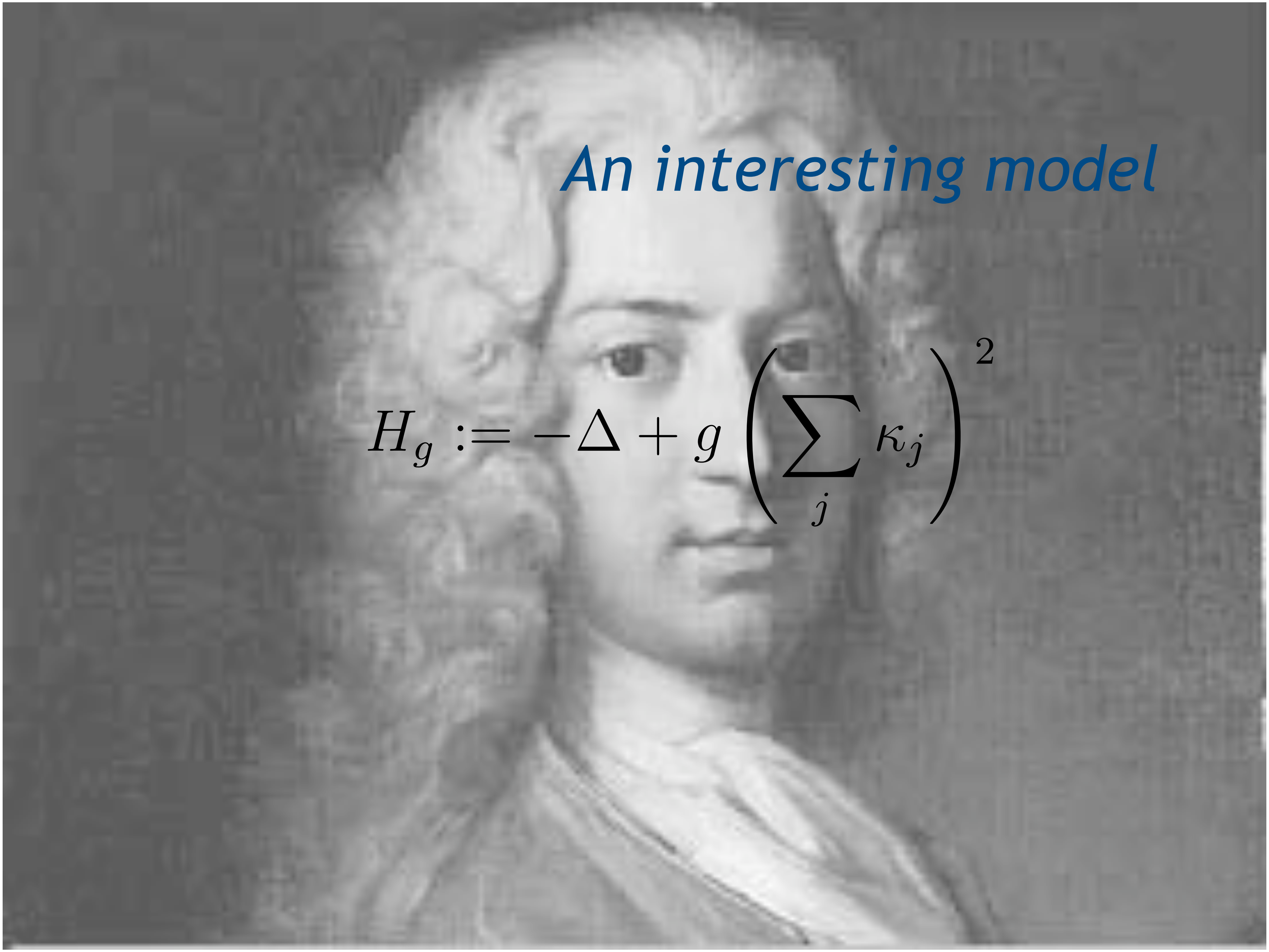
Quadratic sum rule with curvature

Sum rules imply universal bounds on eigenvalue gaps for Schrödinger operators on closed submanifolds in terms of the lower spectrum. Let

$$\delta := \sup_M \frac{(\sum \kappa_j)^2}{4} - V(\mathbf{x})$$

Simplest case is

$$\lambda_2 - \lambda_1 \leq \frac{4}{d}(\lambda_1 + \delta)$$



An interesting model

$$H_g := -\Delta + g\left(\sum_j \kappa_j\right)^2$$

An explicit calculation shows that the bound is sharp for the non-zero eigenvalue gaps of the sphere, for which all the eigenvalues are known and elementary [20]: For simplicity, assume that $d = 2, g = \frac{1}{4}$, and that M is the sphere of radius 1 embedded in $\mathbb{R}^3$. Then $h = 2, \sigma = 1$, and:

$$\lambda_1 = 1; \lambda_2 = \lambda_3 = \lambda_4 = 3; \ldots ; \lambda_{(m-1)^2+1} = \cdots = \lambda_{m^2} = m^2 - m + 1.$$

For $n = m^2$, the calculation shows that $\overline{\lambda_n} = \frac{n+1}{2}$, and $\overline{\lambda_n^2} = \frac{n^2+n+1}{3}$. Hence $D_n = n$, and b) informs us that

$$\begin{aligned} 2\overline{\lambda_{m^2}} - m = m^2 - m + 1 \leq \lambda_{m^2} = m^2 - m + 1 \\ \leq \lambda_{m^2+1} = m^2 + m + 1 \leq 2\overline{\lambda_{m^2}} + m = m^2 + m + 1, \end{aligned}$$

and thus λ_{m^2} equals the lower bound $2\overline{\lambda_{m^2}} - m$ and λ_{m^2+1} equals the upper bound $2\overline{\lambda_{m^2}} + m$.

What about Lieb-Thirring?

What about Lieb-Thirring?

Can establish establish a quadratic “Yang-type inequality, either by commuting with coordinate functions, or by commuting with unitary operators

$$G = \exp(i\, z.x)$$

(use modified trace identity).

Because of the curvature terms, the natural L-T inequality is not in reference to energy 0.

Harrell-Stubbe TAMS to appear

What about Lieb-Thirring?

Similar results for periodic Schrödinger. There is a shift reflecting the periodicity lattice, analogous to the mean curvatures.

Geometrically, the periodicities are connected with the curvature necessary to embed a torus in Euclidean space.

Harrell-Stubbe TAMS to appear

What about Lieb-Thirring?

For semiclassics we need a partial differential inequality:

$$\frac{\partial}{\partial \epsilon}\left(\epsilon^{d/2} R_2(z,\epsilon)\right) \leq \frac{gd}{2}\epsilon^{d/2} R_1(z,\epsilon)$$

$$\partial R_2/\partial z \; = \; 2R_1$$

Harrell-Stubbe TAMS to appear

What about Lieb-Thirring?

$$U(z,\epsilon) := \epsilon^{d/2} R_2(z,\epsilon)$$

$$\frac{\partial U}{\partial \epsilon} \le \frac{gd}{4} \frac{\partial U}{\partial z}$$

$$\xi := \epsilon - \tfrac{4}{gd} z \qquad \frac{\partial U}{\partial \xi} \le 0$$

(gd reflects the curvature (= sup h^2) or, resp. periodicity.)

Harrell-Stubbe TAMS to appear

What about Lieb-Thirring?

For all $\epsilon > 0$ the mapping

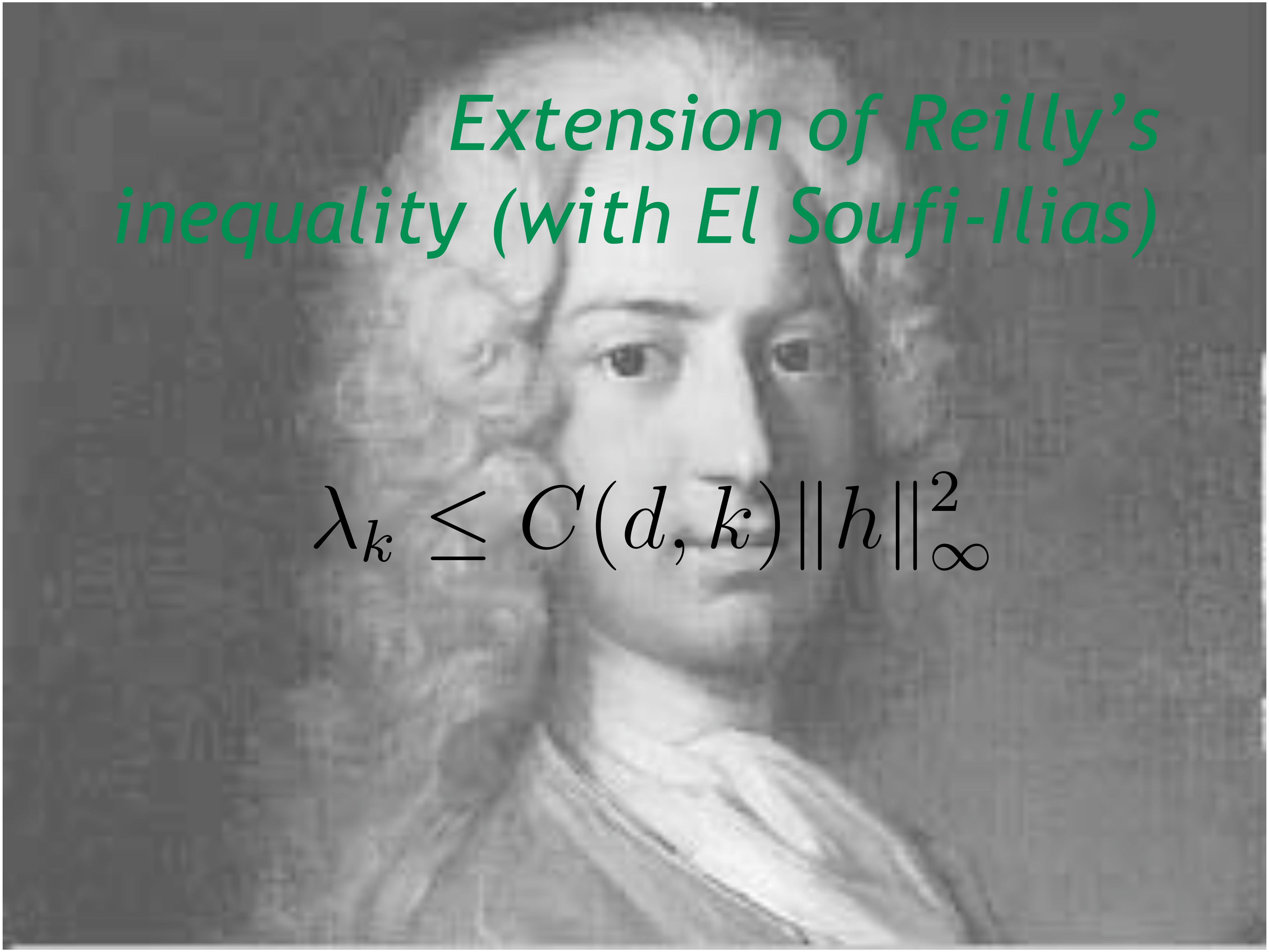
$$\epsilon \mapsto \epsilon^{\frac{d}{2}} R_\sigma(z - \frac{\epsilon g d}{4}) = \epsilon^{\frac{d}{2}} \sum (z - \frac{\epsilon g d}{4} - \lambda_j)_+^\sigma$$

is nonincreasing, and therefore for all $z \in \mathbb{R}$ and all $\epsilon > 0$ the following sharp Lieb-Thirring inequality holds:

$$R_\sigma(z, \epsilon) \leq \epsilon^{-d/2} L_{\sigma,d}^{cl} \int_M \left(V(\mathbf{x}) - \left(z + \frac{gd}{4}\epsilon \right) \right)_-^{\sigma + d/2} d\mathbf{x}.$$

Harrell-Stubbe TAMS to appear

Extension of Reilly's inequality (with El Soufi-Ilias)



$$\lambda_k \leq C(d,k)\|h\|_\infty^2$$

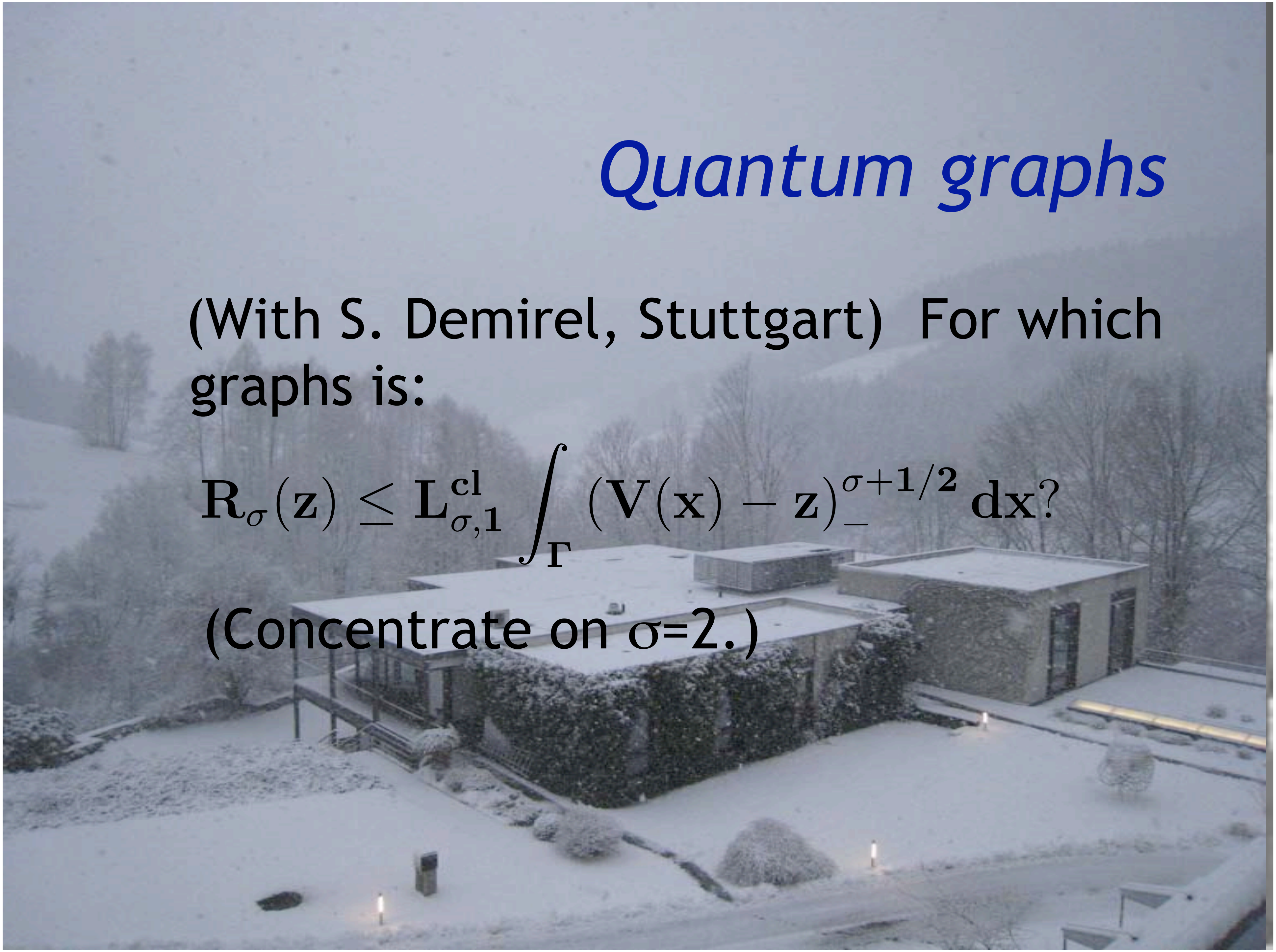
Take-away messages #3

1. On manifolds, sum rules involve mean curvature in an explicit way

2. Sharp for spheres where potential = g h^2.

3. Semiclassical inequality requires a partial differential inequality.

4. Each eigenvalue dominated by mean curvature.



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.)

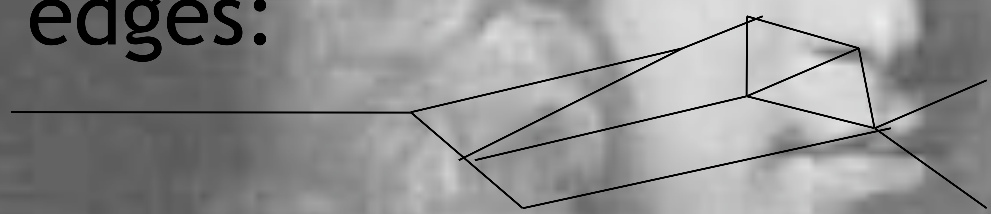
ON SEMICLASSICAL AND UNIVERSAL INEQUALITIES FOR EIGENVALUES OF QUANTUM GRAPHS

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.

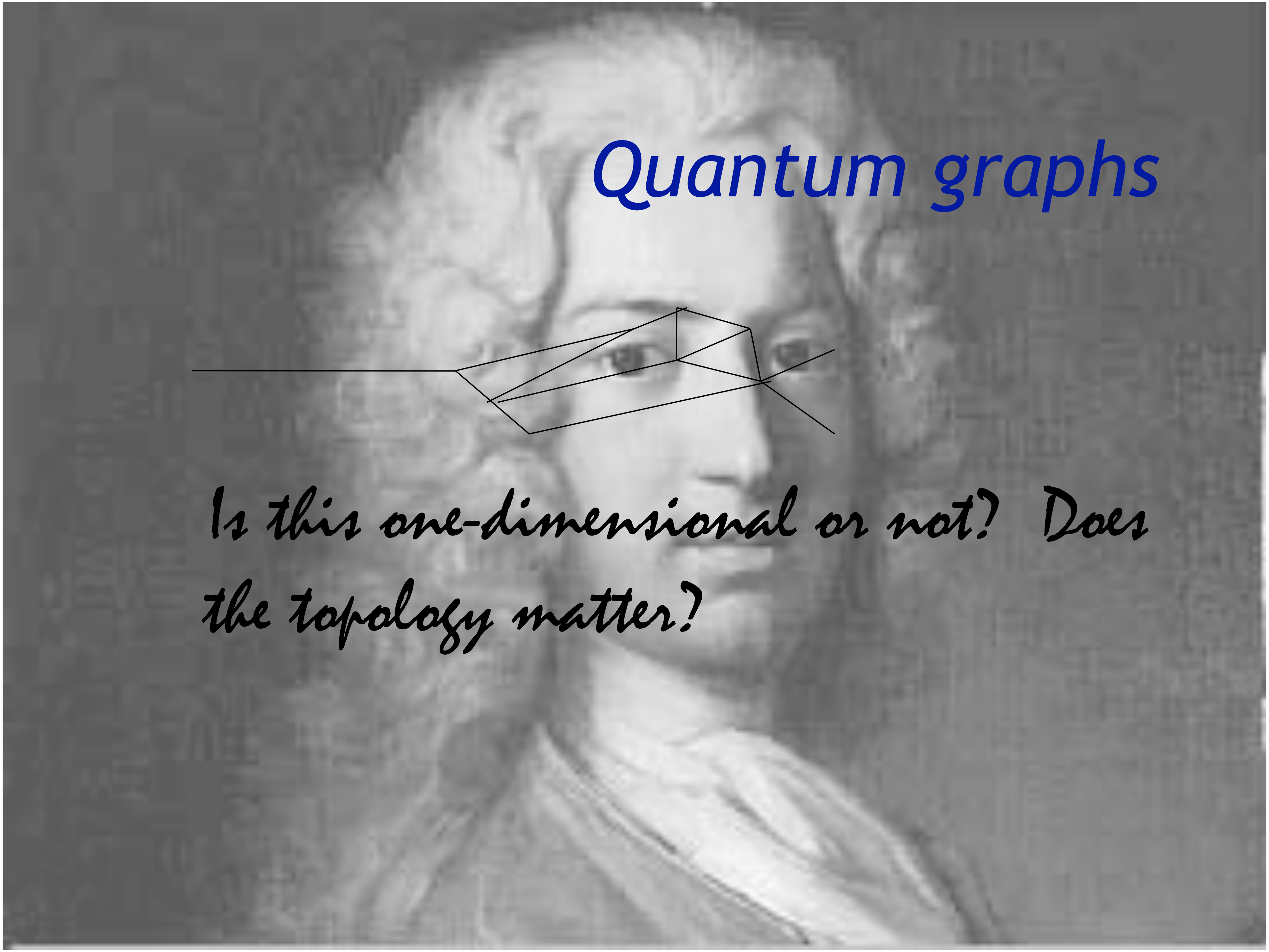
Quantum graphs

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.

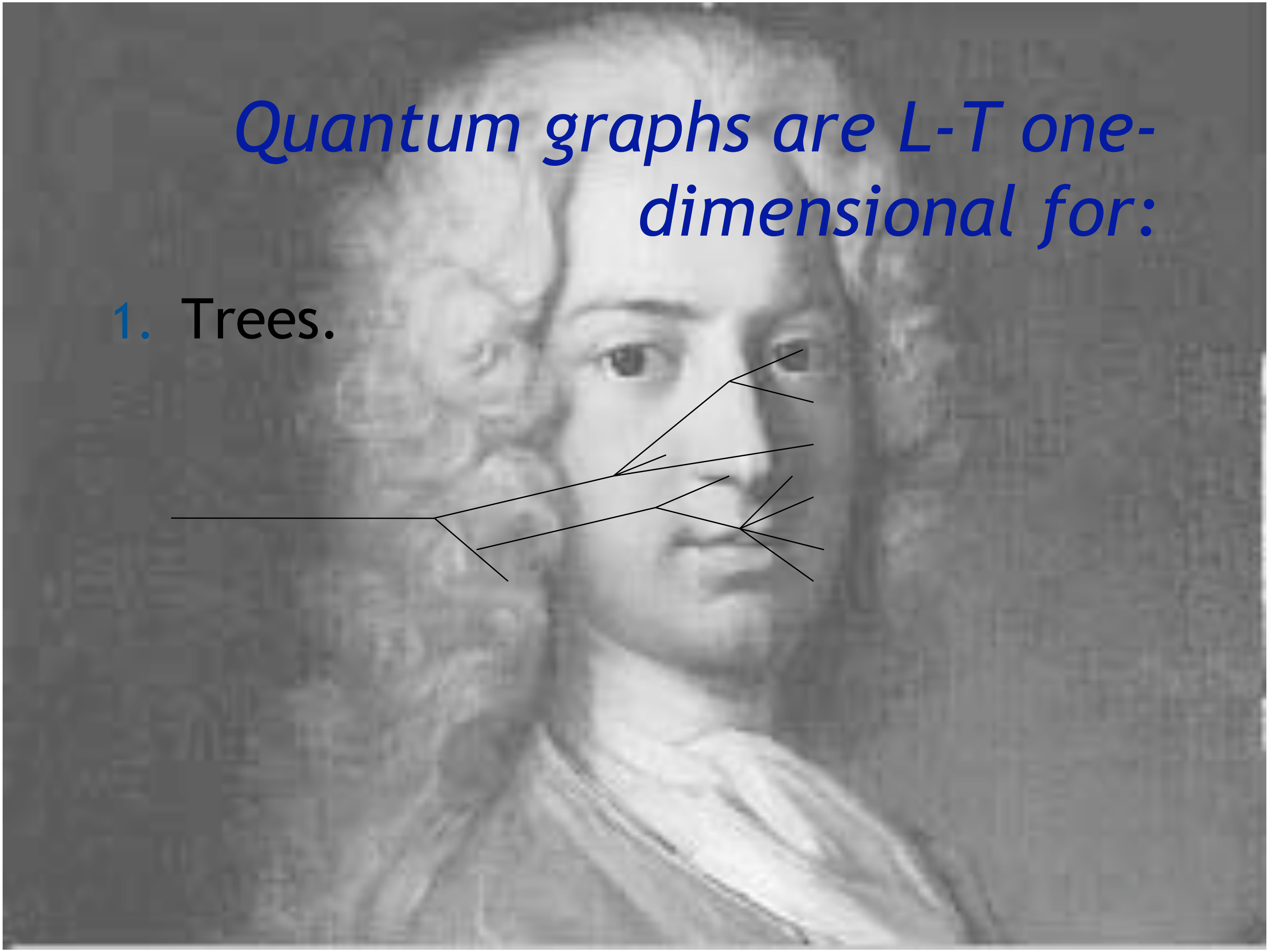
Quantum graphs



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

Quantum graphs are L-T one-dimensional for:

1. Trees.



Quantum graphs are L-T one-dimensional for:

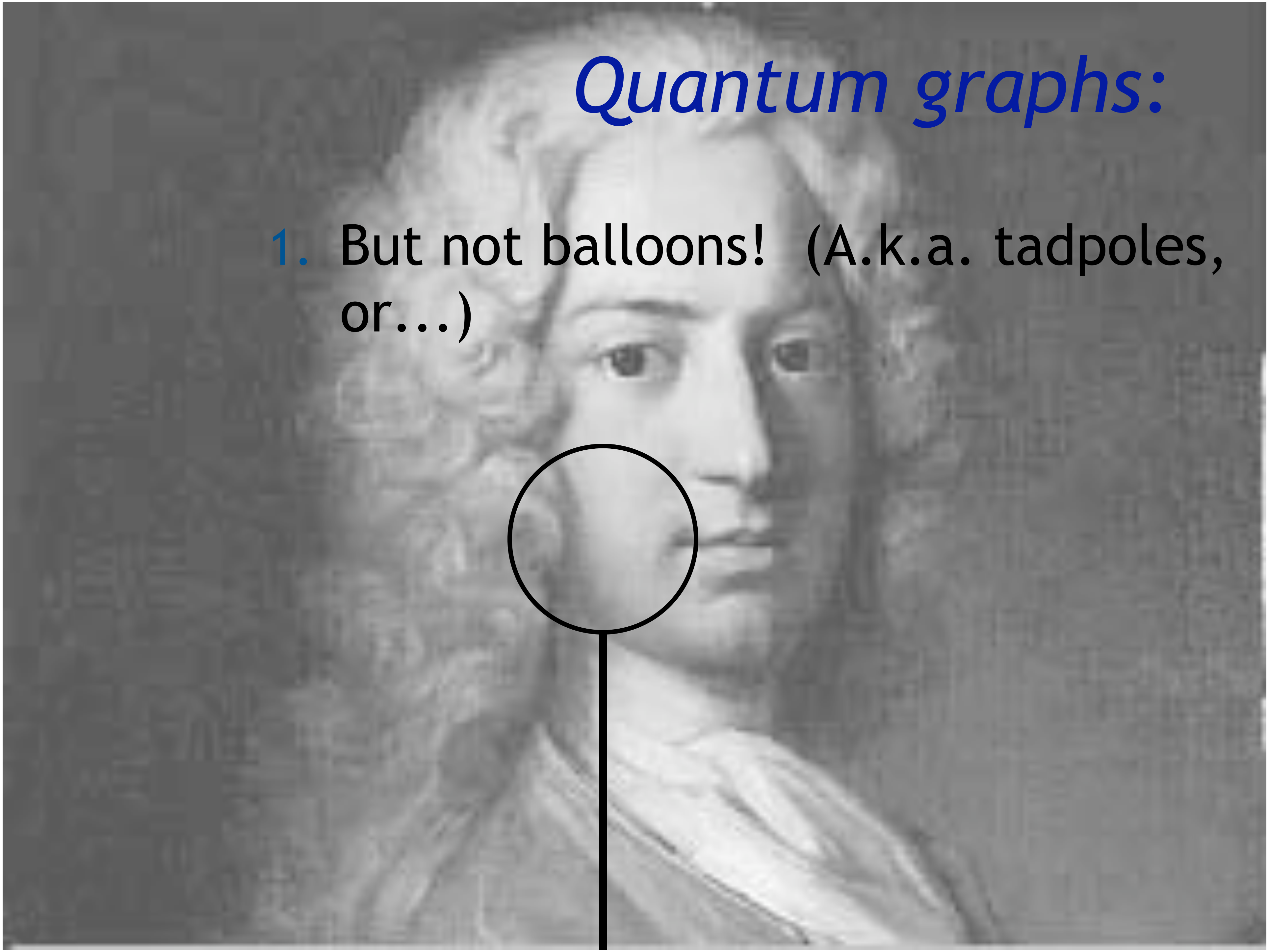
1. Trees.
2. Scottish tartans (infinite rectangular graphs):

Quantum graphs are L-T one-dimensional for:

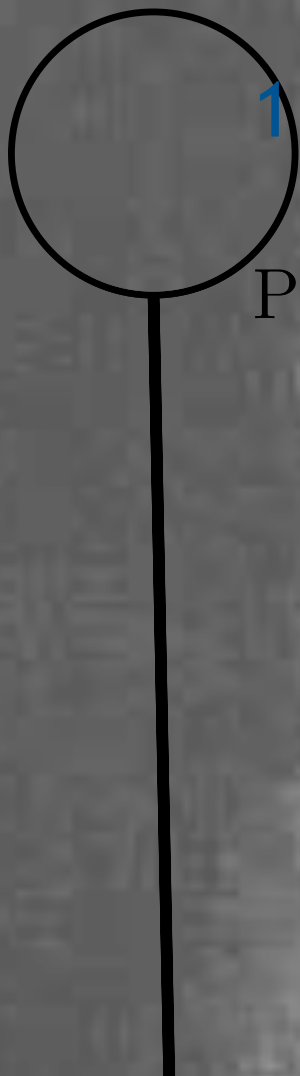
1. Trees.
2. Infinite rectangular graphs.
3. Bathroom tiles, a.k.a. honeycombs, etc.:

Quantum graphs:

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



Quantum graphs:



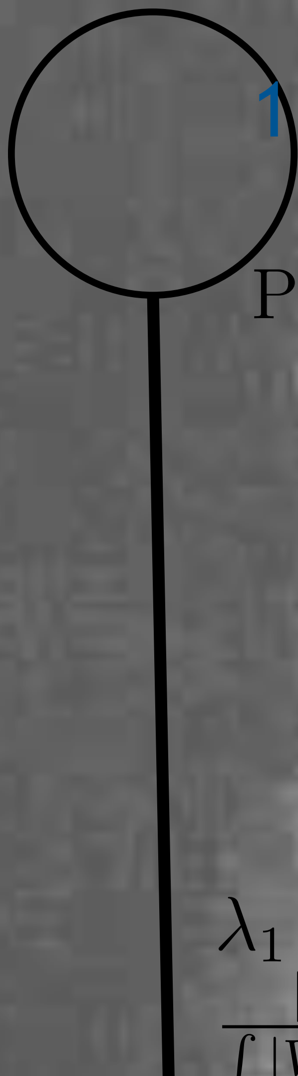
1. But not balloons! (A.k.a. tadpoles, or...)

Put a soliton potential on the loop:

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

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

Quantum graphs:



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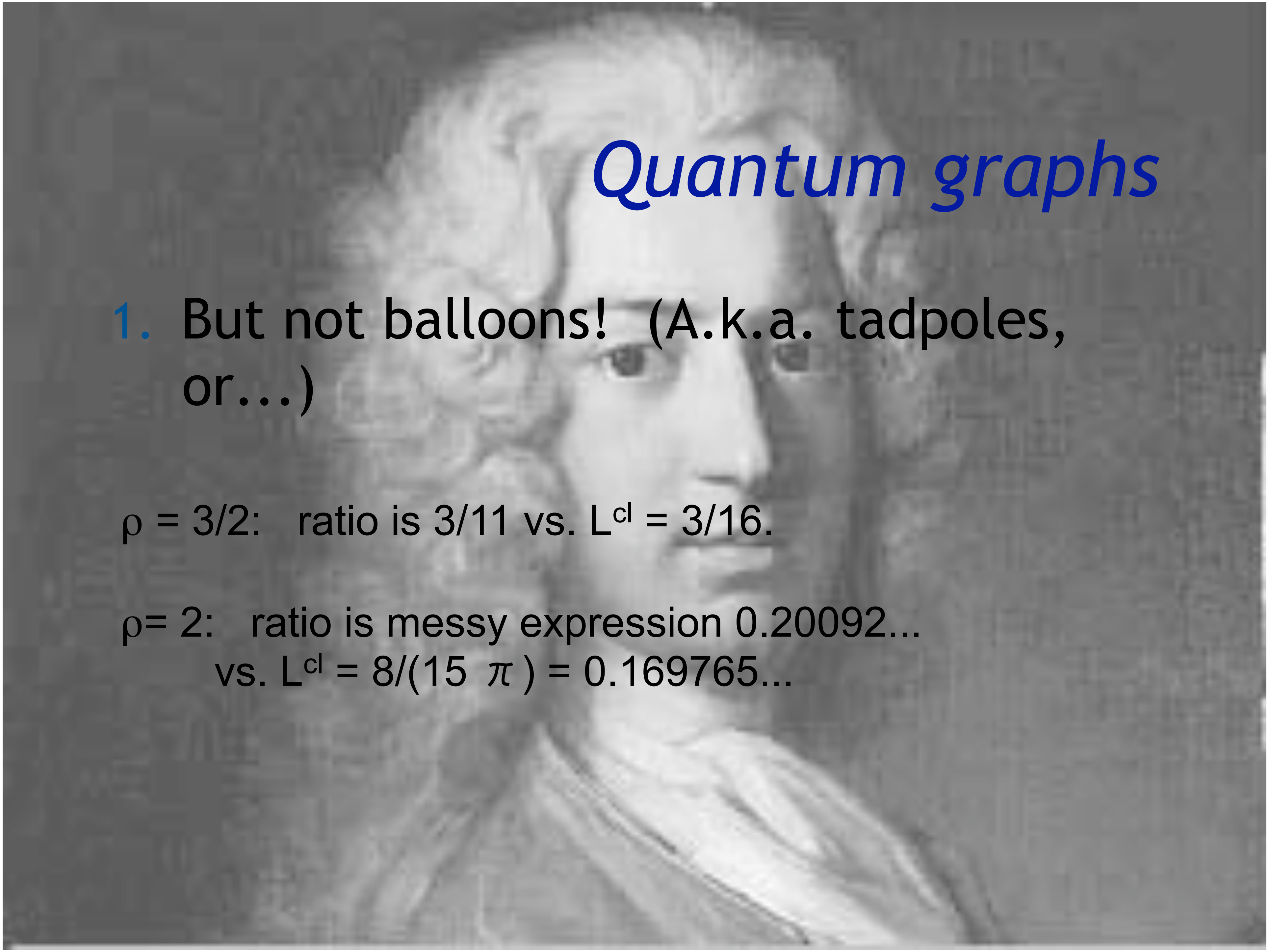
$$V = \frac{-2a^2}{\cosh^2(ax)} \chi_{\text{loop}}$$

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

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

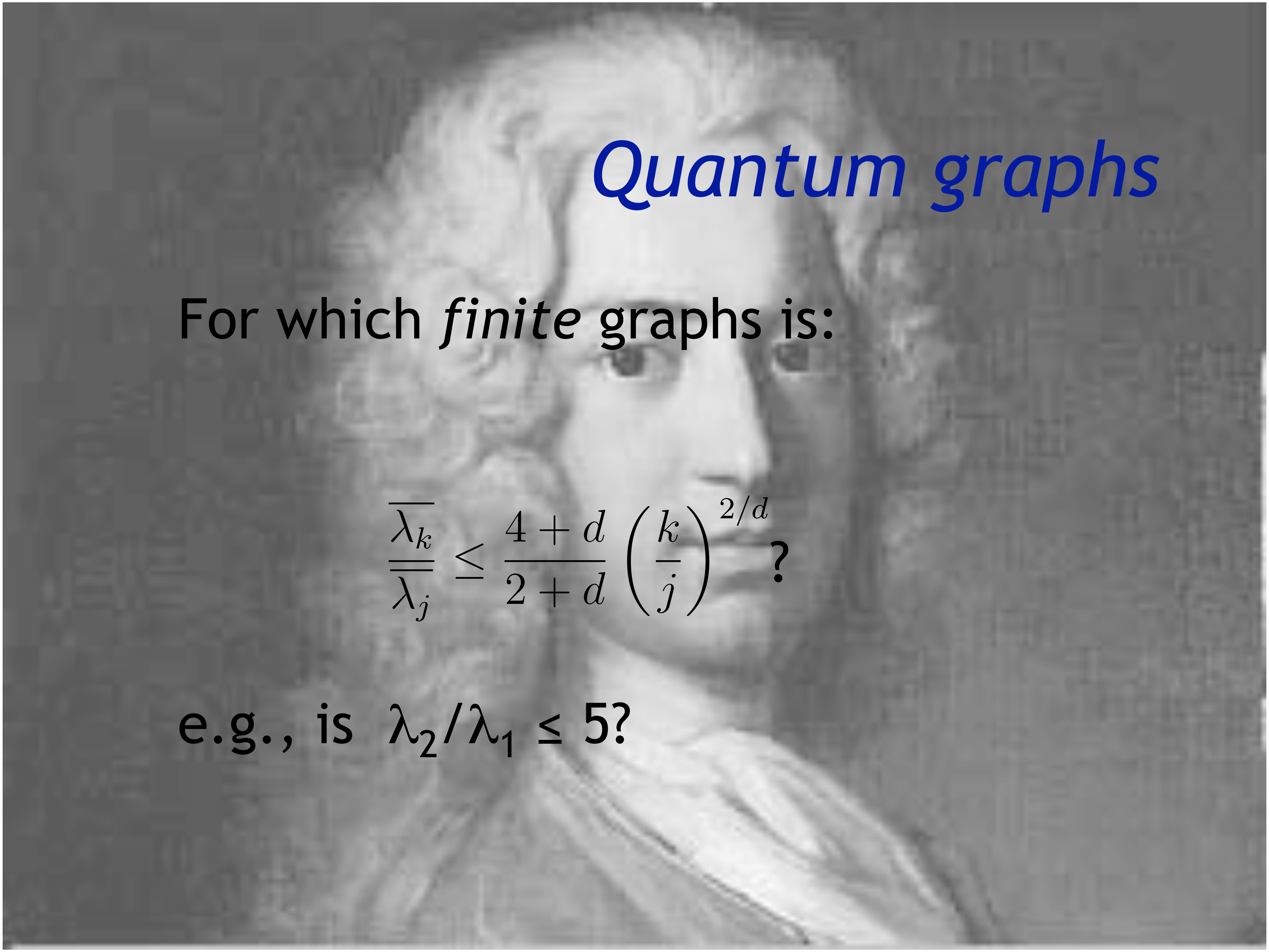


Quantum graphs

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

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

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



Quantum graphs

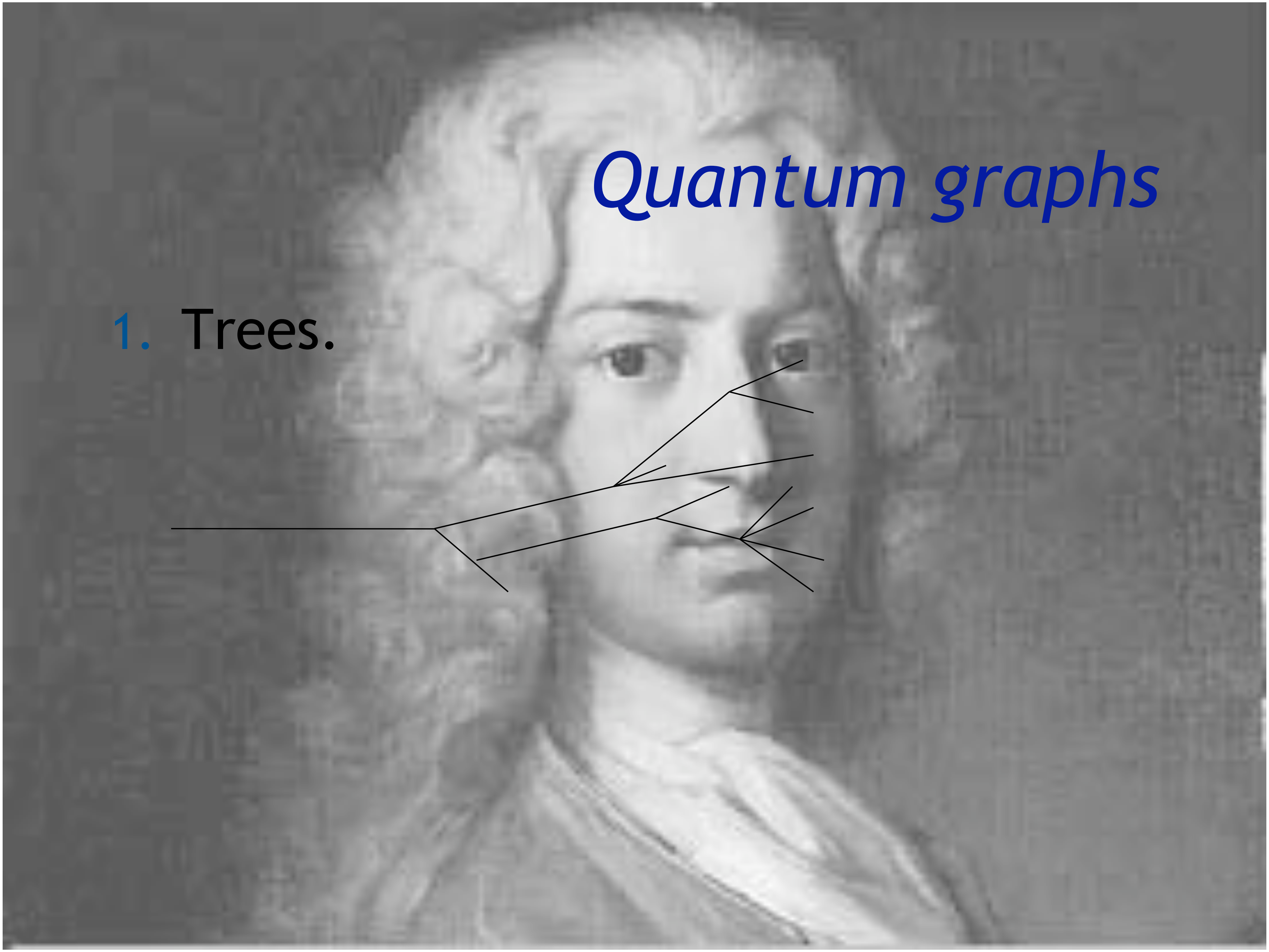
For which *finite* graphs is:

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

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

Quantum graphs

1. Trees.

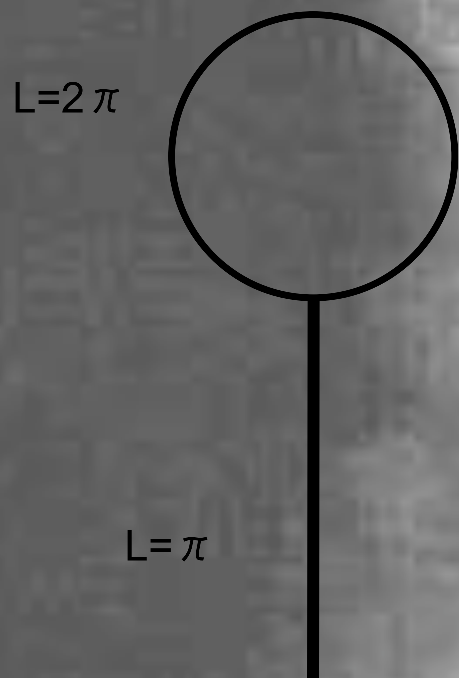


Quantum graphs

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

Quantum graphs

- But not balloons!

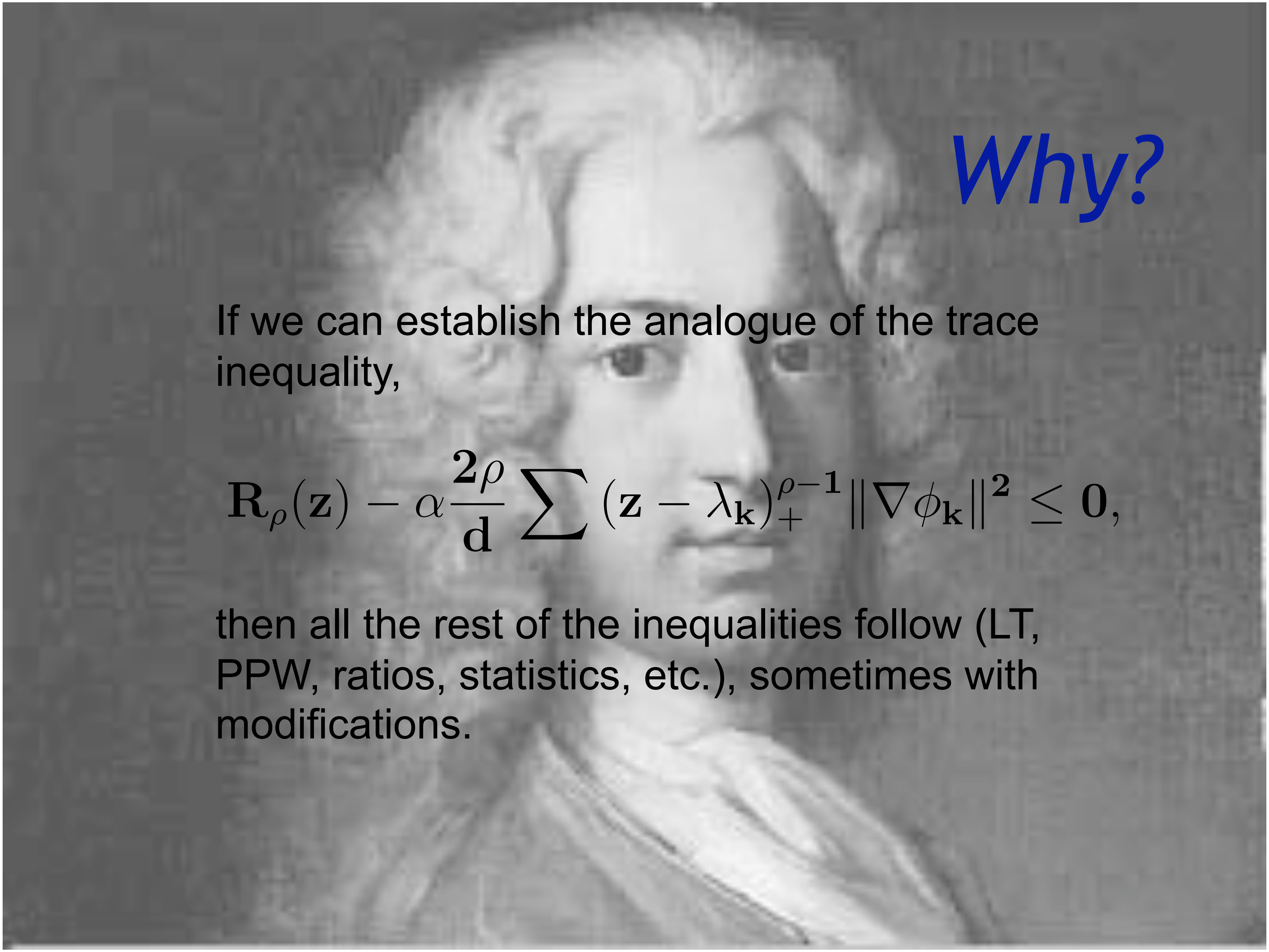


$$\frac{\lambda_2}{\lambda_1} = \left(\frac{\pi - \arctan(1/\sqrt{(2)})}{\arctan(1/\sqrt{(2)})}\right) \doteq 16.8$$

Quantum graphs

- Fancy balloons can have arbitrarily large λ_2/λ_1.


Why?

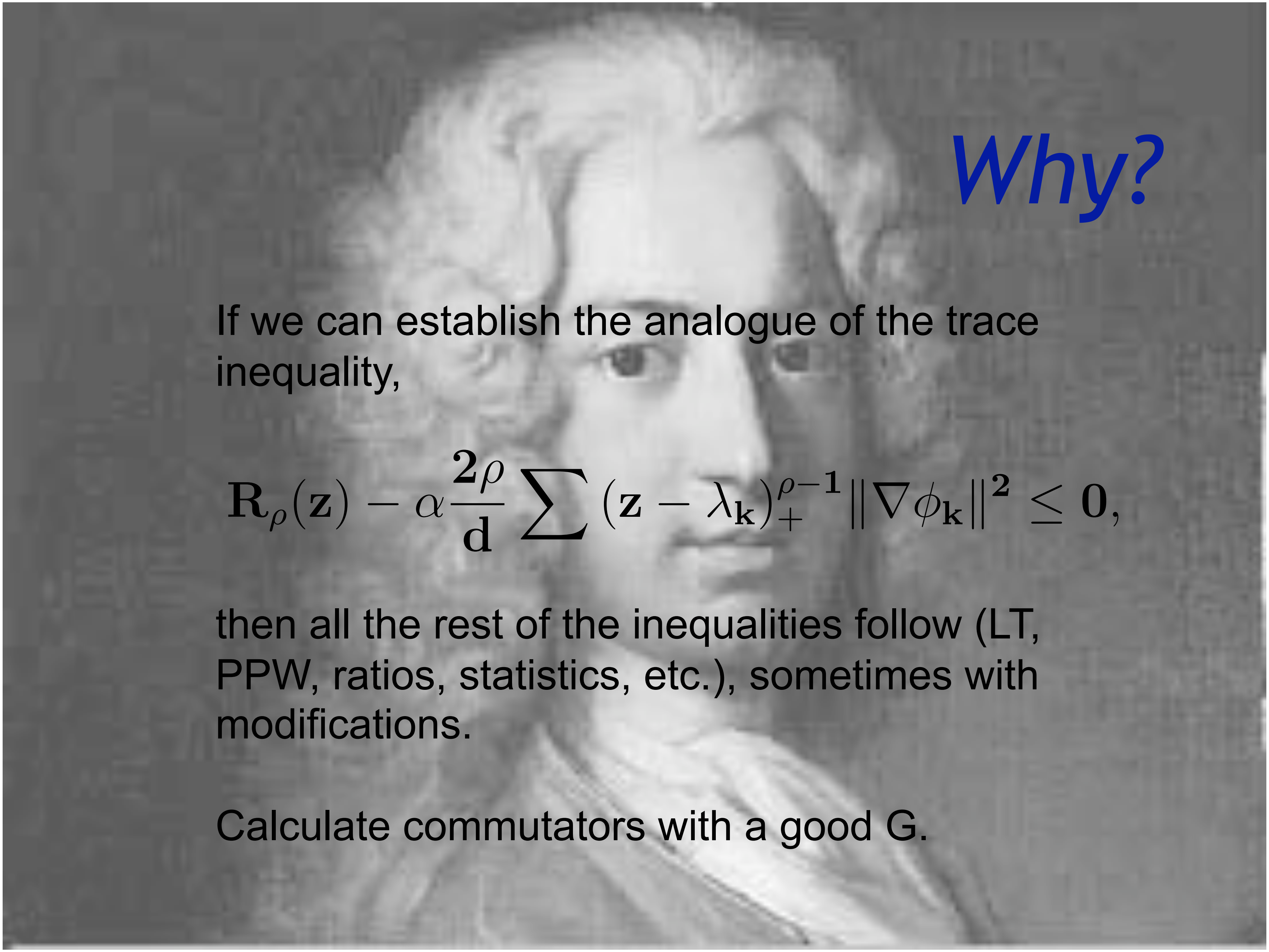


Why?

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.



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

Calculate commutators with a good G.

Suppose G' is cst on each edge and

$\phi \to G\phi$ preserves vertex conditions.

(In std case this means G contin., $\sum \frac{\partial G}{\partial x_i} = 0$ @ V.)

Sum rule becomes

$$\sum_j \sum_k \left((z-\lambda_k)_+^2 \, a_j \|\phi_k\|_{\Gamma_j}^2 - 4\alpha (z-\lambda_j)_+ \, a_j \|\phi_k'\|_{\Gamma_j}^2 \right)$$

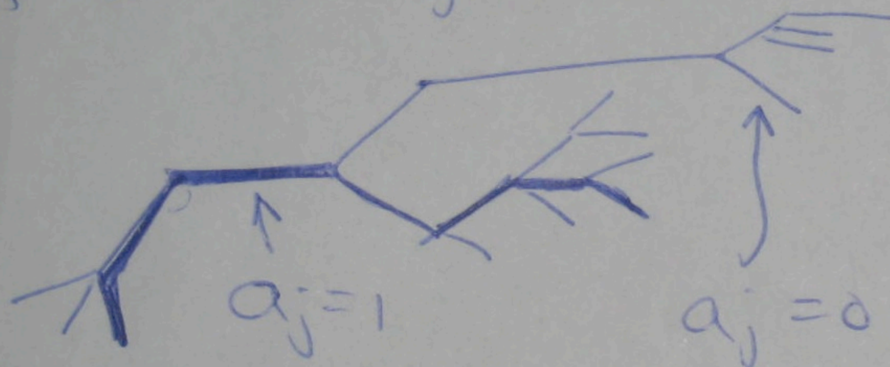
$$= \cdots \leq 0$$

where $|G'(x)|^2 = a_j$ on $\Gamma_j \subset \Gamma$.

$$\boxed{\sum_j \sum_{k\le n} a_j\left((z-\lambda_k)^2\,\|\phi_k\|^2_{\Gamma_j} - 4\alpha(z-\lambda_k)\|\phi_k'\|^2_{\Gamma_j}\right) \le 0}$$

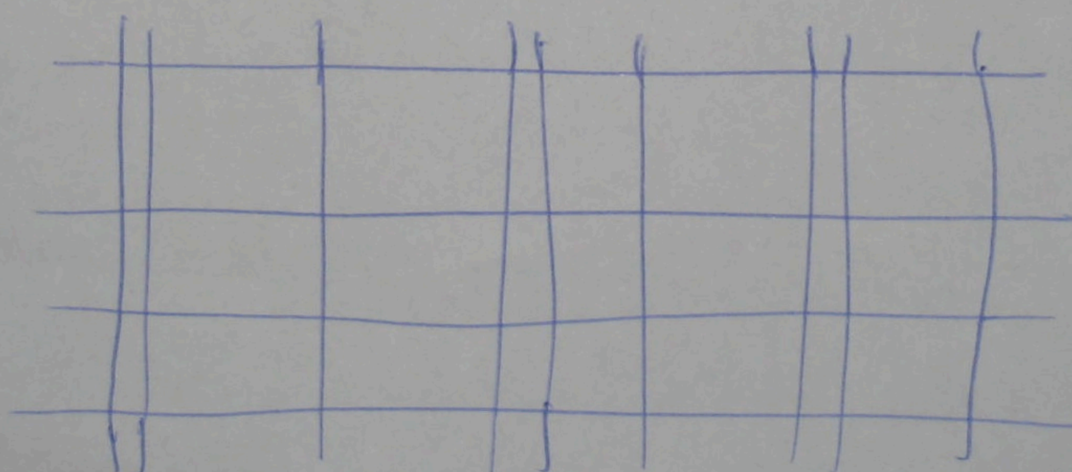
* Can we find a family of such G's and sum, so that we get $\sum_{k\le n}\left((z-\lambda_k)^2 - 4\alpha(z-\lambda_k)\|\phi_k'\|^2\right) \le 0$?

Example. σ = distance along a "transit" in a tree, constant elsewhere.



Example. Scottish tartan, $\sigma = x+y$

$a = 1$
(good).



Sharpest inequalities if a_j always 1

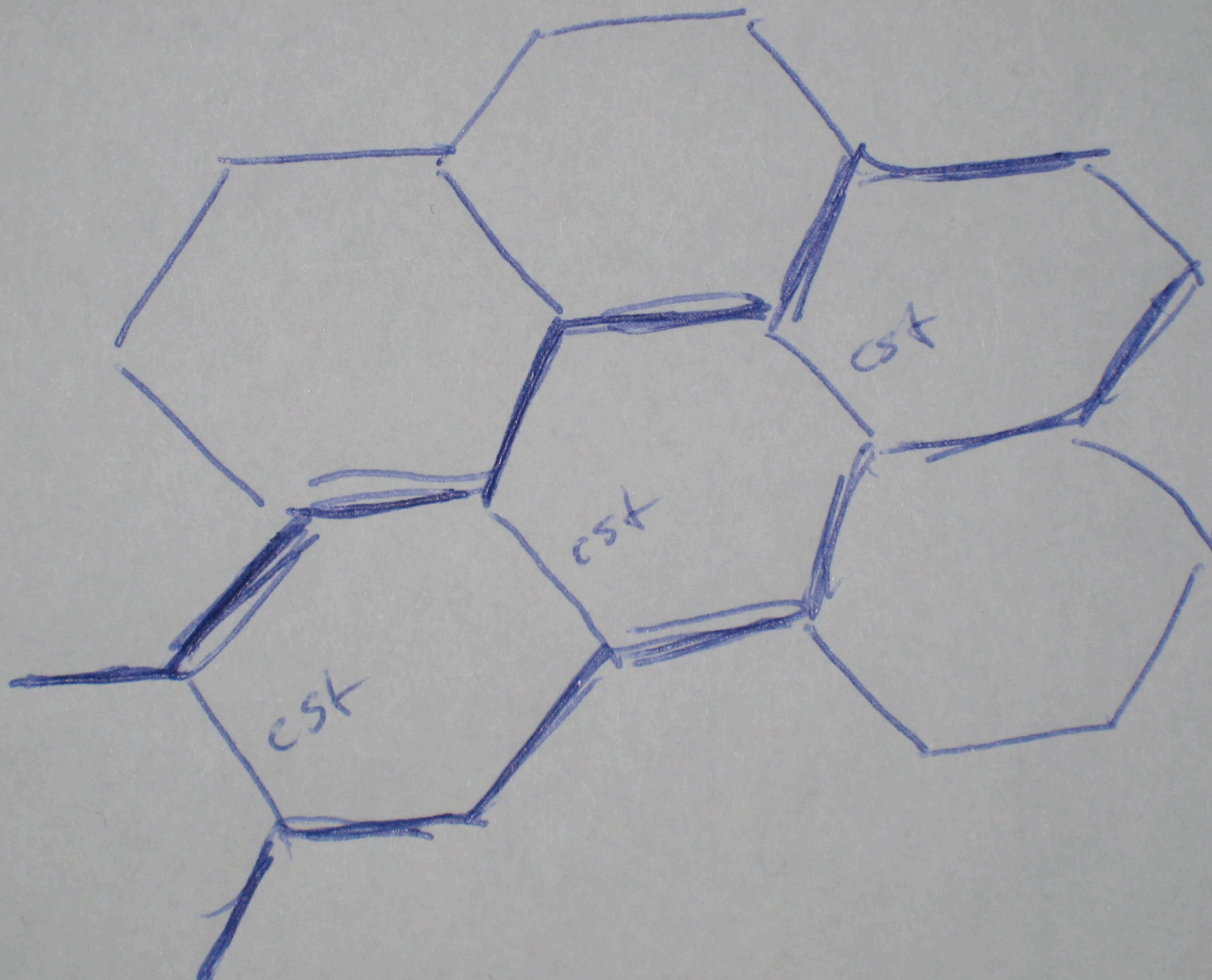
or, equally good, $\sum_{\alpha} a_j^{(\alpha)} \chi_{\Gamma_j} = 1$.

Then:

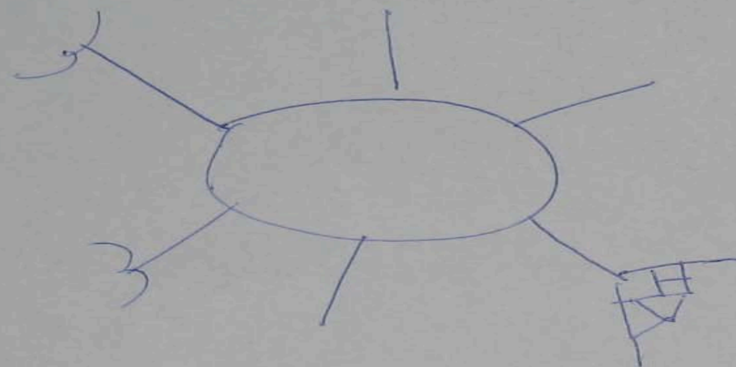
$$R_2(z) := \sum_j (z-\lambda_j)_+^2 \le 4\alpha \sum (z-\lambda_j)_+ T_j$$

$$R_\sigma(z) \le 2\sigma\alpha \sum (z-\lambda_j)_+ T_j \,, \quad \sigma \ge 2$$

$$\le 4 \sum (z-\lambda_j)_+ T_j \quad 1 \le \sigma \le 2$$


cst
cst
cst

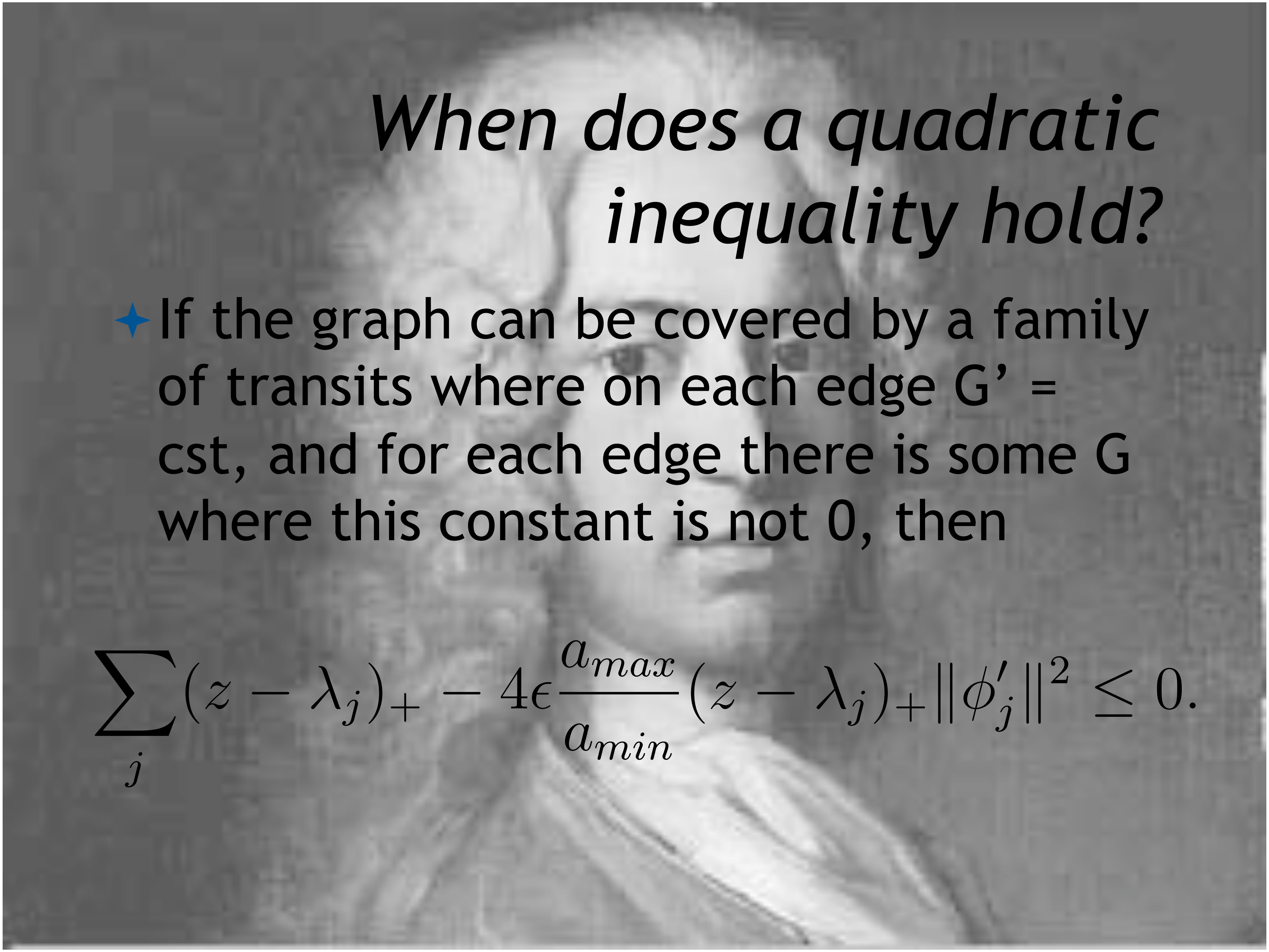
Commutation for loops



Use non-self-adjoint trace formula with $G = e^{iqx_e}$, $q = \frac{2\pi}{L}$, and extend by a constant on exterior parts.

$$T_j \to T_j + \frac{|q|^2}{4},$$

systematically weakening the inequality



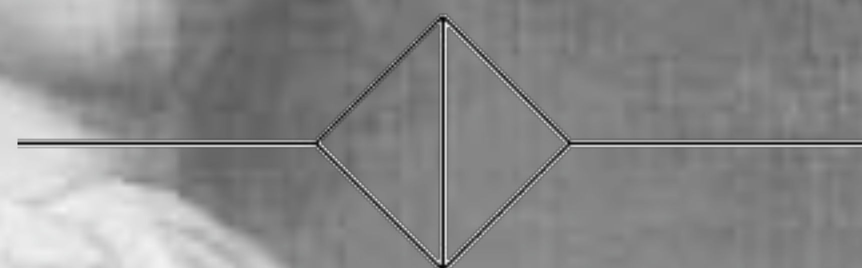
When does a quadratic inequality hold?

- 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

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

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”



Take-away messages #4

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.

Take-away messages #N

THE END