Mathematics of Quantum Mechanics on Thin Structures

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CIMPA

FACULTÉ DES SCIENCES ET TECHNIQUES MARRAKECH

Lecture 2

`You may seek it with trial functions---and seek it with care;
You may hunt it with rearrangements and hope;
You may perturb the boundary with a lump here and there;
You may fool it with some series rope-a-dope---'

Apologies to Lewis Carroll.

The postulates of quantum theory

- Every "observable" is modeled by a self-adjoint operator <A ϕ, ψ> = <ϕ, Aψ> on a Hilbert space. (Complete, normed, linear space. Usually $L^2(\Omega)$, $\langle f, g \rangle := \int_\Omega f(\mathbf{x})\overline{g(\mathbf{x})}dV$.)

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- The possible measurements are sp(A)
  - If A has discrete eigenvalues, it is "quantized."

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$$\|\psi\|^2 = \langle \psi, \psi \rangle = 1$$

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$$\|\psi\|^2 = \langle\psi,\psi\rangle = 1$$

- Expectation values: E(f(A)) =<(A) ψ, ψ>

The postulates of quantum theory

- How do things change in time?
  - There is a Hamiltonian operator, corresponding to the total energy: H, which is a function of momentum **p** and position **x**.

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi.$$

$$\psi(t) = e^{-iHt}\psi(0)$$

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

A brief course on spectral theory

- A *self-adjoint* or *Hermitian* operator on a Hilbert space is a linear mapping with the property that

  $\langle A\varphi,\psi\rangle = \langle\varphi,A\psi\rangle$

  - This means $A = A^*$, the *adjoint* operator
  - $D(A)$ is a dense set but not all of H if A is unbounded. For a differential operator, different boundary conditions (Dirichlet, Neumann) correspond to different choices of $D(A)$.

A brief course on spectral theory

- Hermitian matrices are the self-adjoint operators on the finite-dimensional Hilbert space C^n. The algebraic and analytical properties of self-adjoint operators are similar to those of Hermitian matrices.
  - Diagonalization, orthogonal basis
  - Noncommutative algebra, commutative subalgebra

A brief course on spectral theory

- The *resolvent set* $\rho(H)$ is the set of complex numbers z such that $(H - z)$ has an inverse, known as the *resolvent operator*, $(H - z)^{-1}$, which is continuous.
- The spectrum sp(H) is the complement of $\rho(H)$. The spectrum is a closed set, and if H is self-adjoint, sp(H) is real.

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- The spectrum sp(H) is the complement of $\rho(H)$. The spectrum is a closed set, and if H is self-adjoint, sp(H) is real.
- 2 possibilities: 1. $(H - z)^{-1}$ doesn't exist; or 2. it exists, but not bounded.

A brief course on spectral theory

- An eigenvalue λ of H belongs to sp(H), because if $(H - \lambda)\, u = 0$ for some $u \neq 0$, then $(H - \lambda)$ is not injective. $(H - z)^{-1}$ doesn't exist.
- Eigenvalues are not the only numbers in the spectrum. If a point of the spectrum of a s-a op. is isolated, however, it is an eigenvalue.

A brief course on spectral theory

von Neumann's Spectral Theorem

Suppose $A = A^*$ and $\phi \in \mathcal{H}$, $\phi \in D(A^n)$, $n = 0 \cdots N$. There exists a measure $d\mu_\phi$ supported on $\mathrm{sp}(A)$ such that $\langle \phi, A^n \phi \rangle = \int_{\mathbb{R}} \lambda^n d\mu_\phi(\lambda)$. (In particular, $\|\phi\|^2 = \int_{\mathbb{R}} d\mu_\phi$.) Moreover, for any bounded function f that is continuous on $\mathrm{sp}(A)$, there is a unique bounded operator $f(A)$ such that for any such ϕ, $\langle \phi, f(A)\phi \rangle = \int_{\mathbb{R}} f(\lambda) d\mu_\phi(\lambda)$. The algebra $\{f(A)\}$ is isomorphic to $C[\mathrm{sp}(A)]$, and

$$\|f(A)\|_{\mathrm{sp}} = \sup_{\mathrm{sp}(A)} |f(\lambda)|.$$

Corollary: Rayleigh-Ritz

$$\inf sp(A) = \inf_{\|\varphi\|=1} \langle \varphi, A\varphi \rangle = \inf_{d\mu_\phi} \int \lambda d\mu_\phi$$

(Infimum over probability measures supported on sp(A).)

Corollary: Rayleigh-Ritz

$$\inf sp(A) = \inf_{\|\varphi\|=1} \langle \varphi, A\varphi \rangle = \inf_{d\mu_\phi} \int \lambda d\mu_\phi$$

For $H = -\nabla^2 + V(x)$, φ smooth,

$$\inf sp(H) \leq \frac{\int |\nabla\varphi|^2 + V(x)|\varphi|^2}{\int |\varphi|^2}$$

"Rayleigh quotient."

Three perspicuous examples of spectral analysis

1. Let A be an n×n matrix and Φ an n-vector. Choose a basis of normalized eigenvectors $\{\mathbf{e}_j\}$, so $A\,\mathbf{e}_j = \lambda_j\,\mathbf{e}_j$.
   - Given any function f defined on $\{\lambda_j\}$, f(A) is the diagonal matrix defined by

     $f(A)\,\mathbf{e}_j = f(\lambda_j)\,\mathbf{e}_j$.
   - The measure μ_Φ associated with

     $\Phi = \sum \Phi_j\,\mathbf{e}_j$ is $\sum |\Phi_j|^2\,\delta_{\lambda_j}$

     For instance, $\Phi \bullet A\Phi = \sum |\Phi_j|^2\,\lambda_j$

Three perspicuous examples of spectral analysis

1. Rayleigh-Ritz estimates the lowest eigenvalue from above:

$$\Phi \bullet A\Phi = \Sigma|\Phi_j|^2 \lambda_j \geq \lambda_1 \Sigma|\Phi_j|^2$$

Three perspicuous examples of spectral analysis

2. Let $-\Delta$ be the Laplace operator on the set $L^2(R^d)$ of square-integrable fucntions. There are no eigenfunctions that can be normalized in , but we can “diagonalize” $-\Delta$ with the Fourier transform.

$$\mathcal{F}\left[f\right](\mathbf{k}) = \hat{f}(\mathbf{k}) := \frac{1}{(2\pi)^{d/2}} \int_{R^d} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) dx$$

$$\mathcal{F}^{-1}\left[g\right](\mathbf{x}) = \check{g}(\mathbf{x}) := \frac{1}{(2\pi)^{d/2}} \int_{R^d} e^{+i\mathbf{k}\cdot\mathbf{x}} g(\mathbf{k}) dk$$

Three perspicuous examples of spectral analysis

2. Because for any “test function” φ,

$$\mathcal{F}\left[\frac{\partial \varphi}{\partial x_\alpha}\right](\mathbf{k}) = k_\alpha \hat{\varphi}(\mathbf{k}),$$

$$\mathcal{F}\left[-\Delta \varphi\right]\mathbf{k} = |\mathbf{k}|^2 \hat{\varphi}(\mathbf{k}),$$

and hence for any function f

$$\mathcal{F}\left[f(-\Delta)\varphi\right]\mathbf{k} = f\left(|\mathbf{k}|^2\right)\hat{\varphi}(\mathbf{k}).$$

Three perspicuous examples of spectral analysis

2. .Rayleigh-Ritz tells us the spectrum, while continuous, is nonnegative:

$$\inf sp(-\Delta) = \inf_{||\varphi=1||} \left\langle \hat{\varphi}, |\mathbf{k}|^2 \hat{\varphi} \right\rangle \geq 0$$

Three perspicuous examples of spectral analysis

2. If $u_t = \Delta u$, and we think of u as a finite-dimensional vector and $-\Delta$ as a number ≥ 0, then

$$u(t) = \exp(-(-\Delta)t)\, u(0).$$

With the spectral theorem we define

$\exp(-(-\Delta)t)$ as a bounded operator for any t,

and recover Fourier's solution:

$$u(t,\mathbf{x}) = \mathcal{F}^{-1}\left[e^{-|\mathbf{k}|^2 t}\hat{u}(t,\mathbf{k})\right].$$

Three perspicuous examples of spectral analysis

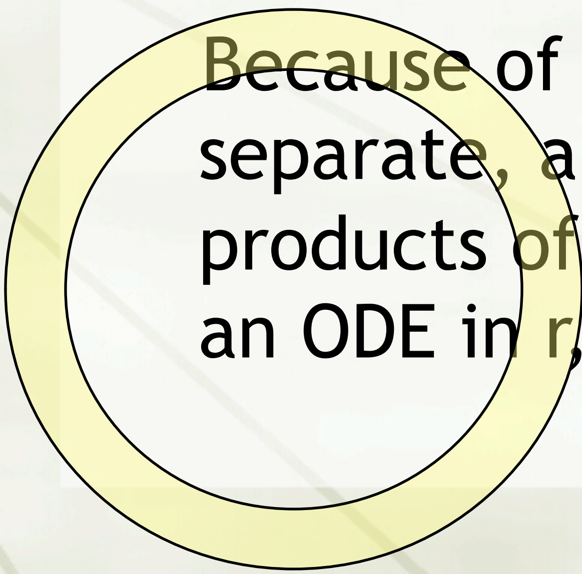
2. **Exercise:** Given a function Φ, what is the associated measure on $sp(-\Delta) = \{\lambda: \lambda \geq 0\}$?

   Hint: Work out the form of μ_Φ by equating λ with $|k|^2$ and changing variables.

Three perspicuous examples of spectral analysis

3. Find the eigenvalues and eigenvectors of the Laplacian on a 2D ring, $1 \le r \le 1+\delta$.

$$\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}$$



Because of the symmetry, variables separate, and the eigenfunctions are products of $\sin(m\ \theta)$ with eigenfunctions of an ODE in r, wich is a version of Bessel’s eqn

Three perspicuous examples of spectral analysis

3. From Kuttler and Sigillito, 1984:

The annulus $a \le r \le b$ has eigenfunctions

$$u_{m,n} = \left[Y_m(k_{m,n})J_m\left(\frac{k_{m,n}r}{a}\right) - J_m(k_{m,n})Y_m\left(\frac{k_{m,n}r}{a}\right)\right][A\cos m\theta + B\sin m\theta], \tag{3.8}$$

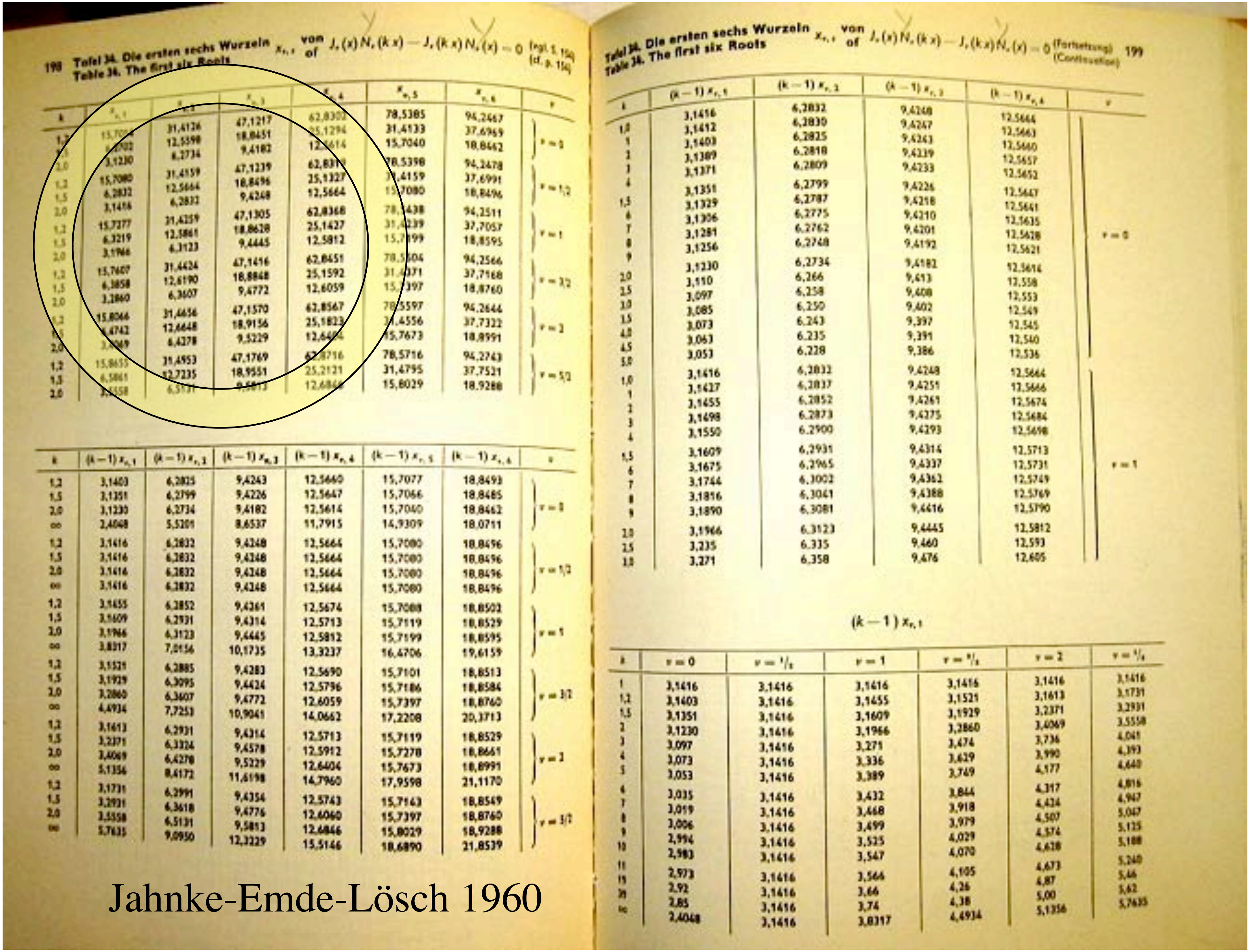
where Y_m is the mth Bessel function of the second kind. The eigenvalues are

$$\lambda_{m,n} = \left(\frac{k_{m,n}}{a}\right)^2, \quad m = 0, 1, 2, \cdots, \ n = 1, 2, \cdots, \tag{3.9}$$

where $k_{m,n}$ is the nth root of

$$Y_m(k)J_m\left(\frac{kb}{a}\right) - J_m(k)Y_m\left(\frac{kb}{a}\right) = 0. \tag{3.10}$$

Tables of these roots are given in [66]. Sectors of an annulus can also be treated similarly.



198 Tafel 34. Die ersten sechs Wurzeln $x_{\nu,s}$ von $J_\nu(x)N_\nu(kx) - J_\nu(kx)N_\nu(x) = 0$ (vgl. S. 15q)
Table 34. The first six Roots $x_{\nu,s}$ of $J_\nu(x)N_\nu(kx) - J_\nu(kx)N_\nu(x) = 0$ (cf. p. 15q)

k	$x_{\nu,1}$	$x_{\nu,2}$	$x_{\nu,3}$	$x_{\nu,4}$	$x_{\nu,5}$	$x_{\nu,6}$	ν
1,2	15,7014	31,4126	47,1217	62,8302	78,5385	94,2467	$\nu = 0$
1,5	6,2702	12,5598	18,8451	25,1294	31,4133	37,6969	
2,0	3,1230	6,2734	9,4182	12,5614	15,7040	18,8462	
1,2	15,7080	31,4159	47,1239	62,8319	78,5398	94,2478	$\nu = 1/2$
1,5	6,2832	12,5664	18,8496	25,1327	31,4159	37,6991	
2,0	3,1416	6,2832	9,4248	12,5664	15,7080	18,8496	
1,2	15,7277	31,4259	47,1305	62,8368	78,5438	94,2511	$\nu = 1$
1,5	6,3219	12,5861	18,8628	25,1427	31,4239	37,7057	
2,0	3,1966	6,3123	9,4445	12,5812	15,7199	18,8595	
1,2	15,7607	31,4424	47,1416	62,8451	78,5504	94,2566	$\nu = 3/2$
1,5	6,3858	12,6190	18,8848	25,1592	31,4371	37,7168	
2,0	3,2860	6,3607	9,4772	12,6059	15,7397	18,8760	
1,2	15,8066	31,4656	47,1570	62,8567	78,5597	94,2644	$\nu = 2$
1,5	6,4742	12,6648	18,9156	25,1823	31,4556	37,7322	
2,0	3,4069	6,4278	9,5229	12,6404	15,7673	18,8991	
1,2	15,8655	31,4953	47,1769	62,8716	78,5716	94,2743	$\nu = 5/2$
1,5	6,5861	12,7235	18,9551	25,2121	31,4795	37,7521	
2,0	3,5558	6,5131	9,5813	12,6866	15,8029	18,9288	

k	$(k-1)\,x_{\nu,1}$	$(k-1)\,x_{\nu,2}$	$(k-1)\,x_{\nu,3}$	$(k-1)\,x_{\nu,4}$	$(k-1)\,x_{\nu,5}$	$(k-1)\,x_{\nu,6}$	ν
1,2	3,1403	6,2825	9,4243	12,5660	15,7077	18,8493	$\nu = 0$
1,5	3,1351	6,2799	9,4226	12,5647	15,7066	18,8485	
2,0	3,1230	6,2734	9,4182	12,5614	15,7040	18,8462	
∞	2,4048	5,5201	8,6537	11,7915	14,9309	18,0711	
1,2	3,1416	6,2832	9,4248	12,5664	15,7080	18,8496	$\nu = 1/2$
1,5	3,1416	6,2832	9,4248	12,5664	15,7080	18,8496	
2,0	3,1416	6,2832	9,4248	12,5664	15,7080	18,8496	
∞	3,1416	6,2832	9,4248	12,5664	15,7080	18,8496	
1,2	3,1455	6,2852	9,4261	12,5674	15,7088	18,8502	$\nu = 1$
1,5	3,1609	6,2931	9,4314	12,5713	15,7119	18,8529	
2,0	3,1966	6,3123	9,4445	12,5812	15,7199	18,8595	
∞	3,8317	7,0156	10,1735	13,3237	16,4706	19,6159	
1,2	3,1521	6,2885	9,4283	12,5690	15,7101	18,8513	$\nu = 3/2$
1,5	3,1929	6,3095	9,4424	12,5796	15,7186	18,8584	
2,0	3,2860	6,3607	9,4772	12,6059	15,7397	18,8760	
∞	4,4934	7,7253	10,9041	14,0662	17,2208	20,3713	
1,2	3,1613	6,2931	9,4314	12,5713	15,7119	18,8529	$\nu = 2$
1,5	3,2371	6,3324	9,4578	12,5912	15,7278	18,8661	
2,0	3,4069	6,4278	9,5229	12,6404	15,7673	18,8991	
∞	5,1356	8,4172	11,6198	14,7960	17,9598	21,1170	
1,2	3,1731	6,2991	9,4354	12,5743	15,7163	18,8549	$\nu = 5/2$
1,5	3,2931	6,3618	9,4776	12,6060	15,7397	18,8760	
2,0	3,5558	6,5131	9,5813	12,6866	15,8029	18,9288	
∞	5,7635	9,0950	12,3229	15,5146	18,6890	21,8539	

Tafel 34. Die ersten sechs Wurzeln $x_{\nu,s}$ von $J_\nu(x)N_\nu(kx) - J_\nu(kx)N_\nu(x) = 0$ (Fortsetzung) 199
Table 34. The first six Roots $x_{\nu,s}$ of $J_\nu(x)N_\nu(kx) - J_\nu(kx)N_\nu(x) = 0$ (Continuation)

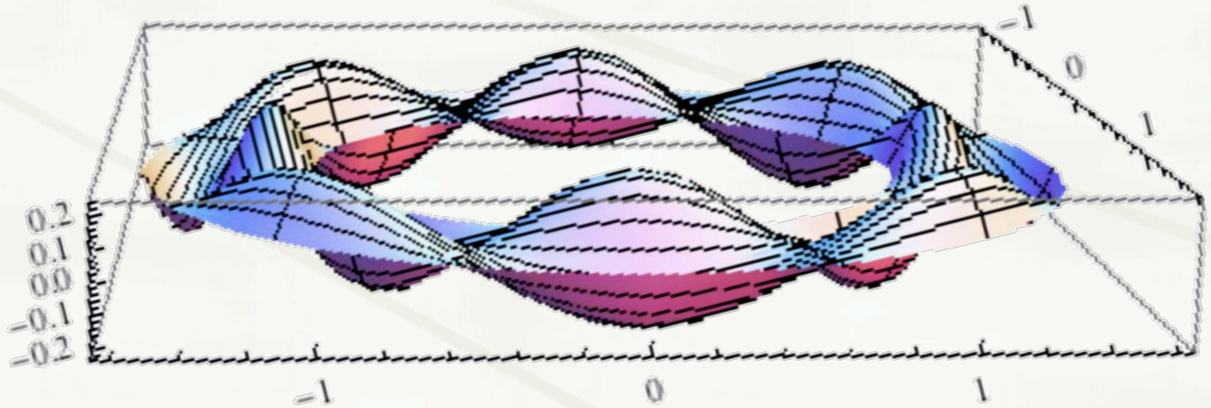
k	$(k-1)\,x_{\nu,1}$	$(k-1)\,x_{\nu,2}$	$(k-1)\,x_{\nu,3}$	$(k-1)\,x_{\nu,4}$	ν
1,0	3,1416	6,2832	9,4248	12,5664	$\nu = 0$
1	3,1412	6,2830	9,4247	12,5663	
2	3,1403	6,2825	9,4243	12,5660	
3	3,1389	6,2818	9,4239	12,5657	
4	3,1371	6,2809	9,4233	12,5652	
1,5	3,1351	6,2799	9,4226	12,5647	
6	3,1329	6,2787	9,4218	12,5641	
7	3,1306	6,2775	9,4210	12,5635	
8	3,1281	6,2762	9,4201	12,5628	
9	3,1256	6,2748	9,4192	12,5621	
2,0	3,1230	6,2734	9,4182	12,5614	
2,5	3,110	6,266	9,413	12,558	
3,0	3,097	6,258	9,408	12,553	
3,5	3,085	6,250	9,402	12,549	
4,0	3,073	6,243	9,397	12,545	
4,5	3,063	6,235	9,391	12,540	
5,0	3,053	6,228	9,386	12,536	
1,0	3,1416	6,2832	9,4248	12,5664	$\nu = 1$
1	3,1427	6,2837	9,4251	12,5666	
2	3,1455	6,2852	9,4261	12,5674	
3	3,1498	6,2873	9,4275	12,5684	
4	3,1550	6,2900	9,4293	12,5698	
1,5	3,1609	6,2931	9,4314	12,5713	
6	3,1675	6,2965	9,4337	12,5731	
7	3,1744	6,3002	9,4362	12,5749	
8	3,1816	6,3041	9,4388	12,5769	
9	3,1890	6,3081	9,4416	12,5790	
2,0	3,1966	6,3123	9,4445	12,5812	
2,5	3,235	6,335	9,460	12,593	
3,0	3,271	6,358	9,476	12,605	

$(k-1)\,x_{\nu,1}$

k	$\nu = 0$	$\nu = 1/2$	$\nu = 1$	$\nu = 3/2$	$\nu = 2$	$\nu = 5/2$
1	3,1416	3,1416	3,1416	3,1416	3,1416	3,1416
1,2	3,1403	3,1416	3,1455	3,1521	3,1613	3,1731
1,5	3,1351	3,1416	3,1609	3,1929	3,2371	3,2931
2	3,1230	3,1416	3,1966	3,2860	3,4069	3,5558
3	3,097	3,1416	3,271	3,474	3,736	4,041
4	3,073	3,1416	3,336	3,629	3,990	4,393
5	3,053	3,1416	3,389	3,749	4,177	4,640
6	3,035	3,1416	3,432	3,844	4,317	4,816
7	3,019	3,1416	3,468	3,918	4,424	4,947
8	3,006	3,1416	3,499	3,979	4,507	5,047
9	2,994	3,1416	3,525	4,029	4,574	5,125
10	2,983	3,1416	3,547	4,070	4,628	5,188
11	2,973	3,1416	3,566	4,105	4,673	5,240
15	2,92	3,1416	3,66	4,26	4,87	5,46
20	2,85	3,1416	3,74	4,38	5,00	5,62
∞	2,4048	3,1416	3,8317	4,4934	5,1356	5,7635

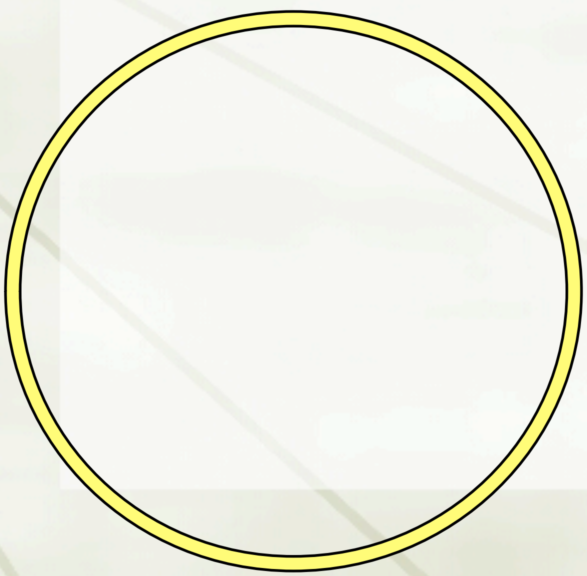
Jahnke-Emde-Lösch 1960

ParametricPlot3D[{r Cos[t], r Sin[t], BesselJ[4, 11.065 r] Cos[4 t]}, {r, 1, 1.592}, {t, 0, 2 Pi}]



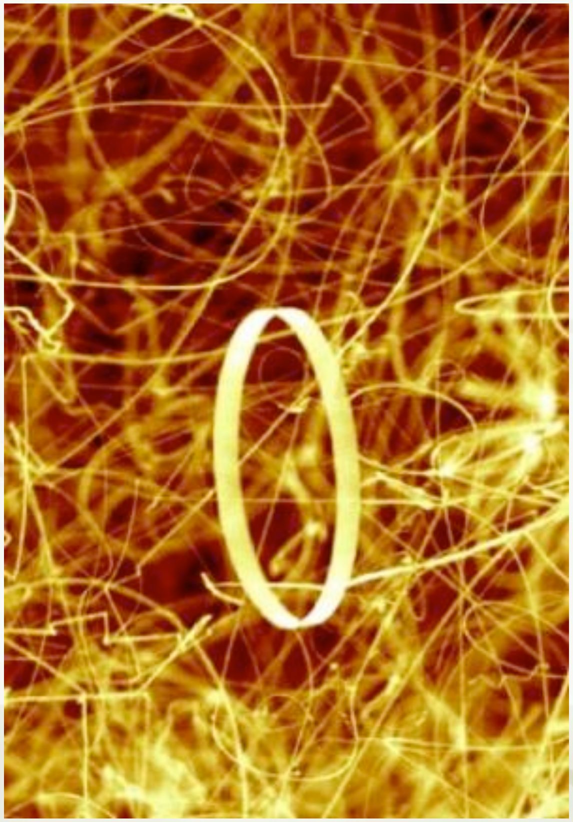
Mathematica 2008

What are the eigenvalues when the ring is thin, i.e., $a = 1$, $b = 1+\delta$?



Zinc oxide quantum wire loop

- Z.L. Wang, Georgia Tech

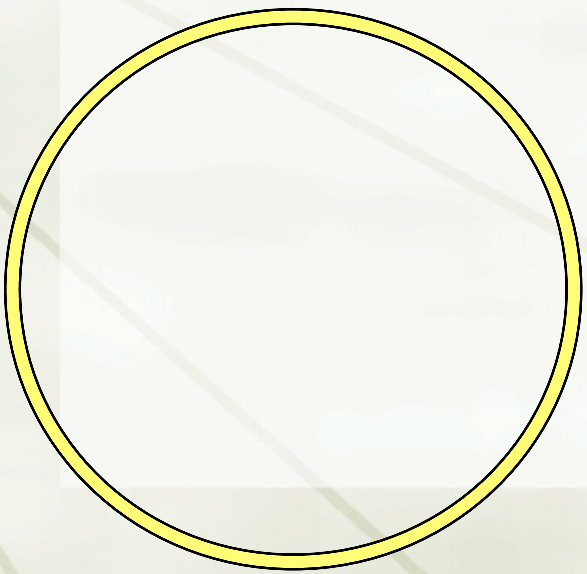


What are the eigenvalues when the ring is thin, i.e., $a = 1$, $b = 1+\delta$?

- ANS: $m^2\pi^2/\delta^2 + 4\, n^2\pi^2 - 1/4 + O(\delta)$

$n = 0, \pm1, \pm2, \ldots;\ m = 1, 2, \ldots$

$$\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}$$



What are the eigenvalues when the ring is thin, i.e., a = 1, b = 1+δ?

- ANS: $m^2\pi^2/\delta^2 + 4\, n^2\pi^2 - 1/4 + O(\delta)$,

n = 0,±1,±2,…; m = 1, 2, …

$$\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}$$

Eigenvalues of the interval (0,δ) (Dirichlet BC)

Eigenvalues of the ring (periodic BC)

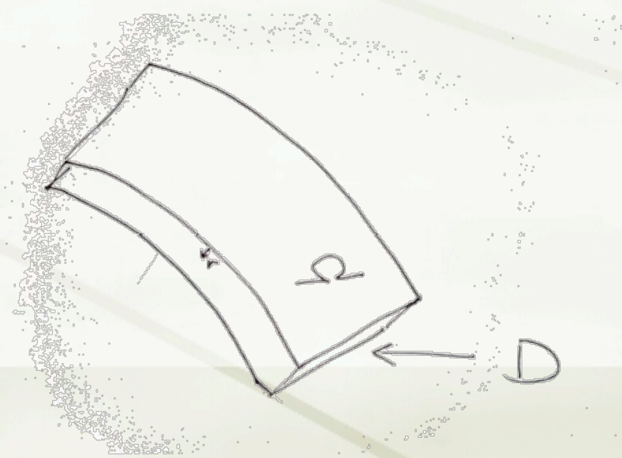
To O(δ) it is as if the variables θ and r separate as *Cartesian* variables. *Except that there is a correction -1/4. This is the effect of curvature.*

Thin structures and local geometry

Thin domain of fixed width
variable r= distance from edge

Energy form in separated variables:

$$\int_D |\nabla_{\|}\, \zeta|^2\, d^{d+1}x + \int_D |\zeta_r|^2\, d^{d+1}x$$



The result:

$$-\nabla_{\|}^{2} + q(\mathbf{x}) = -\Delta_{\Omega} + q(\mathbf{x})$$

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

which reduces to -1/4 when Ω is a circle of radius 1.

Weapons used when hunting for eigenvalues

- Rayleigh-Ritz
- Other variational principles, such as min-max
- Approximate eigenvalues
- Perturbation theory
  - If an eigenvalue and eigenvector are known for A, solve

$$(A + \kappa B)u(\kappa) = \lambda(\kappa)u(\kappa)$$

with power series in κ.

Fun with Rayleigh and Ritz

How does a spectral theorist estimate π²?

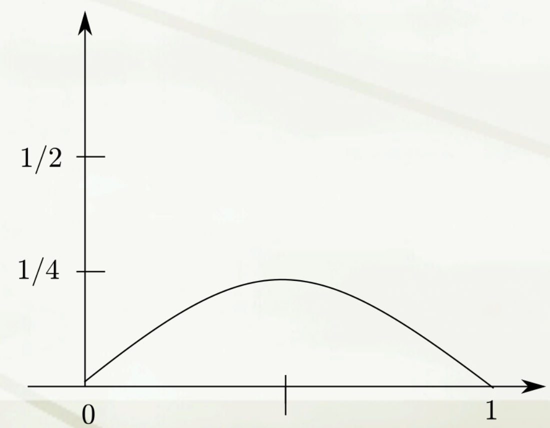
We know $-\frac{d^2}{dx^2}\sin(n\pi x) = n^2\pi^2\sin(n\pi x)$, vanishing BC at $0, 1$, $\lambda_n = n^2\pi^2$.

According to Rayleigh-Ritz,

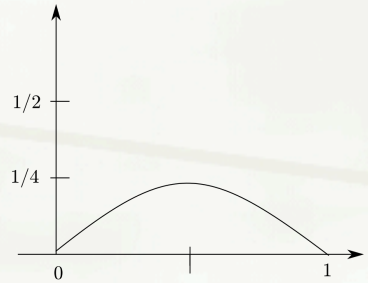
$$\pi^2 \leq \frac{\langle \varphi, \frac{-d^2}{dx^2}\varphi \rangle}{\langle \varphi, \varphi \rangle} = \frac{\int_0^1 |\varphi'(x)|^2 dx}{\int_0^1 |\varphi(x)|^2 dx}.$$

The sine function is transcendental. It would be nicer if φ were a polynomial.

Let's try $\varphi(x) = x(1-x)$, $0 \leq x \leq 1$.



How does a spectral theorist estimate π²?



$$\pi^2 \leq \frac{\int_0^1 (1 + 4x^2 - 4x)dx}{\int_0^1 (x^2 + x^4 - 2x^3)dx} = \frac{1 + 4/3 - 2}{1/3 + 1/5 - 1/2} = 10$$

Cf. 9.8696044. 10 is too large by 1.32%.

What about a lower bound?

Rayleigh and Ritz like to guess that an eigenvalue is

$$\lambda_\kappa \approx \eta_\kappa := \langle\varphi_k, H\,\varphi_k\rangle,$$

where the trial function is chosen cleverly. For λ_1 this is always a bit too high. *If* the eigenvalue is known to be isolated, Temple's inequality offers a counterpart:

$$\lambda_1 \geq \eta_1 - (\langle H\varphi_k, H\,\varphi_k\rangle - \eta_1^2)/(\text{isolation from above})$$

Kato's Improvement of Temple's Inequality

A is a self adjoint operator such that $\mathrm{sp}(A) \cap (\alpha, \beta) = \lambda_*$. For $\varphi \in D(A)$, $\|\varphi\| = 1$, $|\eta| = \langle \varphi, A\varphi \rangle$, $\epsilon^2 = \|A\varphi\|^2 - \eta^2$. Then

$$\epsilon^2 \leq (\beta - \eta)(\eta - \alpha) \Longrightarrow \eta - \frac{\epsilon^2}{\beta - \eta} \leq \lambda_* \leq \eta + \frac{\epsilon^2}{\eta - \alpha}$$

Proof. EXERCISE: Hint:

(1) Assume $\mathrm{sp}(A) \cap (\alpha', \beta') = \phi$. Then $\nu \in \mathrm{sp}(A) \Rightarrow \left| \nu - \frac{\alpha + \beta}{2} \right| \geq \frac{\beta' - \alpha'}{2}$

(2) Square and show $\nu^2 - \eta^2 \geq (\alpha + \beta')\nu - \alpha\beta' - \eta^2$. If $\|\varphi\| = 1$, $d\mu_\phi$ is a probability measure, and by integrating

$$\epsilon^2 \geq (\alpha' + \beta')\eta - \alpha'\beta' - \eta^2 = (\eta - \alpha)(\beta - \eta)$$

Contradicting assumption.

(3) Given, ϵ, η, $\alpha' = \alpha$, choose β' optimally. Given ϵ, η, $\beta' = \beta$, choose α'optimally.

How does a spectral theorist estimate π²?

What About a Lower Bound?

Temple's inequality. We know $\pi > 3$, so $\lambda_2 \geq 4 \cdot 9 = 36$.

$$\lambda_1 \geq \langle \varphi, A\varphi \rangle - \frac{\|A\varphi\|^2 - \langle \varphi, A\varphi \rangle^2}{36 - \langle \varphi, A\varphi \rangle} = 10 - \frac{1}{\phi} \frac{\left(\int_0^1 (\varphi'')^2 dx\right) - 100}{26}$$
$$= 10 - \frac{120 - 100}{26} \doteq 9.23.$$

Improvement. Project into subspace of functions even under $x \leftrightarrow 1 - x$. The second eigenvalue becomes $\lambda_3 > 9 \cdot 9, and$

$$\lambda_1 \geq 10 - \frac{120 - 100}{71} \quad \doteq \quad 9.72.$$

(Too small by 1.5%)

Weapons used when hunting for eigenvalues

- Rayleigh-Ritz
- Other variational principles, such as min-max
  - λ_k = max min $<\varphi, A\varphi>$, φ normalized and orthogonal to a k-1 dimensional subspace.

Weapons used when hunting for eigenvalues

- Rayleigh-Ritz
- Other variational principles, such as min-max
- Approximate eigenvalues, i.e., sequences

$$\|\varphi_n\| = 1, \text{ such that } \|(H - \lambda)\varphi_n\| \to 0.$$

Weapons used when hunting for eigenvalues

- Rayleigh-Ritz
- Other variational principles, such as min-max
- Approximate eigenvalues
- Perturbation theory
  - If an eigenvalue and eigenvector are known for A, solve

$$(A + \kappa B)u(\kappa) = \lambda(\kappa)u(\kappa)$$

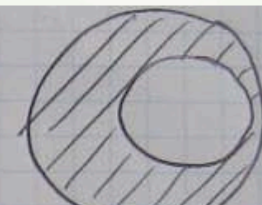
  with power series in κ.

*1. If the volume is fixed, what shape **mini**mizes the fundamental eigenvalue?*

- Answer: The ball. Conjectured by Rayleigh, proved by Faber and Krahn.
- A modern proof combines the Rayleigh-Ritz inequality, the notion of rearrangement, the “co-area formula,” and the isoperimetric inequality.

*2 Cases where Ω is annular and λ_1 is **max**imixed by the circularly symmetric case.*

constant
width.
One curved edge (inner)
fixed at length = 1



$g \to \quad |dx|^2 = dr^2 + (1+Kr)^2 dt^2$ $\qquad K(t)$ - curvature on edge.

$$\int |\nabla\varphi|^2 d^2x = \int_0^\delta \int_0^1 \left(\varphi_r^2 + \frac{\varphi_t^2}{(1+Kr)^2}\right)(1+Kr)\,dt\,dr$$

Rayleigh quotient with φ <u>indep</u> of t:

$$\lambda_1 \le \int_0^\delta \int_0^1 \varphi_r^2 (1+Kr)\,dt\,dr = \int_0^\delta \varphi_r^2 (1+2\pi r)\,dr = \lambda_1^* \text{ if}$$

$\varphi \to u_1 \text{(ann)}$

Spherical Shells. Infinitesimal case.

Suppose $\Omega \cong S^2 \subset \mathbb{R}^3$. $\lambda_{1,2}(-\Delta + q(K))$?

$$q(K) = -\frac{(K_1 - K_2)^2}{4} \qquad \left(\text{similar for } -c^{K_1 K_2}, \text{ etc.}\right)$$

$$\lambda_1 \le \frac{\int |\nabla 1|^2 + \int q(K)}{\int 1} = 0 + \langle q \rangle \le 0$$

$=$ iff sphere. (WHY?)

Same argument for Ω = circle

- $q(\kappa) = -\kappa^2/4$
- $\lambda_1 \le -\langle\kappa^2\rangle/4 \le -\langle\kappa \bullet 1\rangle^2/4$ (Cauchy-Schwarz)

  $= -\pi^2$
- Equality iff sphere. (Why?)

Proof outline for the Faber-Krahn theorem

Spherical rearrangement

- Any (say, continuous, non-negative, compactly supported) function $f(x)$ can be rearranged to a radially decreasing $f^*(x)$ so that
  $\mu(f^*(x) \geq h) = \mu(f(x) \geq h)$.

- Integrals of $g(f(x))$ are unaffected by this rearrangement.

Co-area formula

- Given a (say, smooth, non-negative, compactly supported) function $f(x)$ on Ω (and assuming $\nabla f = 0$ only on a null subset) , what happens when you change variables to include $h = f(x)$?
- Ans: $dV = (dS(f^{-1}(h))/|\nabla f|)\ dh$
- Area on "level set"

Faber-Krahn

- What happens to a Dirichlet integral when you rearrange the function?
- Consider the quantity

$$I = \int_0^{\|f\|_\infty} \int_{f^{-1}(h)} ds \, dh$$

Faber-Krahn

$$I = \int_0^{\|f\|_\infty} \int_{f^{-1}(h)} dS\, dh$$

The Cauchy-Schwarz-Буняковский inequality states $\left(\int g\, h\, du\right)^2 \le \int g^2 du \int h^2 du$,

so

$$I^2 \le \int_0^{\|f\|_\infty} \int_{f^{-1}(h)} |\nabla f|\, dS\, dh \cdot \int_0^{\|f\|_\infty} \int_{f^{-1}(h)} \frac{1}{|\nabla f|}\, dS\, dh$$

$$= \int_\Omega |\nabla f|^2 dV \cdot \mathrm{Vol}(\Omega)$$

Faber-Krahn

Meanwhile, since $f^{-1}(h)$ is the surface bounding the set $\{x: f(x) \ge h\}$, the volume of which is unchanged by symmetrization,

$$\int_{f^{-1}(h)} dS \ge \int_{f^{*-1}(h)} dS \qquad \text{(Isoperimetric thm).}$$

$$\therefore\ I^2 \ge I^{*2} = \int_{\Omega^*} |\nabla f^*|^2 \, dV \cdot \mathrm{Vol}(\Omega)$$

Yet another "isoperimetric theorem," this time for λ_2.

- Consider the thin-domain operator on a closed, simply connected surface in R^3,

$$- \nabla^2 - (\kappa_2 - \kappa_1)^2/4.$$

- The ground state is maximized (at 0) by the sphere. Let's fix the area and ask after the maximum of the second eigenvalue.

Yet another "isoperimetric theorem," this time for λ_2.

Eigenfunctions of a self-adjoint operator, with different eigenvalues, are orthogonal. Therefore if we search over φ orthogonally to u_1,

$$\lambda_2 \leq \langle\varphi, A\,\varphi\rangle/\|\varphi\|^2.$$

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$$\lambda_2 \leq \langle \varphi, A\, \varphi \rangle / \|\varphi\|^2.$$

Problem: We don't know u_1 *a priori*. One way around this is a lemma of J. Hersch:

Yet another "isoperimetric theorem," this time for λ_2.

Lemma. *(J. Hersch). Let Ω be a two-dimensional, closed, smooth Riemannian manifold of the topological type of the sphere, and specify a bounded, positive, measurable function ρ on Ω. Then there exists a conformal transformation $\Phi : \Omega \to S^2 \subset R^3$, embedded in the standard way as the unit sphere, such that*

$$\int_{S^2} \mathbf{x}\rho(\Phi^{-1}(\mathbf{x}))J d\hat{S} = \mathbf{0}. \tag{3}$$

Jacobian

Yet another "isoperimetric theorem," this time for λ_2.

For the trial function φ let's choose one of the Cartesian coordinates x,y,z on S^2, but "pull back" to Ω with the inverse of Hersch's conformal transformation. Let the resulting functions on Ω be called X,Y,Z. What do we know about X,Y,Z?

Yet another "isoperimetric theorem," this time for λ_2.

For the trial function φ let's choose one of the Cartesian coordinates x,y,z on S^2, but "pull back" to Ω with the inverse of Hersch's conformal transformation. Let the resulting functions on Ω be called X,Y,Z. What do we know about X,Y,Z?

1. The functions X,Y,Z are orthogonal, because the functions x,y,z are orthogonal on S^2.
   * Note: The restrictions of x,y,z to S^2 are the spherical harmonics = eigenfunctions:
     - $- \nabla^2 x = 2\ x,$
     - $- \nabla^2 y = 2\ y,$
     - $- \nabla^2 z = 2\ z,$

Yet another "isoperimetric theorem," this time for λ_2.

For the trial function φ let's choose one of the Cartesian coordinates x,y,z on S^2, but "pull back" to Ω with the inverse of Hersch's conformal transformation. Let the resulting functions on Ω be called X,Y,Z. What do we know about X,Y,Z?

1. The functions X,Y,Z are orthogonal.
2. $X^2 + Y^2 + Z^2 = 1$, because $x_1^2 + x_2^2 + x_3^2 = 1$.

Yet another "isoperimetric theorem," this time for λ_2.

For the trial function φ let's choose one of the Cartesian coordinates x,y,z on S^2, but "pull back" to Ω with the inverse of Hersch's conformal transformation. Let the resulting functions on Ω be called X,Y,Z. What do we know about X,Y,Z?

1. The functions X,Y,Z are orthogonal.
2. $X^2 + Y^2 + Z^2 = 1$, because $x_1^2 + x_2^2 + x_3^2 = 1$.
3. Identifying now ρ with u_1,
   $\langle X,u_1\rangle = \int_{S^2} \mathbf{x}\rho(\Phi^{-1}(\mathbf{x}))J d\hat{S} = \mathbf{0}$. Likewise for Y, Z.

Ready to roll with Rayleigh and Ritz:

Let's choose the trial function in

$$R(\zeta) := \frac{\int_\Omega |\nabla \zeta|^2 dS - \frac{1}{4}\int_\Omega (\kappa_2 - \kappa_1)^2 |\zeta|^2 dS}{\int_\Omega |\zeta|^2 dS}$$

as ζ =X, Y, or Z. Considering for example X, conformality implies that

$$\int_\Omega |\nabla X|^2 dS = \int_{S^2} |\nabla x|^2 d\hat{S} = \frac{8\pi}{3}$$

Ready to roll with Rayleigh and Ritz:

Observing that

$$a \leq \frac{b_j}{c_j}$$

$\Rightarrow$

$$a \leq \frac{\sum_j b_j}{\sum_j c_j} :$$

$$\lambda_2 \leq \frac{8\pi - \int_\Omega (\kappa_2 - \kappa_1)^2 dS}{\int_\Omega 1 dS}.$$

Equality iff sphere. Why?