Math 116 : LECTURE 12

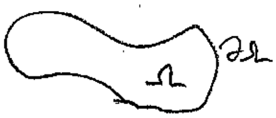
① Barnett
2/14/06

METHOD OF PARTICULAR SOLUTIONS (MPS).

- As we have seen, handling layer potentials correctly requires care (singularities in BIEs).
- Here's a method for the same linear, const-coefficient PDEs, that can solve BVPs and eigenproblems, which is
  - i) even simpler
  - ii) scales the same way, ie $\underset{\text{\# degrees of freedom.}}{N} \propto \overset{\text{wavenumber for Helmholtz.}}{k} \cdot \text{perimeter}$ $(d=2)$ ← means it's a 'boundary method'.
  - iii) a current topic of research.

Let's focus on solving...

Dirichlet Eigenproblem:



$$\begin{cases} (\Delta + k_j^2)\phi_j = 0 & \text{in } \Omega \\ \phi_j = 0 & \text{on } \partial\Omega \end{cases}$$

normalize $\int_\Omega |\phi_j|^2 dx = 1$, choose $\phi_j(\overset{x \in \mathbb{R}^d}{x})$ real

Want: $\left.\begin{array}{l} k_j = \text{eigenwavenumber} \\ \phi_j = \text{eigenmode} \end{array}\right\} j = 1, 2, \cdots \infty$

$\rightarrow k_1 < k_2 \le k_3 \le \cdots$, may have degeneracies $\overbrace{k_i = k_{i+1} = \cdots = k_{i+m-1}}^{m\text{-fold, } \mathrm{Span}\{\phi_j\}_{j=i \cdots i+m-1} = \text{eigenspace,}}$

We don't know k_j's , but start with a guess: wavenumber parameter k.

If $k = k_j$ then there is nontrivial $\underset{(\text{a multiple of } \phi_j)}{\underline{\text{function } u}}$ s.t. ① $(\Delta + k^2) u = 0$ in Ω ← (Helmholtz Eqn.)

② $\int_{\partial\Omega} |u|^2 ds = 0$

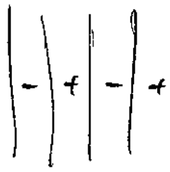
Numerically, we satisfy ① by approximating u by $u = \sum_{i=1}^{N} \alpha_i \xi_i$

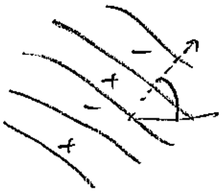
$\vec{a}$ = coeff. vector → ; ↖ 'basis funcs', each satisfies ①.

The basis funcs should be analytically known Helmholtz solutions in Ω, but they need <u>not</u> satisfy the Dirichlet BC (if they did, they would already be eigenmodes!).

Eg. $\xi_i(x) = \begin{cases} \sin(k \hat{d}_i \cdot x) & , 1 \le i \le \frac{N}{2} \\ \cos(k \hat{d}_{i-N/2} \cdot x) & , \frac{N}{2} < i \le N. \end{cases}$ unit direction vectors in $[0, \pi)$

"plane waves"

eg. $\xi_1(x)$ is 

$\xi_{\pi/6}(x)$ is 

these are real-valued Helmholtz solutions (everywhere in $\mathbb{R}^2$) which are easy to evaluate .... 'Particular Solutions'.

Numerically, satisfy ⓘⓘ by minimizing $\int_{\partial\Omega} |u|^2 ds =: \overset{\text{"tension" (on boundary).}}{t[u]}$ for $u \in \mathrm{Span}\{\xi_i\}$

- Clearly, the trivial solution $u \equiv 0$, given when $\vec{a} = \vec{0}$, minimizes $t[u]$
- So modify using assumption that $\{\xi_i\}$ are <u>linearly-independent</u> funcs over Ω,

which means: $u \equiv 0 \Rightarrow \vec{a} = \vec{0}$

and more importantly: $\vec{a} \neq \vec{0} \Rightarrow u$ not identically zero in Ω

An idea is then to use $\|\vec{a}\|_2$ as some kind of norm of u in Ω, and fix it to unity:

$$t(k) := \min_{\|\vec{a}\|_2 = 1} t[u] \quad = \min_{\vec{a} \neq \vec{0}} \frac{t[u]}{\|\vec{a}\|_2^2} \quad , \text{with } u = \sum_i a_i \xi_i$$

If k = some eigenwavenumber k_j,
then would expect as $N \to \infty$, if the basis is 'complete' in some way,
that $t(k) \to 0$, hence Dirichlet BCs become arbitrarily close to being satisfied, $u \to$ eigenmode.

But, if $k \neq k_j$,
no such sequence exists as $N \to \infty$, and $t(k)$ reaches some minimum > 0.

Boundary integral:

As we know, $\int_{\partial\Omega} |u|^2 ds \approx \sum_{j=1}^{M} w_j |u(\overset{\text{boundary points, eg equally spaced in } \theta.}{y_j})|^2$ where weights are eg. $w_j = \Delta\theta \cdot \left.\frac{ds}{d\theta}\right|_{s_j}$

is spectrally convergent for analytic funcs, on analytic $\partial\Omega$.

Note $\sum_j w_j |u(y_j)|^2 = \|\vec{b}\|_2^2$, $\vec{b} \in \mathbb{R}^M$

where $b_j := \sqrt{w_j}\, u(y_j) = \sqrt{w_j} \sum_{i=1}^{N} a_i \xi_i(y_j) = (A\vec{a})_j$

where matrix $A_{ji} := \sqrt{w_j}\, \xi_i(y_j)$, $j = 1 \cdots M$, $i = 1 \cdots N$.

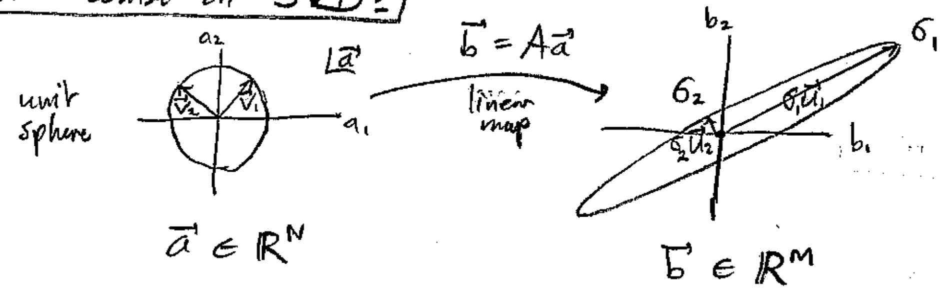
So,
$t[u] \approx \sum_j w_j |u(y_j)|^2 = \|A\vec{a}\|_2^2$ to arbitrary accuracy as choose M large enough.

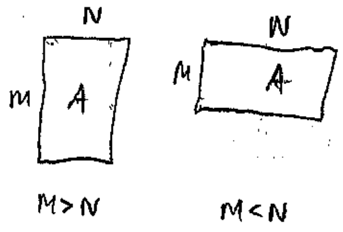
Given k parameter, and basis funcs $\{\xi_j\}$, then minimization problem is now,

$$\text{find } t(k) = \min_{\vec{a} \neq \vec{0}} \frac{\|A\vec{a}\|_2^2}{\|\vec{a}\|_2^2} \qquad (*)$$

This linear algebra problem has known solution, $t(k) = \sigma_{\min}^2$ ← smallest singular value of A.

Crash course on SVD:

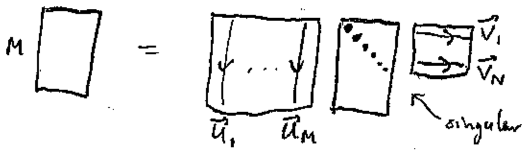




singular values $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_r$, where $r = \min(M,N)$, give semiaxes of ellipsoid, image of unit sphere.
↑ smallest one

Any matrix can be decomposed $A = U \Sigma V^T$ ← diagonal matrix of $\{\sigma_1, \dots \sigma_r\}$

eg M>N case



↖ singular values. $\sigma_1 \cdots \sigma_N$ since $r = N$

U, V orthogonal.

any linear xform = rotation, followed by rescaling along coord axes, followed by rotation.

$\{\vec{u}_k\}$ left singular vectors
$\{\vec{v}_k\}$ right " "

$\text{rank}(A) = \#$ nonzero σ_k's

$\left.\begin{matrix}\vec{v}_1 \\ \vec{v}_r\end{matrix}\right\}$ is the unit vector which is expanded by A $\left\{\begin{matrix}\text{most,} \\ \text{least}\end{matrix}\right.$ giving $\left\{\begin{matrix}A\vec{v}_1 = \sigma_1\vec{u}_1 \\ A\vec{v}_r = \sigma_r\vec{u}_r\end{matrix}\right.$

Theorem: Every $A \in \mathbb{C}^{m \times n}$ has an SVD, $\{\sigma_k\}$ uniquely defined, and if they are distinct then $\{\vec{u}_k\}$ and $\{\vec{v}_k\}$ uniquely defined (up to complex scalar factors of magnitude 1).

(Proof: see Trefethen & Bau, "Numerical Linear Algebra" (SIAM, 1997), induction argument starting by isolating largest direction u_1, etc).

Conclusion: (*) given by $t(k) = \sigma_r^2$, achieved with $\vec{a} = \vec{v}_r$

Note: condition # $\text{cond}(A) = \dfrac{\sigma_{\max}}{\sigma_{\min}} = \dfrac{\sigma_1}{\sigma_r}$, so this blows up when $t(k) \to 0$.
(cf. HW2, Qu. 2).

So, we have found the unit vector $\vec{a}$ which minimizes L_2 norm on $\partial\Omega$, as approximated by the (weighted) ℓ_2-norm on a bunch of boundary points.

This was the original MPS* (Fox, Henrici & Moler, 1967).

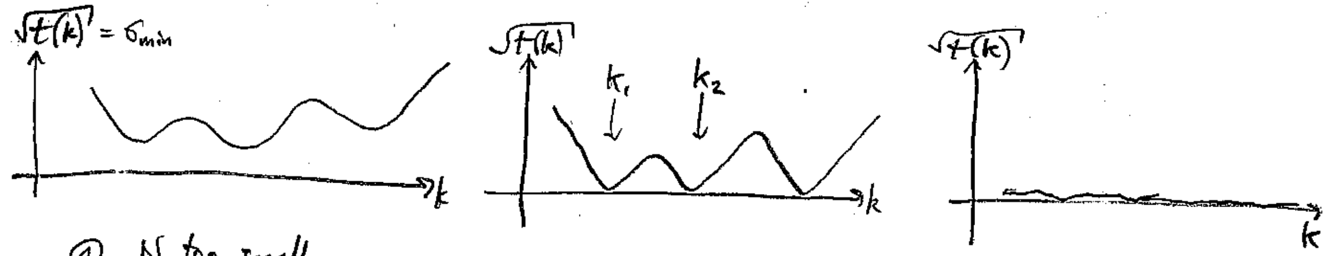
inventor of MatLab; the logo  is MPS on L-shaped domain!

*except different ξ_i were used.

In summary, algorithm: (first pick N).

- i) choose k
- ii) fill A_{ij} matrix
- iii) set $t(k) = \sigma_r$ from SVD(A)
- iv) search along k axis for places where $t(k)$ very small.
  — these are the k_j, and modes ϕ_j have basis coeffs given by corresponding singular vector $\vec{a} = \vec{v}_r$

Typical plots:



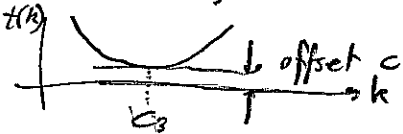
① N too small to represent ϕ_j accurately; never find small boundary values.

② N about right.

③ N too large: at *every* k there are basis combinations with $|\vec{a}|=1$ which are very small on $\partial\Omega$ (and in Ω)

You may use a simple minimum-finding algorithm on $t(k)$:

Eg, since $t(k)$ is approx a parabola



$t(k) \approx c_2(k-c_3)^2+c_1$

Use 3 nearby samples of $t(k)$ at $k^{(1)}, k^{(2)}, k^{(3)}$, to compute offset c_1, curvature c_2 & location c_3. Add this c_3 to the list of samples & remove the $k^{(i)}$ which is *furthest* from c_3. iterate until all 3 k-values in list are within desired accuracy of each other.

Or, if you are willing to package your $t(k)$ function in the right way, you could use MatLab's fminbnd 1d optimization command.

Math 116 : LECTURE 13.

① Barnett
2/16/06

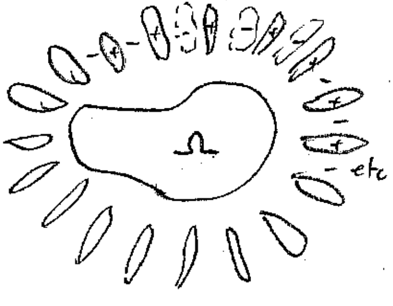
- Fixing the MPS
- Accuracy of MPS

Normalization problem:

- As increase basis size N, there arise funcs $u = \sum_{i=1}^{N} a_i \xi_i$ which are exponentially (in N) small <u>everywhere</u> in $\overline{\Omega}$, but $\|\vec{a}\|_2 = 1$!
- This means $\{\xi_i\}$ exp. close to linearly <u>dependent</u>, A matrix $\to$ (numerically) singular for all k values! ($\sigma_r \approx 0$ $\forall k$, bad).

This is (believed to be) a generic property of basis funcs obeying Helmholtz eqn...

Example for plane waves:



'high angular momentum state' (physicists speak)

$$u(r,\theta) = e^{-i\ell\theta} \cdot J_\ell(kr) = \frac{1}{2\pi i^\ell}\int_0^{2\pi} e^{ikr\cos\phi}\, e^{i\ell(\phi-\theta)}\, d\phi$$

↑ polar coords.

since $J_\ell(z) = \frac{1}{2\pi i^\ell}\int_0^{2\pi} e^{iz\cos\phi + i\ell\phi}\, d\phi$

"Bessel is integral over plane waves $e^{ikr\cos\phi}$, with sinusoidal weight $e^{i\ell\phi}$"

Within any fixed-radius ball $r \le R$, $J_\ell(kr)$ becomes exponentially small, as $\ell \to \infty$,

since, $J_\ell(z) \sim \frac{1}{\Gamma(\ell+1)}\left(\frac{z}{2}\right)^\ell$ asymptotic form for $z \ll \ell$.

Numerically you find singular vectors $\vec{v}_r$ for small σ_r look just like this...

Cure:

(Barnett 2000, Betcke-Trefethen 2004).

$$t[u] := \frac{\int_{\partial\Omega} |u|^2 ds}{\int_\Omega |u|^2 dx} \longleftarrow \text{ensures normalization over } \Omega.$$

and, as before, $t(k) = \min_{u \in \mathrm{span}\{\xi_i\}} t[u]$

We only need to estimate $\int_\Omega |u|^2 dx$ to low accuracy, so use Q interior points.

$\Omega \ni q_j$ $j = 1 \cdots Q$.

$$\int_\Omega |u|^2 dx \approx \frac{1}{Q}\sum_{j=1}^{Q} |u(q_j)|^2 = \|B\vec{a}\|_2^2 \quad \text{where } B_{ji} = \frac{1}{\sqrt{Q}}\xi_i(q_j)$$

Now, once basis representation of u is inserted, get

$$t(k) = \min_{\vec{a} \neq \vec{0}} \frac{\|A\vec{a}\|_2^2}{\|B\vec{a}\|_2^2}$$

this linear algebra problem is solved either by

two are intimately related

i) Generalized SVD : $t(k)$ is σ_r^2, the minimum generalized sing. val.
  – approach of Betcke 2006. "gsvd(a,b)" in matlab.

ii) Generalized eigenvalues. – my approach... happy for you to use.
  $t(k) = \lambda_1$, the lowest generalized eigenvalue of A^TA, B^TB.
  "eig(a'*a, b'*b)" in matlab.

Recall:
- λ an eigenvalue of $F \in \mathbb{C}^{n \times n}$ if $(F - \lambda I)$ singular.
- if A has singular values σ_k then $F = A^TA$ has eigenvalues $\lambda_k = \sigma_k^2$
- λ is a generalized eigenvalue of the matrix 'pencil' (F, G), $F, G \in \mathbb{C}^{n \times n}$, if $(F - \lambda G)$ singular.
- if (A,B) have gen. sing. vals. σ_k then 'pencil' (A^TA, B^TB) has gen. eigvals $\lambda_k = \sigma_k^2$.

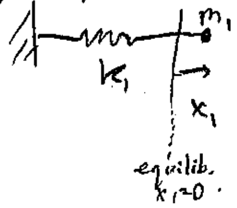
Note $F = A^TA$ and $G = B^TB$ are symmetric positive semi-definite, $\forall A, B$.

Numerical detail : F & G both become singular as N increases
(their condition #s are exponentially large in N, above a certain N_0).
$\Rightarrow$ matlab's eig(F,G) will eventually fail. (QZ algorithm).
A regularization method is described in my preprint to cure this;
I imagine you can keep N small enough to avoid this.

Another application of Generalized Eigenvalue Problem: (an interlude).

Normal modes of (linearized) elastic systems

1 mass, 1 spring

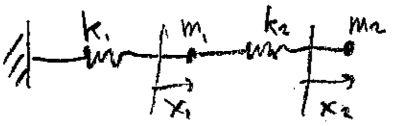


$$m_1\ddot{x}_1 \overset{\text{Newton's 2nd Law}}{=} F_1 \overset{\text{Hooke's Law}}{=} -k_1 x_1$$

ie $\ddot{x}_1 + \frac{k_1}{m_1}x_1 = 0$,

$$\boxed{\begin{array}{l} x_1(t) = a\cos\overset{\omega_1}{\sqrt{\tfrac{k_1}{m_1}}}\,t + b\sin\sqrt{\tfrac{k_1}{m_1}}\,t \\ \text{general solution} \\ = \mathrm{Re}\left[Ae^{-i\omega_1 t}\right],\quad A\in\mathbb{C} \end{array}}$$

2 masses, 2 springs



$$m_1\ddot{x}_1 = F_1 = -k_1x_1 + k_2(x_2-x_1)$$

$$m_2\ddot{x}_2 = F_2 = -k_2(x_2-x_1)$$

ie
$$\underbrace{\begin{pmatrix} m_1 & 0 \\ 0 & m_2\end{pmatrix}}_{\text{'mass' (inertia) matrix}}\begin{pmatrix}\ddot{x}_1\\ \ddot{x}_2\end{pmatrix} = -\underbrace{\begin{pmatrix} k_1+k_2 & -k_2 \\ -k_2 & k_2\end{pmatrix}}_{\text{'spring matrix'. (symmetric by Newt. 3rd Law)}}\begin{pmatrix}x_1\\ x_2\end{pmatrix}$$

ie (*) $\underline{\underline{M}}\,\ddot{\vec{x}} = -\underline{\underline{K}}\,\vec{x}$

note $\begin{cases} E_k = \text{Kinetic energy} = \frac{1}{2}\dot{\vec{x}}^T\underline{\underline{M}}\,\dot{\vec{x}} \\ E_p = \text{Potential energy} = \frac{1}{2}\vec{x}^T\underline{\underline{K}}\,\vec{x}\end{cases}$

N masses : $\underline{\underline{M}}$, $\underline{\underline{K}}$ are symmetric, positive definite. → on physical grounds (E_p, E_k bounded from below).

Look for particular time-harmonic solutions $\vec{x}(t) = \vec{v}\,e^{-i\omega t}$ (real part taken implicitly)

$$\partial_t^2\Big\{\ \ddot{\vec{x}}(t) = -\omega^2\vec{v}\,e^{-i\omega t}$$

so (*) is $-\omega^2\underline{\underline{M}}\,\vec{v}\,e^{-i\omega t} = -\underline{\underline{K}}\,\vec{v}\,e^{-i\omega t}$

ie $\underline{\underline{K}}\,\vec{v} = \omega^2\underline{\underline{M}}\,\vec{v}$, ie $\begin{cases}\vec{v} \\ \omega^2\end{cases}$ is generalized $\begin{cases}\text{eigenvector}\\ \text{eigenvalue}\end{cases}$ of pencil $(\underline{\underline{K}},\underline{\underline{M}})$.

General solution $\vec{x}(t) = \sum_{j=1}^{N} A_j\vec{v}_j\,e^{-i\omega_j t}$ ← you may now match any initial conditions

Note g-eigenvalues ω_j^2 are extremal values of $\frac{\vec{x}^T\underline{\underline{K}}\,\vec{x}}{\vec{x}^T\underline{\underline{M}}\,\vec{x}} =: R[\vec{x}] = \frac{\text{"}E_p\text{"}}{\text{"}E_k\text{"}}$, Rayleigh quotient, cf. Lecture 18

Barnett 2/21/06

MATH 116 ~ LECTURE 14.

MPS Accuracy:

say $\begin{cases} E \\ u \end{cases}$ is an approximate $\begin{cases} \text{eigenvalue} \\ \text{eigenmode} \end{cases}$, can we bound how close they are to a true $\begin{cases} E_j \\ \phi_j \end{cases}$?

Such bounds are called 'a posteriori' ("after the fact").

... contrast 'a priori' bounds, which tell you stuff without numerical calcs.

Simplest type: right BCs, but PDE not satisfied exactly (typical Finite Element case)

Given fine $u \in L^2_0(\Omega)$, $E > 0$, define residual $R_E[u] := \dfrac{\|(\Delta+E)u\|_{L^2(\Omega)}}{\|u\|_{L^2(\Omega)}}$

$\llcorner$ ie $u = 0$ on $\partial\Omega$.

note if $\begin{cases} u = \phi_j \\ E = E_j \end{cases}$ then numerator vanishes, denom $= 1$.

Thm: $\boxed{\min_j |E - E_j| \leq R_E[u]}$ ← distance to nearest E_j.

Proof. since $\{\phi_j\}$ form complete orthonormal basis for $L^2(\Omega)$, $u = \sum_{j=1}^{\infty} a_j \phi_j$ for $\{a_j\} \in l_2$

with $a_j = \langle \phi_j, u \rangle$

So $(\Delta+E)u = \sum a_j (E - E_j) \phi_j$

recall Parseval (Plancherel's thm) $\|\sum \alpha_j \phi_j\|^2_{L^2(\Omega)} = \sum |\alpha_j|^2$

So $\|(\Delta+E)u\|^2_{L^2(\Omega)} = \sum_j a_j^2 (E - E_j)^2 \underset{\text{positive terms}}{\geq} \left[\min_j (E-E_j)^2\right] \cdot \underbrace{\sum_j a_j^2}_{= \|u\|^2_{L^2(\Omega)}}$

QED.

There are corresponding bounds on eigenmode L^2-error, $\|u - \phi_j\|_{L^2(\Omega)}$ where j is the such that $|E - E_j|$ is minimum.

MPS type: wrong BCs, PDE satisfied exactly.

Let $u \in L^2(\Omega)$, $E > 0$. define boundary residual $T_E[u] := \dfrac{\|u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}}$

↖ need not be zero on $\partial\Omega$.

& Let $(\Delta+E)u = 0$ in Ω (1)

note it's $\sqrt{t[u]}$ from last time.

Thm: $\boxed{\min_j \frac{|E-E_j|}{E_j} \le C_\Omega T_E[u]}$

Fox-Henrici-Moler '67
Moler-Payne '68.
Kuttler-Sigillito '84 review.

Proof, 2 stages

$\boxed{\text{Stage i)}}$ Let u_0 satisfy $\begin{cases} \Delta w = 0 & \text{in } \Omega \\ w = u & \text{on } \partial\Omega \end{cases}$ (2) ie w is 'harmonic extension' of bdry values of u.

Lemma: $\min_j \frac{|E-E_j|}{E_j} \le \frac{\|w\|_{L^2(\Omega)}}{\|u\|_{L^2(\Omega)}}$

Proof. $u - w \in L^2_0(\Omega)$

using $u = \sum_j \langle\phi_j, u\rangle \phi_j$

$$\min_j \left|\frac{E-E_j}{E_j}\right|^2 \cdot \|u\|^2_{L^2(\Omega)} \le \sum_j \left|\frac{E-E_j}{E_j} \langle\phi_j, u\rangle\right|^2$$ since positive terms in sum.

$$= \sum_j \left|\frac{-\langle\Delta(u-w), \phi_j\rangle + \langle u, \Delta\phi_j\rangle}{E_j}\right|^2$$ since $-\Delta(u-w) = Eu$

$$= \sum_j \left|\frac{-\langle u-w, \Delta\phi_j\rangle + \langle u, \Delta\phi_j\rangle}{E_j}\right|^2$$ since Δ self-adjoint in $L^2_0(\Omega)$.

$$= \sum_j |\langle u, \phi_j\rangle|^2 = \|w\|^2_{L^2(\Omega)}$$

proves the lemma.

$\boxed{\text{Stage ii)}}$ Lemma $\|w\|_{L^2(\Omega)} \le \sqrt{\frac{1}{q_1}} \|w\|_{L^2(\partial\Omega)}$ for $\Delta w = 0$ in Ω.

where q_1 is the lowest 'Steckloff eigenvalue' satisfying

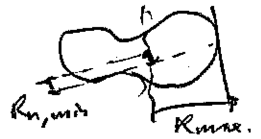
$$\begin{cases} \Delta^2 u = 0 & \text{in } \Omega \\ \Delta u - q u_n = 0 & \text{on } \partial\Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

note: biharmonic!

See Kuttler-Sigillito '68.

the connection of this obscure eigenvalue problem to harmonic funcs is "Fichera duality".

For Ω star-shaped, it's known $q_1 \ge \frac{E_1^{1/2} R_{n,\min}}{2 R_{\max}}$



Since $w = u$ on $\partial\Omega$, combining i) & ii) proves the Thm.

Thus we have <u>a-posteriori bounds on error in E_j from MPS</u> ... also error bounds on ϕ_n exist.

Math 116 ∼ LECTURE 15.

Today: • how to compute inner products of Helmholtz solutions (eg eigenmodes) using boundary values alone. = v. fast!

this with improve your MPS code, but is not crucial.

Aside on computing $\|u\|_{L^2(\Omega)}$ efficiently

in HW3,(3) I suggested you use $\int_\Omega |u|^2 dx \approx \frac{\text{vol}(\Omega)}{Q} \sum_{j=1}^{Q} u(q_j)^2$

q_j are random interior points.

Obviously this was a total hack designed to get you going easily (Betcke & Trefethen use too!) Since u is a Helmholtz solution in Ω, you can in fact do much better.

First let's solve a more general problem: compute $\int_\Omega uv\, dx$ where

$$(\Delta + E_u)u = 0 \quad (1)$$
$$(\Delta + E_v)v = 0 \quad (2)$$

using <u>only boundary values</u> of u, v.

$$(E_u - E_v)\int_\Omega uv\, dx \overset{(1),(2)}{=} \int_\Omega (u\Delta v - v\Delta u)\, dx \overset{GT2}{=} \int_{\partial\Omega} u\overset{\text{normal deriv.}}{v_n} - v u_n \, ds$$

So for $E_v \neq E_u$, $\int_\Omega uv\, dx = \frac{1}{E_u - E_v} \int_{\partial\Omega} uv_n - vu_n \, ds$

↑ a boundary integral that can be done using quadrature.

This is $O(\underset{\text{wavenumber}}{k}\underset{\text{cavity size}}{L})$ times faster than doing domain integral accurately.

We want case $u = v$ & $E_u = E_v$, so above fails!

Proceed by noticing core of GT2 was

$$\vec\nabla \cdot (u\vec\nabla v) = -E_v uv + \vec\nabla u \cdot \vec\nabla v$$
$$\vec\nabla \cdot (v\vec\nabla u) = -E_u uv + \vec\nabla u \cdot \vec\nabla v.$$

We found a linear combo of these equations which left <u>only</u> uv on RHS. The LHS is then $\vec\nabla \cdot (\text{something})$, which you push to $\partial\Omega$ via Div. Thm.

We can do this in a way that uv RHS coeff. is nonzero when $E_u = E_v$, amazingly!

Lemma: $(E_u = E_v = E)$

$$\int_\Omega uv\, dx = \frac{1}{2E}\int_{\partial\Omega} \vec x \cdot \hat n \left(Euv - \vec\nabla u \cdot \vec\nabla v\right) + (\vec x \cdot \vec\nabla u) v_n + (\vec x \cdot \vec\nabla v) u_n \, ds \quad \text{in } d = 2.$$

Proof: Write action of div on vectors, in a matrix of coefficients:

$$\vec{\nabla}\cdot\begin{bmatrix}\vec{x}uv\\ u\vec{\nabla}v\\ v\vec{\nabla}u\\ \vec{x}(\vec{\nabla}u\cdot\vec{\nabla}v)\\ (\vec{\nabla}u)(\vec{x}\cdot\vec{\nabla}v)\\ (\vec{\nabla}v)(\vec{x}\cdot\vec{\nabla}u)\end{bmatrix} = \underbrace{\begin{bmatrix}\overset{\text{\# dimensions of space}}{d} & 1 & 1 & & & \\ -E_v & & & 1 & & \\ -E_u & & & 1 & & \\ & & & d & 1 & 1\\ & -E_u & & 1 & 1 & \\ & & -E_v & 1 & & 1\end{bmatrix}}_{\text{'M'}}\begin{bmatrix}uv\\ u\vec{x}\cdot\vec{\nabla}v\\ v\vec{x}\cdot\vec{\nabla}u\\ \vec{\nabla}u\cdot\vec{\nabla}v\\ \vec{\nabla}u\cdot(x\cdot\vec{\nabla})\vec{\nabla}v\\ \vec{\nabla}v\cdot(\vec{x}\cdot\vec{\nabla})\vec{\nabla}u\end{bmatrix}$$

We can solve our algebra problem as a linear algebra one in $\mathbb{R}^6$!

Eg, symbolically take determinant in Mathematica, $\det(M) = (E_u - E_v)^2$

$\det M = 0$ for $E_u = E_v$. $\Rightarrow$ not invertible

However, when $E_u = E_v$, want linear comb. of rows of M which $= \overbrace{[\underset{\substack{\uparrow\\ uv\text{ term.}}}{1}, 0, \cdots 0]}^{\hat{e}_1^T}$.

This is equiv. to solving $\hat{e}_1 = M\vec{\xi}$ for vector $\vec{\xi} \in \mathbb{R}^6$.

You may check $\vec{\xi} = \frac{1}{2E}[E, \frac{d}{2}-1, \frac{d}{2}-1, -1, 1, 1]^T$ works. for $E = E_u = E_v$.

Thus (reading off coeffs in $\vec{\xi}$).

$$\vec{\nabla}\cdot\left[E\vec{x}uv + \left(\frac{d}{2}-1\right)(u\vec{\nabla}v + v\vec{\nabla}u) - \vec{x}(\vec{\nabla}u\cdot\vec{\nabla}v) + (\vec{\nabla}u)(\vec{x}\cdot\vec{\nabla}v) + (\vec{\nabla}v)(\vec{x}\cdot\vec{\nabla}u)\right] = uv$$

note, eg $\vec{\nabla}u\cdot(\vec{x}\cdot\vec{\nabla})\vec{\nabla}v = (\partial_i u)x_j\partial_j\partial_i v$ useful for algebra

"Einstein" notation (summation over i,j assumed).

For case $d=2$, take $\int_\Omega dx$, then use Div. Thm., swap LHS $\leftrightarrow$ RHS:

$$\int_\Omega uv\,dx = \frac{1}{2E}\int_{\partial\Omega}\hat{n}\cdot\left[\vec{x}uv - \vec{x}(\vec{\nabla}u\cdot\vec{\nabla}v) + (\vec{\nabla}u)(\vec{x}\cdot\vec{\nabla}v) + (\vec{\nabla}v)(\vec{x}\cdot\vec{\nabla}u)\right]ds$$

- This Lemma also gives rapid computation of $\int_R \phi_j^2\,dx$ over any subregion $R\subset\Omega$!
- **Note**: set $u = v$, and $u = 0$ on $\partial\Omega$, get

$\vec{x}\cdot\hat{n}$ = "Morawetz multiplier".

$$\boxed{\int_\Omega u^2\,dx = \frac{1}{2E}\int_{\partial\Omega}\vec{x}\cdot\hat{n}\,(u_n)^2\,ds}$$

Useful "Rellich-type" boundary normalization formula for eigenmodes! [Rellich, 1940].

Math 116 — LECTURE 16

Barnett
2/28/06.

- Asymptotic expansions
- EBK quantization for 'regular' modes
- billiard dynamics

Asymptotic expansions:

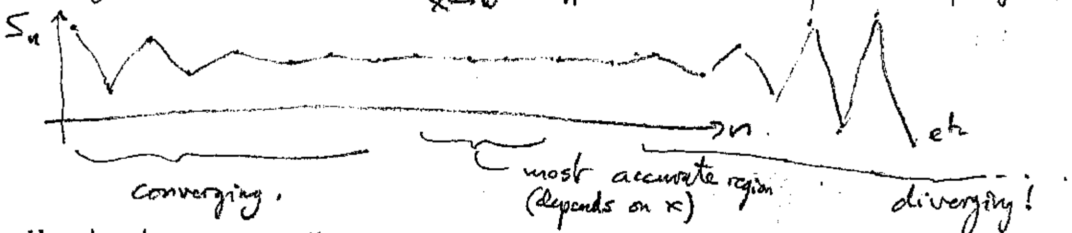
We care about approximating a quantity which depends on a parameter x, in a limit $x \to 0$ or $x \to \infty$.

Power series

$$a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n = \sum_{j=0}^{n} a_j x^j = S_n$$

As in taylor series we may have, for fixed x, $\lim_{n\to\infty}$ of above exists (convergent series)

Asym. expansion: for any fixed n, $\lim_{x\to 0} S_n$ exists, but for fixed x, $\lim_{n\to\infty} S_n$ doesn't.



Despite their ultimate divergence, they are very useful.

Eg. exponential integral $E_1(x)$ in limit $x \to \infty$. [Fowler ('97) book]

$$E_1(x) := \int_x^\infty \frac{e^{-t}}{t}\,dt$$

by parts

$$= \left[-\frac{e^{-t}}{t}\right]_x^\infty - \int_x^\infty \frac{e^{-t}}{t^2}\,dt$$

by parts

$$= \frac{e^{-x}}{x} + \left[\frac{e^{-t}}{t^2}\right]_x^\infty + 2!\int_x^\infty \frac{e^{-t}}{t^3}\,dt$$

repeated

$$= \underbrace{e^{-x}\left(\frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \cdots (-1)^{n-1}\frac{(n-1)!}{x^n}\right)}_{\text{asymp. expansion: first few terms give good approx. for large } x.} + \overbrace{(-1)^n n! \int_x^\infty \frac{e^{-t}}{t^{n+1}}\,dt}^{=:\text{remainder } R_n}$$

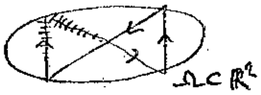
Note $|R_n| < \frac{e^{-x}(n-1)!}{x^n}$ vanishes as $o(x^{1-n})$ as $x \to \infty$., so this gives order of convergence wrt x.

Ratio between successive terms in series $= \frac{n-1}{x} \Rightarrow \forall$ fixed x, series diverges as $n \to \infty$

Such (divergent) series are incredibly useful in applied math. Eg, asymptotics of waves.

Einstein–Brioullin–Keller (EBK) Quantization.

How to find asymptotic (large wavenumber k) expressions for modes living on stable rays, eg.



see Keller–Rubinow, (1960) Ann. Phys. 9, 24-75

Assumption: $$u = \sum_{j=1}^{N} A_j \, e^{ikS_j} + O\left(\frac{1}{k}\right)$$

N finite, sum of 'waves'.

S_j: phase function (real), A_j: amplitude func. (complex) } both slowly-changing funcs of position x.

ie no fast (k) oscillations.

Substitute $u = Ae^{ikS}$ into $(\Delta + k^2)u = 0$:

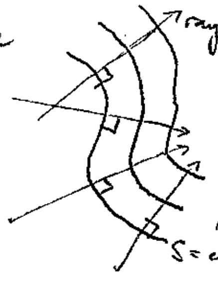
deriv. $$\vec{\nabla} u = \vec{\nabla} A \, e^{ikS} - ikA\vec{\nabla} S \, e^{ikS}$$

$$\Delta u = \Delta A \, e^{ikS} - ik\left[2\vec{\nabla} S\cdot\vec{\nabla} A \, e^{ikS} + \Delta S A e^{ikS}\right] - k^2|\vec{\nabla} S|^2 A e^{ikS}$$

Equate terms in k^2: $$|\vec{\nabla} S|^2 = 1 \qquad \text{(i) "eikonal" equation.}$$

in k: $$2\vec{\nabla} S\cdot\vec{\nabla} A + A\Delta S = 0 \qquad \text{(ii)}$$

If level curve of S known, (i) tells you that the next level curve obtained by transport along lines (rays) orthogonal to the level curve



.... Huygens' Principle.

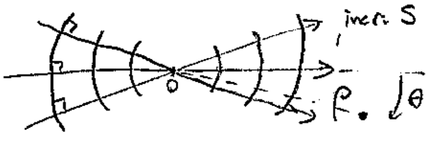
Let t measure distance along a ray, $S(t) = S_0 \pm t$

$\vec{\nabla} S$ // to rays

$\Rightarrow$ (ii) becomes $$2\frac{dA}{dt} + (\Delta S)A = 0,$$

an ODE which has exact solution $$A(t) = A_0 e^{-\frac{1}{2}\int_0^t \Delta S(t')\,dt'}$$

consider polar coords centered at a focal point.

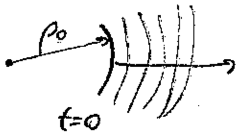


$\rho = t$ our coord along rays.

$$\Delta S = \underbrace{\partial_{\rho\rho} S}_{\text{zero since } \partial_\rho S = \text{const.}} + \frac{1}{\rho}\underbrace{\partial_\rho S}_{1} + \underbrace{\frac{1}{\rho^2}\partial_{\theta\theta} S}_{\text{zero since } S \text{ const. on wavefronts.}}$$

so $$\Delta S = \frac{1}{\rho} = \text{Gaussian curvature of wavefront, } G(t) \begin{cases} > 0 & \text{for })))\rightarrow \text{ diverging} \\ < 0 & \text{for } (((\leftarrow \text{ converging} \end{cases}$$

Note $G(t) = \frac{1}{\rho_0+t}$ where ρ_0 is radius of curvature at $t=0$.

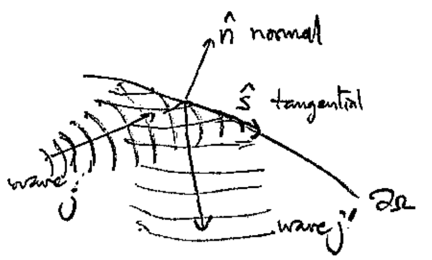


So $\int_0^t \Delta S(t')\,dt' = \int_0^t \frac{dt'}{\rho_0+t'} = \ln(\rho_0+t) - \ln\rho_0$

⇒ soln. to (ii) can be written. $A(t) = A_0 e^{-\frac{1}{2}\ln\frac{\rho_0+t}{\rho_0}} = A_0\left(\frac{\rho_0}{\rho_0+t}\right)^{1/2}$ (iii)

tells you amplitude has sqrt singularity as pass through focus.
Expect this by conservation of flux (energy).

Boundary conditions -



For Each wave j impinging on ∂Ω, there must be another (reflected) wave j' which cancels its value on ∂Ω.

choose Dirichlet $u=0$ on ∂Ω.

$$A_j e^{ikS_j} + A_{j'} e^{ikS_{j'}} = 0 \quad \text{on } \partial\Omega$$

we wish to hold for a sequence of different k values.

⇒ $S_j = S_{j'}$ on ∂Ω

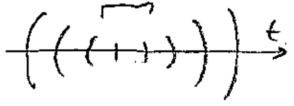
Since $\frac{\partial S_j}{\partial s} = \frac{\partial S_{j'}}{\partial s}$, (i) gives $\frac{\partial S_j}{\partial n} = \pm \frac{\partial S_{j'}}{\partial n}$

↳ only − relevant, otherwise 2 waves equivalent.

This is geometric reflection law $\theta_r = \theta_i$

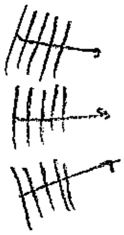
Also $A_j = -A_{j'}$ on ∂Ω (phase change of π).

Phase change at focal point:

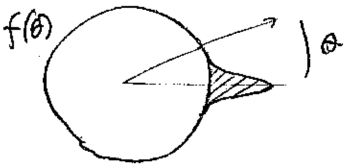


(iii) suggests that if A real on one side, pure imaginary on other, ie factor $e^{i\pi/2}$
This is in fact true; there is a phase loss of $\pi/2$ on passing through focus.
This is standard result of paraxial (ie close-to-axis propagating) gaussian beam optics.

Why?



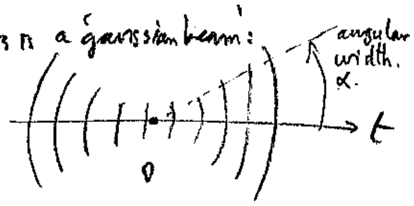
consider narrow angular distribution of plane waves



angular width α.

$$u(x) = \int_{-\pi}^{\pi} f(\theta) e^{ik\hat{d}_\theta\cdot x}\, d\theta \quad \text{with } f(\theta) = e^{-\frac{\theta^2}{2\alpha^2}} \text{ (gaussian).}$$

This is a gaussian beam:



consider $u(t)$, the value along the direction $\theta=0$.

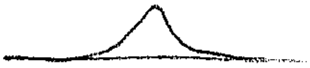
$$u(t) = \int_{-\pi}^{\pi} e^{ikt\cos\theta}\, e^{-\frac{\theta^2}{2\alpha^2}}\, d\theta$$

use $\cos\theta = 1-\frac{\theta^2}{2!}+O(\theta^4)$

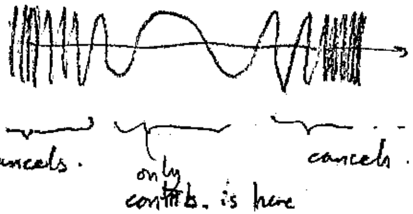
$$= \underbrace{e^{ikt}}_{\text{undisturbed (plane wave) phase.}} \int_{-\pi}^{\pi} \underbrace{e^{-\frac{1}{2}(ikt+\frac{1}{\alpha^2})\theta^2 + O(\theta^4)}}_{e^{if(\theta)}}\, d\theta.$$

$e^{if(\theta)}$ with f stationary at $\theta=0$; only $f''(\theta)$ important, "stationary phase approximation".

Recall $\int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2}}dx = a\sqrt{2\pi}$



Imag. (osc.) version $\int_{-\infty}^{\infty} e^{-i\frac{x^2}{2a^2}} = e^{-i\pi/4}a\sqrt{2\pi}$



can prove by contour integration. (Fresnel integral).

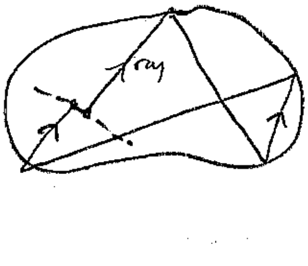
For $|kt| \gg \frac{1}{\alpha^2}$, ie away from beam 'waist',

$$u(t) \approx e^{ikt}\cdot\int e^{-\frac{1}{2}kt\theta^2}d\theta = e^{ikt}\sqrt{\frac{2\pi}{kt}}\cdot\begin{cases} e^{-i\pi/4} & t>0 \\ e^{+i\pi/4} & t<0 \end{cases}$$

Therefore there's a phase (loss) of $e^{-i\pi/2}$. (this happens gradually through beam waist).

Quantization condition:

ray must eventually close (finite # bounces), making a single-valued eigenmode u.



Round-trip phase difference δS_j must be integer multiple of 2π, call n

Ie, $$\underbrace{k\oint \vec{\nabla} S\cdot d\vec{\ell}}_{\text{this is just length of orbit, L.}} = 2\pi\left(n+\frac{m}{4}+\frac{b}{2}\right)$$

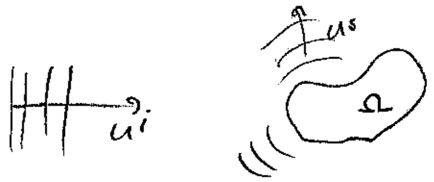
m = # focal points.

b = # bounces off Dirichlet BCs.

Math 116 — LECTURE 17.

① Barnett 3/2/06

Physical optics approx. to scattering: (Kirchhoff's approx; good for $k \to \infty$, short wavelength).



$u = u^i + u^s$ $\qquad$ $u = 0$ on $\partial\Omega$ (sound soft) $\qquad$ $(\Delta + k^2)u = 0$ in $\mathbb{R}^d \setminus \bar{\Omega}$.

First derive a new exact formulation of scattering:

u^s is radiating so GRF applies ($x \in \mathbb{R}^d \setminus \bar{\Omega}$), $u^s(x) = \int_{\partial\Omega} u^s(y) \frac{\partial \Phi(x,y)}{\partial n_y} - u^s_n(y) \Phi(x,y) \, ds_y$

u^i is entire soln. over $\mathbb{R}^d$ (is not radiating) so GRF doesn't apply, but...

GT2 inside: Fix $x \in \mathbb{R}^d \setminus \bar{\Omega}$

$$\int_\Omega \underbrace{u^i(y) \Delta \Phi(x,y) - \Phi(x,y) \Delta u^i(y)}_{-k^2 u^i(y) \Phi(x,y) + k^2 u^i(y) \Phi(x,y) = 0\text{, since both Helmholtz solns in } \Omega} dy = \int_{\partial\Omega} u^i \frac{\partial \Phi}{\partial n_y}(x,y) - \Phi(x,y) u^i_n \, ds_y$$

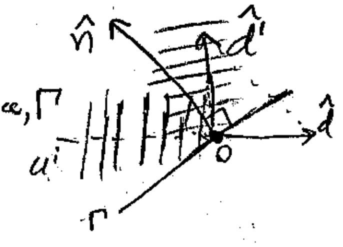
Add the above: $\quad \underset{\text{write } u - u^i}{u^s(x)} = \int_{\partial\Omega} \underset{\text{apply BCs.}}{u(y)} \frac{\partial \Phi}{\partial n_y}(x,y) - u_n(y) \Phi(x,y) \, ds_y$

$$\Rightarrow \quad \boxed{u(x) = u^i(x) - \int_{\partial\Omega} u_n(y) \Phi(x,y) \, ds_y} \quad (1)$$

exact, "Lippmann-Schwinger type".

↑ note: u here too ⇒ not easy to solve

Now for plane surface, Γ (passing through origin)



$u^i = e^{ik\hat{d}\cdot x}$
$u^s = -e^{ik\hat{d}'\cdot x}$

where $\hat{d}' = \hat{d} - 2\hat{n}(\hat{d}\cdot\hat{n})$ is reflected ray direction.

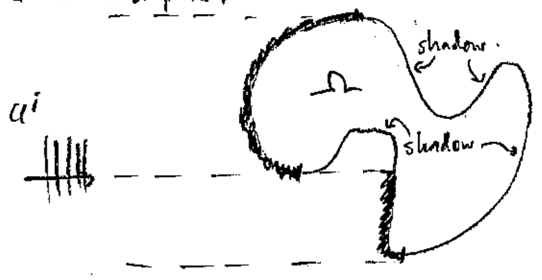
Notice $u^s = -u^i$ on Γ $\qquad$ since $x \cdot \hat{n} = 0$ defines Γ.

$\frac{\partial u^s}{\partial n} = \frac{\partial u^i}{\partial n}$ on Γ $\qquad$ since $\frac{\partial u^s}{\partial n} = ik \underbrace{\hat{n} \cdot (\hat{d} - 2\hat{n}(\hat{d}\cdot\hat{n}))}_{-\hat{d}\cdot\hat{n}} e^{ik\hat{d}'\cdot x}$

So here $u_n = 2u^i_n$ exactly.

We approximate $u_n \approx 2u^i_n$ on the 'illuminated' side of general obstacle, insert into (1).

Illuminated parts:



in special case of convex Ω we may use $\hat{d}\cdot\hat{n} \begin{cases} < 0 & \text{illum.} \\ > 0 & \text{shadow.} \end{cases}$

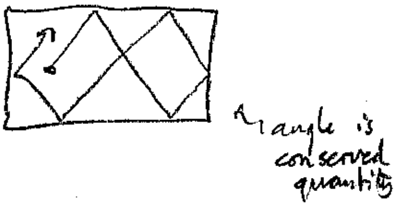
Clearly computing illum. region for nonconvex is harder.

For convex Ω this approximation is often good. – in fact it is the basis of correction schemes for rapid scattering codes (Chandler-Wilde '05)

Note no BIE equation had to be solved! ($O(N^3)$ if do naively ⇒ slow part).

Ray dynamics in cavities: free motion of point particle, with law of reflection.

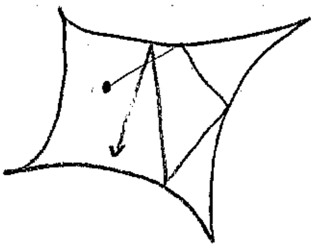
rect.



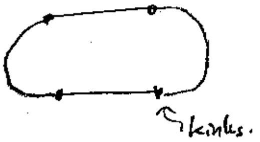
ellipse

Integrable. (families on tori)

(Keller showed how to find modes asymptotically, "EBK" quantization, 1960).



'dispersing' billiard
Sinai
(proven ergodic, 1970)



$\partial\Omega$ is C^1, not C^2.

stadium
(Bunimovich).

Chaotic. = ergodic ⇒ no families.

(No known way to find approximations to modes, other than numerical PDE solutions eg. MPS, BIE, Scaling...).

See reviews by Sinai, Notices AMS, 2004.
Porter & Lansel, Notices AMS Feb 2006.
Lai-Sang Young, NYU.

or dynamical systems books.

3/7/06
Barnett

Lecture 18 ~ MATH 116.

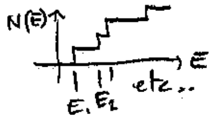
WEYL'S PROBLEM: How do Dirichlet-eigenvalues E_n behave as $n\to\infty$?

$$-\Delta\phi_n = E_n\phi_n \quad \text{in } \Omega$$
$$\phi_n = 0 \quad \text{on } \partial\Omega$$

Define level counting function $N(E) = \#\{n : E_n \leq E\}$

Note $\frac{dN}{dE} = \underbrace{\rho(E)}_{\text{level density}} = \sum_{n=1}^{\infty}\delta(E-E_n)$, formally

N defines an integration measure $\int f(E)\,dN(E)$
$= \int f(E)\rho(E)\,dE$



Weyl's Asymptotic formula ('law'):

$$N(E) = \begin{cases} \frac{\mathrm{Vol}(\Omega)}{4\pi}E + \underbrace{O}_{\text{big 'oh'}}(E^{1/2}) & \text{for } \Omega\subset\mathbb{R}^d,\ d=2 \\ \frac{\mathrm{Vol}(\Omega)}{(4\pi)^{d/2}\Gamma(\frac{d}{2}+1)}E^{d/2} + O(E^{\frac{d-1}{2}}) & d\geq 2 \end{cases}$$

eg denom. is $6\pi^2$ for $d=3$

Remarks:

- The bound is sharp because of examples such as the disk (sphere, etc) for which fluctuations from first term are as large as $cE^{\frac{d-1}{2}}$.
- Since $\mathrm{Vol}(B^d)$, the d-dim unit ball, is $\frac{\pi^{d/2}}{\Gamma(d/2+1)}$, we could write

$$N(E) \sim \frac{1}{(2\pi)^d}\underbrace{\mathrm{Vol}(\Omega)\mathrm{Vol}(B^d)k^d}_{\text{volume of phase space } \overset{\text{position}}{\Omega}\times \overset{\text{velocity (speed}=|k|)}{B^d_k}}$$

ball radius k

"Each mode occupies fixed phase space volume".

- Weyl's law was first proved by elementary means by Weyl (1912),

via $\boxed{\text{'minimax'}}$:
$$E_n = \max_{v_1,v_2\cdots v_{n-1}}\left[\min_{\substack{u\perp \mathrm{Span}\{v_1,\cdots v_{n-1}\}\\ u=0 \text{ on } \partial\Omega}} \frac{\int_\Omega |\nabla u|^2dx}{\int_\Omega u^2dx}\right]$$

which then tells us, eg. E_n cannot increase if Ω changed to $\Omega^*\supset\Omega$.

Let's examine Weyl's method, in d=2. (see eg, Garabedian's PDE book, Ch.11).

Proof of minimax:

Choose $u \in C_0^2(\Omega)$, twice cont. differentiable funcs which vanish on $\partial\Omega$.

The eigenfunction expansion $u = \sum a_j \phi_j$

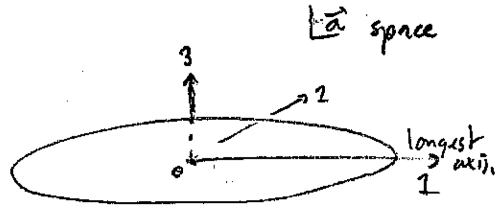
GT1 $\int_\Omega \vec{\nabla} u \cdot \vec{\nabla} u \, dx + \int_\Omega u \Delta u \, dx = \int_{\partial\Omega} \overset{0}{\cancel{u}} u_n \, ds = 0$

gives $\int_\Omega |\nabla u|^2 dx = -\int_\Omega u \Delta u \, dx = -\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_i a_j \underbrace{\int_\Omega \phi_i \overbrace{\Delta \phi_j}^{-E_j \phi_j} dx}_{-E_j \delta_{ij}}$

$= \sum_j E_j a_j^2$

also $\int_\Omega u^2 dx = \sum_j a_j^2$ Parseval

So $R[u] := \dfrac{\int_\Omega |\nabla u|^2 dx}{\int_\Omega u^2 dx} = \dfrac{\sum E_j a_j^2}{\sum a_j^2}$
(Rayleigh quotient)



defines hyper-ellipsoid $R[u] = 1$, axes aligned along coordinates

Note $R[u] \geqslant E_1$ which proves minimax for $n=1$.

It will turn out $v_j = \phi_j$, $j = 1, \ldots n-1$, gives the optimal choice for $v_1 \cdots v_{n-1}$

i) With this choice, $a_j = 0$ for $j < n$ so $\min\limits_{u \perp \text{Span}\{v_1 \cdots v_{n-1}\}} R[u] = \min\limits_{\{a_j\}, j \geqslant n} \dfrac{\sum_{j=n}^{\infty} E_j a_j^2}{\sum_{j=n}^{\infty} a_j^2}$

$= E_n$.

ii) If $V := \text{Span}\{v_1 \cdots v_{n-1}\}$ differs from $\text{Span}\{\phi_1 \cdots \phi_{n-1}\}$
then can find $u \perp V$ s.t. $u \in \text{Span}\{\phi_1 \cdots \phi_{n-1}\} = \sum_{j=1}^{n-1} a_j \phi_j$, with $\sum_{j=1}^{n-1} a_j^2 = 1$,

giving $R[u] = \sum_{j=1}^{n-1} E_j a_j^2 \leq E_{n-1} \leq E_n$.

Combining i) & ii) proves it. (Garabedian p. 395)

Bounding eigenvalues by contained and containing domains:

Thm if $\Omega \subset \Omega^*$ then $E_n \geq E_n^*$ for all $n = 1, 2, \cdots$

Pf. extend funcs $\left\{\begin{matrix} v_1, \cdots v_{n-1} \\ u \end{matrix}\right.$ as zero in $\Omega^* \setminus \Omega$

Then if $u \perp \text{Span}\{v_1 \cdots v_{n-1}\}$ holds over Ω, also does over Ω^*

Also $R^*[u] = R[u]$, where $*$ indicates integrals in Ω^*.

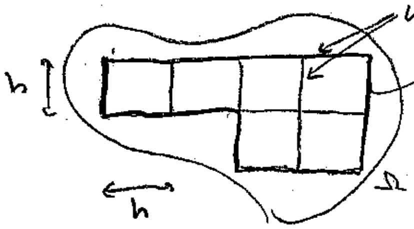
But since subspace of trial func is enlarged, $\min_{\substack{u \perp V \\ u=0 \text{ on } \partial\Omega^*}} R^*[u] \leq \min_{\substack{u \perp V \\ u=0 \text{ on } \partial\Omega}} R[u]$

Using minimax, E_n^* then cannot exceed E_n.

General rule: $\left\{\begin{matrix} \text{enlarging} \\ \text{restricting} \end{matrix}\right.$ the linear space of trial funcs means E_n cannot $\left\{\begin{matrix} \text{increase} \\ \text{decrease} \end{matrix}\right.$

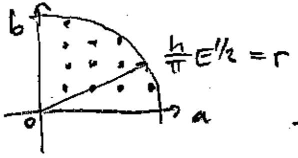
- As our restricted space choose:

$u=0$ on all boundaries of squares in lattice contained in Ω.



Each Dirichlet square has spectrum $E_n = \left(\frac{\pi}{h}\right)^2 (a^2 + b^2)$ (modes = $\sin a\pi\frac{x}{h} \sin b\frac{\pi x}{h}$) for $a, b \in \mathbb{N}$

Then $N(E)$ for each square = # lattice points of $\mathbb{N}^2$ lying within radius $\frac{h}{\pi}E^{1/2}$ of origin.



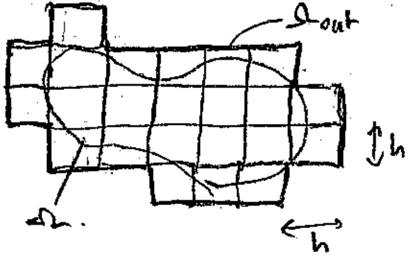
Thus $N(E) = \frac{\pi}{4}r^2 + O(r)$

$= \frac{h^2}{4\pi}E + O(E^{1/2})$

Ie each square already obeys Weyl's law. (area = h^2)

Disjoint regions have independent spectra $\Rightarrow$ $N_{in}(E) = \frac{\text{vol}(\Omega_{in})}{4\pi}E + O(E^{1/2})$.

- As enlarged space choose covering squares, each with Neumann BCs ('free' membranes), similar argument gives $N_{out}(E) = \frac{\text{vol}(\Omega_{out})}{4\pi}E + O(E^{1/2})$



Thus asymptotically, $\lim_{E\to\infty} \frac{N_{in}(E)}{E} = \frac{\mathrm{vol}(\Omega_{in})}{4\pi}$

$$\lim_{E\to\infty} \frac{N_{out}(E)}{E} = \frac{\mathrm{vol}(\Omega_{out})}{4\pi}$$

Our bounds on eigenvalues E_n mean

$$N_{in}(E) \leq N(E) \leq N_{out}(E)$$

ie $$\frac{\mathrm{vol}(\Omega_{in})}{4\pi} \leq \lim_{E\to\infty} \frac{N(E)}{E} \leq \frac{\mathrm{vol}(\Omega_{out})}{4\pi}$$

Finally we may take arbitrarily small squares h, giving $\mathrm{vol}(\Omega_{in}) \to \mathrm{vol}(\Omega)$, $\mathrm{vol}(\Omega_{out}) \to \mathrm{vol}(\Omega)$

Thus. $$\underline{\lim_{E\to\infty} \frac{N(E)}{E} = \frac{\mathrm{vol}(\Omega)}{4\pi}}$$ QED. "Exhaustion method".

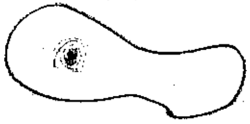
Heat trace asymptotics:

Historically, the next step (Carleman, '30's). [see Baltes & Hilf, Spectra of Finite Systems, book (1976)]

Heat equation $u_t = \Delta u$ in $\Omega \times [0,\infty)$

$u = 0$ on $\partial\Omega \times [0,\infty)$

Time evolution ...



t small

t large

initial condition $u(x,0) = u_0(x)$

$u_0 \in L^2(\Omega)$

Solution by mode decomposition : (1) $$u(x,t) = \sum_{j=1}^{\infty} a_j e^{-E_j t} \phi_j(x)$$ sep. of variables.

check satisfies PDE ! $a_j = \langle \phi_j, u_0 \rangle$

Write as evolution operator, $u(x,t) = (K_t u_0)(x,t) = \int_\Omega K(x,y;t)\, u_0(y)\, dy$ (2)

where $K_t = e^{t\Delta}$ has kernel $K(x,y;t) = \sum_{j=1}^{\infty} e^{-E_j t} \phi_j(x) \phi_j(y)$ (3)

(formally solves PDE)

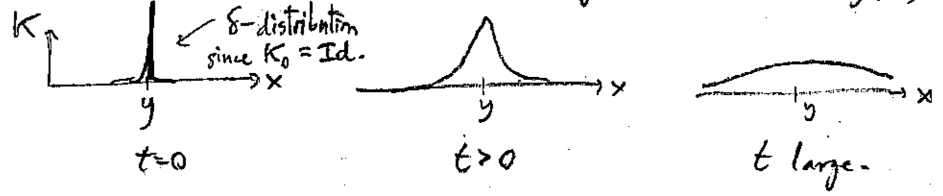
Why? Check (1) correctly given when stick kernel into (2).

Trace (integral along diagonal) is, using (3),

$$\mathrm{Tr}\, e^{t\Delta} := \int_\Omega K(x,x;t)\,dx = \sum_{j=1}^{\infty} e^{-E_j t}\int_\Omega \phi_j(x)^2\,dx = \sum_{j=1}^{\infty} e^{-E_j t}$$

Note can write as $\mathrm{Tr}\, e^{t\Delta} = \int_0^\infty e^{-Et}\rho(E)\,dE = \int_0^\infty e^{-Et}\,dN(E)$ $\boxed{\text{Laplace transform of level density}}$

Missing ingredient? We know things about $K(x,y;t)$ from PDEs!



In $\boxed{\text{free space}}$, $\Omega = \mathbb{R}^d$, K is analytically known, eg Fourier transform (spatial)

$$\hat{f}(k) := \int_{\mathbb{R}^d} f(x)\, e^{-ik\cdot x}\,dx \qquad \text{FT}$$

$$f(x) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \hat{f}(k)\, e^{ik\cdot x}\,dk \qquad \text{inv. FT}.$$

FT of heat eqn: $\hat{u}_t = \widehat{\Delta u} = -|k|^2\hat{u}$

which decouples into ODE for each k value, solved by $\hat{u}(k,t) = e^{-|k|^2 t}\,\hat{u}_0(k)$

$e^{t\Delta}$ therefore multiplies by $e^{-|k|^2 t}$ in k-space, ie convolves by inv. FT of $e^{-|k|^2 t}$ in x-space.

convolution kernel $K(\cdot x;t) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}}$

ie $K(x,y;t) = (4\pi t)^{-d/2} e^{-\frac{1}{4t}|x-y|^2}$

easy to derive using $e^{-\frac{x^2}{2}}$ is its own FT, and $\int_{-\infty}^{\infty} e^{-x^2/2}\,dx = \sqrt{2\pi}$.

Approx. K by freespace kernel: $K(x,x;t) \approx (4\pi t)^{-d/2}$
(exponentially good for small t, everywhere apart from near $\partial\Omega$).

$$\Rightarrow \int_0^\infty e^{-Et}\rho(E)\,dE = \int_\Omega K(x,x;t)\,dx = \frac{\mathrm{vol}(\Omega)}{(4\pi t)^{d/2}}$$

But we know the following Laplace transform:

$$L[E^\alpha] := \int_0^\infty e^{-Et}E^\alpha\,dE = \frac{\Gamma(\alpha+1)}{t^{\alpha+1}}$$

follows from $\int_0^\infty e^{-E}E^\alpha\,dE := \Gamma(\alpha+1)$ gamma defn.

Choosing $\alpha+1 = \frac{d}{2}$ gives $\rho(E) = \frac{1}{\Gamma(\frac{d}{2})} \frac{\mathrm{vol}(\Omega)}{(4\pi)^{d/2}} E^{\frac{d}{2}-1}$

This integrates $N(E) = \int_0^E \rho(E) dE'$ to the given Weyl Law form.

Why did ρ come out smooth? (It's a sum of δ-distributions!)

This was due to the free-space approximation. (free space has continuous Δ spectrum)

- However, rigorously you may prove $K(x,x;t) \sim (4\pi t)^{-d/2}$ $\forall x \in \Omega$
  small-t asymptotics.

Then you can use Tauberian Thm. of Karamata (1931):

Thm. let L be slowly varying function (ie $\forall a>0$, $\frac{L(ax)}{L(x)} \to 1$ as $x\to\infty$)

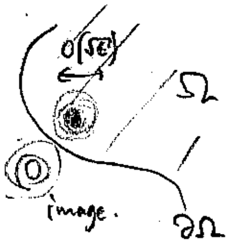
Then for $\sigma \geq 0$, $\int_0^\infty e^{-E/y} dN(E) \sim y^\sigma L(y)$ as $y \to \infty$

iff $N(E) \sim \frac{y^\sigma L(y)}{\Gamma(1+\sigma)}$ as $y \to \infty$

see Borwein reviews.

note y is t^{-1} for us, and $\sigma = +d/2$

- Intuitively, you may see $K(x,x;t)$ only differs from free space within $O(\sqrt{t})$ distance of $\partial\Omega$, and within this distance, method of images can be used...



This gives, eg, in d=2,

$$\bar{N}(E) \sim \frac{\mathrm{vol}(\Omega)}{4\pi} E \pm \frac{\mathrm{perim}(\partial\Omega)}{4\pi} E^{1/2} + \dots$$

smoothed version of

$+\}$ for $\{$Neumann BCs
$-\}$ $\}$Dirichlet

corner, curvature terms.

Notice this is no longer a rigorous bound on $N(E)$, which remains as before.

- In the 70's (Balian & Bloch, Hörmander), wave trace methods arrived allowing better results.
  Eg. pseudodifferential operators (ΨDOs)... ie $u_{tt} = \Delta u$ propagation.