Consider functions on a ring of points $\mathbb{Z}/N\mathbb{Z}$.
They could be represented by column vectors
with the convention $\psi_m \equiv \psi_n$
whenever $m \equiv n \pmod N$.

$$\vec{\psi} = \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{bmatrix}$$

Consider the circular shift operator
with $(\hat{C}\vec{\psi})_n = \psi_{n-1}$.
We have $\hat{C}^N = \hat{I}$.

$$\hat{C} = \begin{bmatrix} 0 & 1 & & & & \\ & 0 & 1 & & 0 & \\ & & 0 & 1 & & \\ & 0 & & & \ddots & 1 \\ & & & & 0 & 1 \\ 1 & & & & & 0 \end{bmatrix}$$

We will call an operator
$\hat{A}$ *translation invariant* if $\hat{C}\hat{A} = \hat{A}\hat{C}$, i.e.,
$\hat{A}$ commutes with the shift $\hat{C}$ (and thus all
shifts $\hat{C}^n$). Equivalently, $A_{ij} = A_{i+n \,(\mathrm{mod}\,N),\, j+n\,(\mathrm{mod}\,N)}$,
or $\hat{A}$ is a circulant matrix. In this case
the eigenvectors of $\hat{C}$ which are
$(\xi = e^{2\pi i/N})$ are also the
eigenvectors of $\hat{A}$, with the
eigenvalues

$$\vec{w}_n \propto \begin{bmatrix} 1 \\ \xi^n \\ \xi^{2n} \\ \vdots \\ \underbrace{\xi^{(N-1)n}}_{=\,\xi^{-n}} \end{bmatrix}$$

$$\lambda_n = \sum_{k=0}^{N-1} A_{0k}\, \xi^{kn} = \sum_{k=0}^{N-1} A_{0k}\, e^{\frac{2\pi i k n}{N}} \; -$$

— a discrete Fourier transform of $\hat{A}$'s row
(or column, as $A_{0k} = A_{-k,0}$).

Consider equations of the type

$$a_n \psi_{k+n} + a_{n-1}\psi_{k+n-1} + \dots + a_2\psi_{k+2} + a_1\psi_{k+1} + a_0\psi_k = 0 \qquad (*)$$

for all $k \in \mathbb{Z}$. This equation couples $n+1$ points, it is an analog of n^{th} order ODE. It is translation invariant, and we can look for exponential solutions: $\psi_k \propto \lambda^k$. The function $\psi: \mathbb{Z} \to \mathbb{C}$, $\psi: k \mapsto \lambda^k$ is the solution of $(*)$ if

$$a_n\lambda^n + a_{n-1}\lambda^{n-1} + \dots + a_2\lambda^2 + a_1\lambda + a_0 = 0$$

the characteristic equation of $(*)$

The equation for λ has n roots: $\lambda_1, \lambda_2, \dots, \lambda_n$; and the general solution of $(*)$ looks like (if all λ_m's are distinct) $\psi_k = \sum_{m=1}^{n} A_m \lambda_m^k$.

arbitrary constants

In the case of repeated roots of the characteristic equation the situation is similar to ODEs — an exponential solution is deformed by a polynomial. For example, consider

analog of $\psi''=0$ — $\psi_{k+2} - 2\psi_{k+1} + \psi_k = 0$

$$\lambda^2 - 2\lambda + 1 = (\lambda-1)^2 = 0,$$

the solutions are $\psi_k = \underbrace{(Ak+B)\cdot 1^k}_{\text{all linear functions}}$.

MATH 583B

due ~~January 31~~ February 1, 2019

Principles and Methods of Applied Mathematics

Section 001, Spring 2019 (instructor: Misha Stepanov)

Homework 7

1. Consider the space X of two-sided sequences u_n, $-\infty < n < \infty$ (or mappings $u : \mathbf{Z} \to \mathbf{C}$) such that $\sum_{n=-\infty}^{\infty} |u_n|^2 < \infty$. The inner product is defined as $\langle u, v\rangle = h \sum_{n=-\infty}^{\infty} u_n^* v_n$ (h is the grid step size). Consider the operator $\hat{L}$ defined by $(\hat{L}u)_n = -\frac{1}{2}(u_{n+1} - 2u_n + u_{n-1})/h^2$.

(a) By wrapping integers into a ring, $\mathbf{Z} \to \mathbf{Z}/N\mathbf{Z}$, consider the operator $\hat{L}_N$ (acting on the mappings $\mathbf{Z}/N\mathbf{Z} \to \mathbf{C}$) with the same formula. Find the eigenvalues and eigenvectors of $\hat{L}_N$. Find the resolvent $\hat{R}_E = (E - \hat{L}_N)^{-1}$. (It is going to be a Toeplitz $N \times N$ matrix. You can represent it by a function on $\mathbf{Z}/N\mathbf{Z}$ — in the case of translation invariance we have $A(x \mid y) = A(x - y \mid 0)$ for the integral kernel of some operator $\hat{A}$.)

(b) Find $\hat{L}^*$.

(c) Find the resolvent $\hat{R}_E = (E - \hat{L})^{-1}$ (it is going to be an infinite size matrix, which you can represent by a function on $\mathbf{Z}$). Find point, continuous, and residual spectra.

(d) Find $\|\hat{L}\|$.

(e) Find the resolvent of $\hat{L}$ in the limit $h \to 0$, where $R_E(n) \to R_E(x = hn)$ — a function on $\mathbf{R}$.

This is going to be relevant for the part **(e)**: If we think about the matrix with elements A_{ij} as the "integral kernel" of operator $\hat{A}$, then it is reasonable to define the action by $\hat{A}$ as $(\hat{A}\vec{\psi})_i = \underbrace{h\sum_j}_{} A_{ij}\psi_j$

integration, one grid site has the weight h - grid step size

Then the identity operator $\hat{I}$ has the "integral kernel" $I_{ij} = \frac{1}{h}\delta_{ij}$, which is the discretization of $I(x \mid y) = \delta(x-y)$.

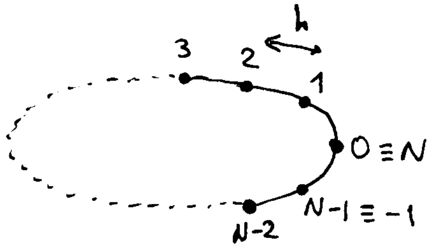
The integral kernels of $\hat{L}$ and $\hat{L}_N$ become $L_{ij} = \dfrac{2\delta_{ij} - \delta_{i,j+1} - \delta_{i,j-1}}{2h^3}$.

discretization of $-\frac{1}{2}\delta''(x-y)$

We have $(E\hat{I} - \hat{L})\hat{R}_E = \hat{I}$, or

$$h\sum_k (E\hat{I} - \hat{L})_{ik} (R_E)_{kj} = I_{ij} = \frac{1}{h}\delta_{ij}.$$

(a)



As the matrix of $\hat{L}_N$ is a circulant one, the normalized eigenvectors of $\hat{L}_N$ are

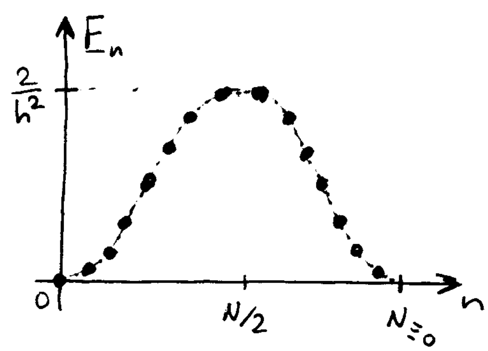
$$\vec{w}_n = \frac{1}{\sqrt{hN}} \begin{bmatrix} 1 \\ \xi^n \\ \xi^{2n} \\ \vdots \\ \underbrace{\xi^{(N-1)n}}_{\xi^{-n}} \end{bmatrix}$$

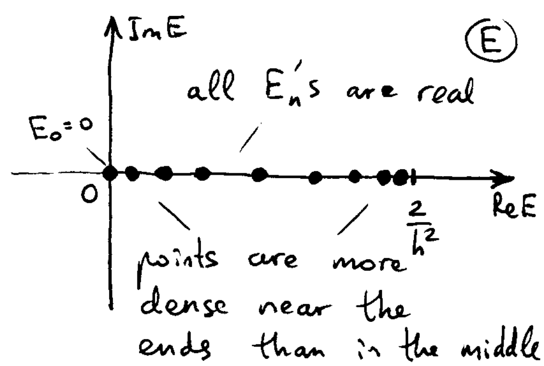
because of h in the inner product

Once the eigenvectors are known, it is easy to find the eigenvalues E_n ($\hat{L}_N \vec{w}_n = E_n \vec{w}_n$):

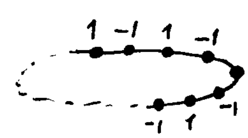
$hN =: L$ is the length of the ring

$$E_n = -\tfrac{1}{2}\left(\xi^n - 2 + \xi^{-n}\right)/h^2 = \frac{1 - \frac{\xi^n + \xi^{-n}}{2}}{h^2} = \frac{1 - \cos\left(\frac{2\pi n}{N}\right)}{h^2}$$





If N is even, then $E_{\frac{N}{2}} = \frac{2}{h^2}$ is realized on



The resolvent $\hat{R}_E$ can be expressed as

$$\hat{R}_E = \sum_{n=0}^{N-1} \underbrace{\vec{w}_n \frac{1}{E - E_n} \vec{w}_n^{\,\dagger}}_{\text{outer product}}, \quad \text{and} \quad \left((E - \hat{L}_N)\hat{R}_E\right)_{ij} = \frac{1}{h}\delta_{ij}.$$

Because of $\frac{1}{\sqrt{h}}$ in both $\vec{w}_n$ and $\vec{w}_n^{\,\dagger}$

This expression for $\hat{R}_E$ can be viewed as diagonalization of $\hat{R}_E$, that has same with $\hat{L}_N$ eigenvectors, or the statement that $\hat{L}_N$ and $\hat{R}_E$, being translation invariant, are diagonalized by the discrete Fourier transform.

Let us find the explicit expression for $\hat{R}_E$. As the matrix of $\hat{R}_E$ is a circulant one, we can find just the 1st column of $\hat{R}_E$ — $(\hat{R}_E)_{m0} =: R_m$, and let $(\hat{R}_E)_{mn} = R_{m-n \,(\mathrm{mod}\, N)}$. The equations for R_m look like

$$\begin{cases} \left(E - \frac{1}{h^2}\right) R_0 + \dfrac{R_1 + \overset{\equiv R_{N-1}}{R_{-1}}}{2h^2} = \dfrac{1}{h} & (1) \\ \left(E - \frac{1}{h^2}\right) R_m + \dfrac{R_{m+1} + R_{m-1}}{2h^2} = 0, \quad 0 < m < N & (2) \end{cases}$$

The characteristic equation of eq. (2)

$$\lambda^2 - 2(1 - Eh^2)\lambda + 1 = 0$$

has 2 roots: $\lambda_{1,2} = 1 - Eh^2 \pm ih\sqrt{E(2 - Eh^2)}$.

Notice that $\lambda_2 = \frac{1}{\lambda_1}$, so we will use just $\lambda := \lambda_1$.

The general solution of (2) looks like

$R_m = \underbrace{A \lambda^m + B \lambda^{-m}}_{\text{arbitrary constants}}$, the expression that should be used for $0 \leq m \leq N$.

The constants A and B are found from $R_0 \equiv R_N$ and eq. (1):

$$\begin{cases} A + B = A\lambda^N + B\lambda^{-N} \Longrightarrow B = \lambda^N A \\ 2(Eh^2 - 1) R_0 + R_1 + R_{N-1} = 2h & (3) \end{cases}$$

We have $2(1-Eh^2) = \lambda_1 + \lambda_2 = \lambda + \frac{1}{\lambda}$, so we rewrite eq. (3) as

$$-\left(\lambda+\frac{1}{\lambda}\right)\underbrace{(A+B)}_{\substack{\parallel \\ R_0}} + \underbrace{A\lambda + \frac{B}{\lambda}}_{\substack{\parallel \\ R_1}} + \underbrace{A\lambda^{N-1} + B\lambda^{1-N}}_{\substack{\parallel \\ R_{N-1}}} = 2h$$

which, using $B = \lambda^N A$, simplifies to

$$\left(\lambda + \lambda^{N-1} - \frac{1}{\lambda} - \lambda^{N+1}\right) A = 2h \quad \text{or} \quad A = \frac{2h}{(\lambda-\frac{1}{\lambda})(1-\lambda^N)}.$$

The resolvent operator $\hat{R}_E$ is equal to

$$R_m = \frac{2h(\lambda^m + \lambda^{N-m})}{(\lambda-\frac{1}{\lambda})(1-\lambda^N)}.$$

In this expression λ could be both λ_1 or λ_2, as changing λ to $1/\lambda$ doesn't change R_m.

As a function of the spectral parameter E the resolvent $\hat{R}_E$ has singularities whenever the denominator $(\lambda-\frac{1}{\lambda})(1-\lambda^N) = 0$, which happens when $\lambda = \pm 1$ or $\underbrace{\lambda^N = 1}$. happens when $E = E_n$ for some n

singularity at $\lambda = -1$ in the case of odd N is cancelled by $\lambda^m + \lambda^{N-m} = (-1)^m - (-1)^{-m} = 0$ in the numerator

We have $\lambda - \frac{1}{\lambda} = 2ih\sqrt{E(2-Eh^2)}$.

Notice that in the limit $h \to 0$ with fixed $L = hN$ and continuous variable $x = mh$ we get

$$R_E(x) = R_{\frac{x}{h}} = \frac{e^{i\sqrt{2E}\,x} + e^{i\sqrt{2E}\,(L-x)}}{i\sqrt{2E}\left(1-e^{i\sqrt{2E}\,L}\right)}$$

— the resolvent of $\hat{L} = -\frac{1}{2}\frac{d^2}{dx^2}$ on the circle of length L $\left(\lambda = 1 + ih\sqrt{2E} + O(h^2)\right)$.

(B) (i) We have $L_{ij} = \dfrac{2\delta_{ij} - \delta_{i,j+1} - \delta_{i,j-1}}{2h^3}$, so $L_{ij} = L_{ji}$ – the matrix of $\hat{L}$ is real symmetric, so $\hat{L}^* = \hat{L}$.

(ii) $$\langle \vec{u}, L\vec{v} \rangle = h \sum_{n=-\infty}^{\infty} u_n^* \frac{v_{n+1} - 2v_n + v_{n-1}}{-2h^2} =$$

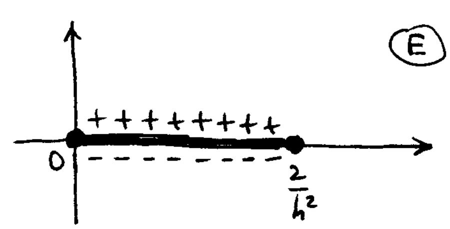
$$= \frac{1}{2h} \sum_{n=-\infty}^{\infty} \Big(2u_n^* v_n - \underset{\text{shift } -1}{u_n^* v_{n+1}} - \underset{\text{shift } +1}{u_n^* v_{n-1}} \Big) =$$

$$= \frac{1}{2h} \sum_{n=-\infty}^{\infty} \Big(2u_n^* v_n - u_{n-1}^* v_n - u_{n+1}^* v_n \Big) =$$

$$= h \sum_{n=-\infty}^{\infty} \frac{u_{n+1}^* - 2u_n^* + u_{n-1}^*}{-2h^2} v_n =$$

$$= \langle \hat{L}\vec{u}, \vec{v} \rangle, \text{ so } \hat{L}^* = \hat{L}.$$

(C) We have $\lambda_{1,2} = 1 - Eh^2 \pm ih\sqrt{E(2 - Eh^2)}$. Let us use the branch of $\sqrt{E(2-Eh^2)}$ that is analytic in the exterior of $[0, \frac{2}{h^2}]$ and has the following sign:



As $\lambda_1 \lambda_2 = 1$, we have $|\lambda_1| = 1$ only when $\lambda_1 = \lambda_2^*$, or when $1 - Eh^2 = \operatorname{Re} \lambda_{1,2}$ and $h\sqrt{E(2-Eh^2)} = \pm \operatorname{Im} \lambda_{1,2}$.

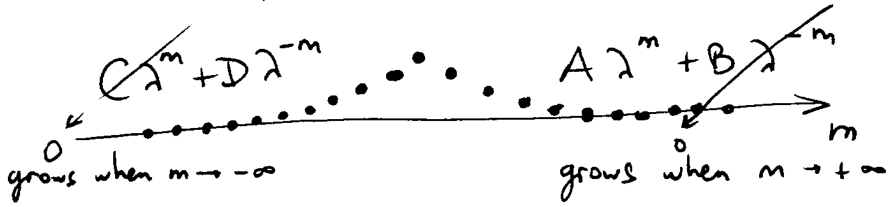
This happens only when E is real and $E(2-Eh^2) \geq 0$, or when $E \in [0, \frac{2}{h^2}]$. Everywhere in the exterior we have either $|\lambda_1| < 1$ or $|\lambda_1| > 1$: $|\lambda_1|$ is a [non-analytic but] continuous function of E, so any two points with $|\lambda_1|<1$ and $|\lambda_1|>1$ would contain a point with $|\lambda_1|=1$ somewhere on any path connecting them, and it is always possible to choose a path that avoids $[0, \frac{2}{h^2}]$. (Check Zhukovsky's function, construct its inverse, compare with $\lambda_{1,2}$.)

With our branch of $\sqrt{E(2-Eh^2)}$ we have

$$\lambda_{1,2}\Big(\underbrace{\tfrac{1}{h^2}+iy}_{E=}\Big) = -i\underbrace{y}_{\text{positive}}h^2 \pm i\underbrace{\sqrt{1+y^2h^4}}_{\text{positive}}, \text{ so it}$$

is $|\lambda_1|<1$ there (and thus everywhere outside of $[0, \frac{2}{h^2}]$), while $|\lambda_2|>1$. We will use $\lambda := \lambda_1 = \frac{1}{\lambda_2}$.

(i) The equations for R_m are the same as in part **(a)**, and their solution looks like



As $R_0 = R_0$, we have $A = D$. The eq. (2) is now

$$\underbrace{\left(E - \frac{1}{h^2}\right)}_{-(\lambda+\frac{1}{\lambda})/2h^2} A + \frac{2A\lambda}{2h^2} = \frac{1}{h} \implies A = \frac{2h}{\lambda - \frac{1}{\lambda}} = \frac{1}{i\sqrt{E(2-Eh^2)}}.$$

The resolvent operator has the form

$$R_m = A\lambda^{|m|} = \frac{\left(1-Eh^2+ih\sqrt{E(2-Eh^2)}\right)^{|m|}}{i\sqrt{E(2-Eh^2)}}.$$

(ii) We have $R_m = \lim_{N\to\infty} \dfrac{2h(\lambda^m+\lambda^{N-m})}{(\lambda-\frac{1}{\lambda})(1-\lambda^N)}$ - expression valid for $0 \le m \le N$

For $m \geq 0$ we get $(\lambda^N \xrightarrow[N\to\infty]{} 0)$ $R_m = \dfrac{2h\lambda^m}{\lambda-\frac{1}{\lambda}}$.

For $m<0$ we can notice that (α) by symmetry $R_{-m} = R_m$, or (β) $m<0$ corresponds to $m \to m+N$ being very large, close to N, so $\lambda^m \to 0$, while $\lambda^{N-m} \to \lambda^{|m|}$, so we get $R_{m<0} \to \dfrac{2h\lambda^{|m|}}{\lambda-\frac{1}{\lambda}}$.

(iii) Consider eqs. (1) and (2) and do the "inverse Fourier series" transform (I'll write it in the form of z-transform):

$$R(z) := \sum_{m=-\infty}^{\infty} R_m z^m, \quad R_m = \frac{1}{2\pi i}\oint_{|z|=1} dz\, \frac{R(z)}{z^{m+1}}.$$

From

$$2(Eh^2-1)R_m + R_{m+1} + R_{m-1} = 2h\delta_{m0}$$

we get

$$2(Eh^2-1)R(z) + \frac{R(z)}{z} + zR(z) = 2h.$$

$$R(z) = -\frac{h}{1 - Eh^2 - \frac{z + \frac{1}{z}}{2}}.$$ By going back from z to m variable, we get

$$R_m = \left\{ \begin{array}{l} z = e^{i\theta} \\ dz = iz\, d\theta \end{array} \right\} = -\frac{h}{2\pi}\int_0^{2\pi} d\theta \, \frac{e^{-im\theta}}{1 - Eh^2 - \cos\theta}.$$

This is the analog of $\hat{R}_E = \sum_{n=0}^{N-1} \frac{\vec{w}_n \, \vec{w}_n^{\dagger}}{E - \frac{1 - \cos\left(\frac{2\pi n}{N}\right)}{h^2}}$ expression.

It defines an analytic function of E whenever $1 - Eh^2$ is not a possible value of $\cos\theta$ (which sits in $[-1, 1]$), i.e., $E \notin [0, \frac{2}{h^2}]$.
Use MATH 583A Fall 2016 Final Exam, problem 5 to show that the answer coincides with the one from (i) and (ii).

Spectrum: The "eigenfunctions" of $\hat{L}$ would look like $A\lambda^m + B\lambda^{-m}$, which either exponentially grow at $+\infty$ or $-\infty$, or don't decay (if $E \in [0, \frac{2}{h^2}]$). They are out of ℓ^2, so the point spectrum is empty. $\hat{L}^* = \hat{L}$, so the residual spectrum is empty too. Whenever $E \notin [0, \frac{2}{h^2}]$ R_m exponentially decays, so $\hat{R}_E$ is bounded — we are in the resolvent set. $[0, \frac{2}{h^2}]$ is the continuous spectrum of $\hat{L}$.

Let us show that the resolvent operator $\hat{R}_0 = -\hat{L}^{-1}$, corresponding to $E=0$, is indeed defined on the dense subspace. We can set $R_m = h\,|m|$, or

$$\left((-\hat{L})^{-1}\vec{\psi}\right)_m = h\sum_{n=-\infty}^{\infty} h\,|m-n|\,\psi_n$$ - discretization of

$$\left(\left(\frac{1}{2}\frac{d^2}{dx^2}\right)^{-1}\psi\right)(x) = \int_{-\infty}^{\infty} dy\,|x-y|\,\psi(y).$$ One will not be able to act by $\hat{L}^{-1}$ on any $\vec{\psi}$ from l^2, as the sum could diverge, or the result could be out of l^2.

For simplicity (the idea is same) let us deal with continuous case $L^2(\mathbb{R})$. Let us truncate $\psi(x)$:

$$\psi_T(x) = \begin{cases} \psi(x), & |x|<T; \\ 0, & |x| \geq T. \end{cases}$$ By increasing T we can make $\|\vec{\psi} - \vec{\psi}_T\|$ being arbitrarily small. Now consider truncated-shifted

$$\psi_{TS}(x) = \psi_T(x) - \begin{cases} A_+, & 0 \leq x < W; \\ A_-, & -W < x < 0; \\ 0, & |x| \geq W. \end{cases}$$

We set $A_\pm := \frac{1}{2W}\int_{-T}^{T} dx\,\psi(x) \pm \frac{1}{W^2}\int_{-T}^{T} dx\,x\,\psi(x)$,

in order to have $\int_{-\infty}^{\infty} dx\,\psi_{TS}(x) = \int_{-\infty}^{\infty} dx\,x\,\psi_{TS}(x) = 0.$

This ensures that $\left(\frac{1}{2}\frac{d^2}{dx^2}\right)^{-1}\vec{\psi}_{TS}$ has compact support ($\vec{\psi}_{TS}$ has compact support too). The norm

$$\|\vec{\psi}_T - \vec{\psi}_{TS}\|^2 = W\left(A_+^2 + A_-^2\right) \xrightarrow[W\to\infty]{} 0$$ can be made arbitrarily small by increasing W,

so $\|\vec{\psi} - \vec{\psi}_{TS}\| \leq \|\vec{\psi} - \vec{\psi}_T\| + \|\vec{\psi}_T - \vec{\psi}_{TS}\|$ can be made small too.

(d) $$\|\hat{L}\vec{u}\|^2 = \frac{1}{4h^4}\sum_{n=-\infty}^{\infty}|u_{n+1}-2u_n+u_{n-1}|^2 \le$$

$$\le \frac{1}{4h^4}\sum_{n=-\infty}^{\infty}\left(|u_{n+1}|+2|u_n|+|u_{n-1}|\right)^2 =$$

$$= \frac{1}{4h^4}\sum_{n=-\infty}^{\infty}\left(|u_{n+1}|^2+4|u_n|^2+|u_{n-1}|^2+4|u_{n+1}||u_n|+4|u_n||u_{n-1}|+2|u_{n+1}||u_{n-1}|\right) \le$$

interpret as inner product $\langle\vec{u},\vec{v}\rangle \le \|\vec{u}\|\cdot\|\vec{v}\|$

$$\le \frac{1}{4h^4}\left(\|\vec{u}\|^2+4\|\vec{u}\|^2+\|\vec{u}\|^2+4\|\vec{u}\|^2+4\|\vec{u}\|^2+2\|\vec{u}\|^2\right) =$$

$$= \frac{4\|\vec{u}\|^2}{h^4} \implies \|\hat{L}\| \le \sqrt{\frac{4}{h^4}} = \frac{2}{h^2}$$

Consider $u_n = \begin{cases}(-1)^n, & 0 \le n < w;\\ 0 & \text{otherwise}.\end{cases}$ Then

$$\vec{u} = \;\dots\; 0 \;\; 0 \;\; \overbrace{1 \;\; -1 \;\; 1 \;\; -1 \;\; \dots \;\; 1 \;\; -1}^{w} \;\; 0 \;\; \dots$$

$$\hat{L}\vec{u} = \;\dots\; 0 \;\; -\frac{1}{2h^2} \;\; \frac{3}{2h^2} \;\; -\frac{2}{h^2} \;\; \frac{2}{h^2} \;\; -\frac{2}{h^2} \;\; \dots \;\; \frac{2}{h^2} \;\; -\frac{3}{2h^2} \;\; \frac{1}{2h^2} \;\; 0 \dots$$

with $\|\hat{L}\vec{u}\| / \|\vec{u}\| \longrightarrow 2/h^2$ as $W \to \infty$.

$$\sup \frac{\|\hat{L}\vec{u}\|}{\|\vec{u}\|} \ge \frac{2}{h^2} \implies \|\hat{L}\| = \frac{2}{h^2}$$

(e) We have $\lambda = 1 + ih\sqrt{2E} + O(h^2)$, while $A \xrightarrow[h\to 0]{} 1/i\sqrt{2E}$. $m = \frac{x}{h}$, so

$$R_E(x) = \lim_{h\to 0} A\lambda^{|m|} = \lim_{h\to 0}\frac{\left(1+ih\sqrt{2E}\right)^{\frac{|x|}{h}}}{i\sqrt{2E}} =$$

$$= \frac{e^{i\sqrt{2E}\,|x|}}{i\sqrt{2E}}$$ – the resolvent of $\hat{\mathcal{L}} = -\frac{1}{2}\frac{d^2}{dx^2}$ on the real line