Chapter 24 Sturm-Liouville problem

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Reference: [1] Veerle Ledoux, Study of Special Algorithms for solving Sturm-Liouville and Schrodinger Equations.

[2] 王信華教授, chapter 8, lecture note of Ordinary Differential equation

Existence and uniqueness [1]

Sturm-Liouville equation: $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y$ on interval $(0,a)$

Assumptions:

1 $p(x)$ is continuous differentiable on closed interval $[0,a]$, or say $p\in C^1[0,a]$, and $p>0$ on $(0,a)$

$$\begin{matrix}\lim_{x\to0} p(x)=p(0)\\ \lim_{x\to a} p(x)=p(a)\end{matrix} \text{, and } \begin{matrix}\lim_{x\to0} p'(x)=p'(0)\\ \lim_{x\to a} p'(x)=p'(a)\end{matrix} \text{, and } \min\{p(x):0\le x\le a\}=p_{\min}>0$$

2 $q(x)$ is continuous on closed interval $[0,a]$, or say $q\in C[0,a]$

3 $w(x)\in C[0,a]$, and $w>0$ on $(0,a)$

Proposition 1.1: Sturm-Liouville initial value problem $\begin{cases}-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y\\ y(0)=y_0,\quad \frac{dy}{dx}(0)=y_0^{(1)}\end{cases}$ is unique on $[0,a]$ under three assumptions.

proof: as before, we re-formulate it as integral equation and apply "contraction mapping principle"

$$\frac{dy}{dx}(x)=\frac{1}{p(x)}\left[p(0)\,y_0^{(1)}+\int_0^x\left(q(s)-Ew(s)\right)y(s)\,ds\right]$$

$$y(x)=y_0+p(0)\,y_0^{(1)}\int_0^x\frac{1}{p(s)}ds+\int_0^x\frac{1}{p(t)}\left[\int_0^t\left(q(s)-Ew(s)\right)y(s)\,ds\right]dt$$

Let $C([0,a])=\{f:[0,a]\to R \text{ is continuous}\}$ be continuous space equipped with norm $\|f\|_\infty=\max\{|f(x)|:0\le x\le a\}$

Existence and uniqueness [2]

1 $C([0,a])$ is complete under norm $\|f\|_\infty = \max\{|f(x)| : 0 \le x \le a\}$

2 define a mapping $T : C[0,a] \to C[0,a]$ by $(Ty)(x) = y_0 + p(0)\, y_0^{(1)} \int_0^x \frac{1}{p(s)} ds + \int_0^x \frac{1}{p(t)} \left[\int_0^t \big(q(s) - Ew(s)\big) y(s)\, ds \right] dt$

$$(T\varphi)(x) - (T\psi)(x) = \int_0^x \frac{1}{p(t)} \left[\int_0^t \big(q(s) - Ew(s)\big)\big(\varphi(s) - \psi(s)\big) ds \right] dt$$

$$\Big\downarrow$$

extract supnorm $\|\varphi - \psi\|_\infty$

$$\left|(T\varphi)(x) - (T\psi)(x)\right| \le \int_0^x \frac{1}{p_{\min}} \left[\int_0^t \left(\|q\|_\infty + |E|\|w\|_\infty\right) \|\varphi - \psi\|_\infty\, ds \right] dt$$

$$\Big\downarrow$$

$$\left|(T\varphi)(x) - (T\psi)(x)\right| \le \frac{\|q\|_\infty + |E|\|w\|_\infty}{2p_{\min}} x^2 \|\varphi - \psi\|_\infty$$

$$\Big\downarrow$$

$$\|T\varphi - T\psi\|_\infty \le \left(\frac{\|q\|_\infty + |E|\|w\|_\infty}{2p_{\min}} a^2 \right) \|\varphi - \psi\|_\infty$$

T is a contraction mapping if $\frac{\|q\|_\infty + |E|\|w\|_\infty}{2p_{\min}} a^2 < 1$ $\longrightarrow$ *Existence and uniqueness*

Fundamental matrix

Sturm-Liouville equation: $-\dfrac{d}{dx}\left(p(x)\dfrac{dy}{dx}\right)+q(x)\,y=Ew(x)\,y$ on interval $(0,a)$

$\Big\downarrow$ Transform to ODE system by setting $z(x)=p(x)\dfrac{dy}{dx}$

$\dfrac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix}=\begin{pmatrix} 0 & \dfrac{1}{p(x)} \\ q(x)-Ew(x) & 0 \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix}$ has two fundamental solutions $\begin{pmatrix} y_1 \\ z_1 \end{pmatrix}, \begin{pmatrix} y_2 \\ z_2 \end{pmatrix}$ satisfying $\begin{pmatrix} y_1(0) \\ z_1(0) \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} y_2(0) \\ z_2(0) \end{pmatrix}=\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\Big\downarrow$

Solution of initial value problem $\left\{\begin{array}{l} -\dfrac{d}{dx}\left(p(x)\dfrac{dy}{dx}\right)+q(x)\,y=Ew(x)\,y \\ y(0)=y_0, \quad \dfrac{dy}{dx}(0)=y_0^{(1)} \end{array}\right.$ is $y(x)=y_0 y_1(x)+\left(p(0)\,y_0^{(1)}\right)y_2(x)$

Definition: fundamental matrix of $-\dfrac{d}{dx}\left(p(x)\dfrac{dy}{dx}\right)+q(x)\,y=Ew(x)\,y$ is $\Phi(x)=\begin{pmatrix} y_1 & y_2 \\ z_1 & z_2 \end{pmatrix}=\begin{pmatrix} y_1 & y_2 \\ p(x)\,y_1' & p(x)\,y_2' \end{pmatrix}$

satisfying $\Phi(0)=\begin{pmatrix} y_1(0) & y_2(0) \\ z_1(0) & z_2(0) \end{pmatrix}=\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$

Question: Can we expect that we have two linear independent fundamental solutions, say

$$\alpha y_1(x)+\beta y_2(x)=0 \text{ on } [0,a] \longrightarrow \alpha=\beta=0$$

Abel's formula [1]

Consider general ODE system of dimension two: $\frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} a_{11}(x) & a_{12}(x) \\ a_{21}(x) & a_{22}(x) \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix}$ with $\Phi(x) = \begin{pmatrix} y_1 & y_2 \\ z_1 & z_2 \end{pmatrix}$, $\Phi(0) = I_2$

$$\frac{d}{dx}\det\Phi(x) = \det\begin{pmatrix} y_1' & y_2' \\ z_1 & z_2 \end{pmatrix} + \det\begin{pmatrix} y_1 & y_2 \\ z_1' & z_2' \end{pmatrix}$$

(from product rule)

$$\det\begin{pmatrix} y_1' & y_2' \\ z_1 & z_2 \end{pmatrix} = \det\begin{pmatrix} a_{11}y_1 + a_{12}z_1 & a_{11}y_2 + a_{12}z_2 \\ z_1 & z_2 \end{pmatrix} = \det\begin{pmatrix} a_{11}y_1 & a_{11}y_2 \\ z_1 & z_2 \end{pmatrix} = a_{11}\det\begin{pmatrix} y_1 & y_2 \\ z_1 & z_2 \end{pmatrix} = a_{11}\det\Phi$$

$$\det\begin{pmatrix} y_1 & y_2 \\ z_1' & z_2' \end{pmatrix} = \det\begin{pmatrix} y_1 & y_2 \\ a_{21}y_1 + a_{22}z_1 & a_{21}y_2 + a_{22}z_2 \end{pmatrix} = \det\begin{pmatrix} y_1 & y_2 \\ a_{22}z_1 & a_{22}z_2 \end{pmatrix} = a_{22}\det\Phi$$

$$\downarrow$$

$$\frac{d}{dx}\det\Phi(x) = (a_{11}(x) + a_{22}(x))\det\Phi(x) = trA \cdot \det\Phi(x)$$

$$\downarrow$$

$$\det\Phi(x) = \det\Phi(0)\exp\left(\int_0^x trA(s)\,ds\right)$$

$$\downarrow$$

$\det\Phi(0) \neq 0 \Leftrightarrow \det\Phi(x) \neq 0$ implies $y_1(x), y_2(x)$ are linearly independent

First order ODE $\frac{dy}{dx} = \lambda(x)\,y$

$$\frac{dy}{y} = \lambda(x)\,dx \longrightarrow \int_{y(0)}^{y}\frac{dy}{y} = \int_0^x \lambda(s)\,ds$$

$$\longrightarrow \log\frac{y(x)}{y(0)} = \int_0^x \lambda(s)\,ds$$

Abel's formula [2]

$$\frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} a_{11}(x) & a_{12}(x) \\ a_{21}(x) & a_{22}(x) \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix} = A(x)\begin{pmatrix} y \\ z \end{pmatrix}$$

with fundamental matrix $\Phi(x) = \begin{pmatrix} y_1 & y_2 \\ z_1 & z_2 \end{pmatrix}$, $\det\Phi(0) \neq 0$

Abel's formula: $\det\Phi(x) = \det\Phi(0)\exp\left(\int_0^x trA(s)\,ds\right)$

⇒

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) + q(x)\,y = Ew(x)\,y$$

$$\Big\downarrow\; z(x) = p(x)\frac{dy}{dx}$$

$$\frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} 0 & \dfrac{1}{p(x)} \\ q(x) - Ew(x) & 0 \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix}$$

$\det\Phi(x) = \det\Phi(0) \quad \forall x \in [0,a]$ since $trA = 0$

Definition: Wronskian $W(\phi_1,\phi_2) \triangleq \det\begin{pmatrix} \phi_1 & \phi_2 \\ \phi_1' & \phi_2' \end{pmatrix}$, then fundamental matrix of Sturm-Liouville equation can be expressed as

$$\Phi(x) = \begin{pmatrix} y_1 & y_2 \\ z_1 & z_2 \end{pmatrix} = \begin{pmatrix} y_1 & y_2 \\ p(x)\,y_1' & p(x)\,y_2' \end{pmatrix} = p(x)W(y_1,y_2)$$

In our time-independent Schrodinger equation, we focus on eigenvalue problem

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) + q(x)\,y = Ew(x)\,y \xrightarrow{p(x)=\frac{1}{2},\,q(x)=V,\,w(x)=1} \left(-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x), \quad \psi(0) = \psi(\pi) = 0$$

Definition: boundary condition $\psi(0) = \psi(\pi) = 0$ is called Dirichlet boundary condition

Question: What is "solvability condition" of Sturm-Liouville Dirichlet eigenvalue problem?

Dirichlet eigenvalue problem [1]

Dirichlet eigenvalue problem: $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)\,y=Ew(x)\,y,\ \ y(0)=y(a)=0$

Observation:

① If (ψ,E) is eigen-pair of Dirichlet eigenvalue problem, then $\psi\in C[0,a]$,in fact, $\psi\in C^2[0,a]$

$$\frac{d^2\psi}{dx^2}=\frac{(q-Ew)\psi-\frac{dp}{dx}\frac{d\psi}{dx}}{p}$$ is continuous on closed interval $[0,a]$

Exercise: $p,q,w:analyitc \longrightarrow \psi:analyitc$

② Under assumption $w(x)\in C[0,a]$, and $w>0\ \text{on}\ (0,a)$, we can define inner-product

$\langle\phi\,|\,\psi\rangle_W \triangleq \int_0^a \phi^*(x)\psi(x)w(x)dx$ where $\phi^*(x)$ is complex conjugate of $\phi(x)$

1 If ***w*** is not positive, then such definition is not an "inner-product"

2 $\langle\phi\,|\,\psi\rangle$ is Dirac Notation, different from conventional form used by Mathematician

Thesis of Veerle Ledoux: $\langle y_i, y_j\rangle=\int_a^b y_i\ y_j^*\ wdx$

Matrix computation: $u^H v=\begin{pmatrix}u_1^* & u_2^* & u_3^*\end{pmatrix}\begin{pmatrix}v_1\\v_2\\v_3\end{pmatrix}$ $\xleftrightarrow[v\to\psi]{u\to\phi}$ Dirac Notation: $\langle\phi\,|\,\psi\rangle$

Dirichlet eigenvalue problem [2]

3 Define differential operator $L=\frac{1}{w(x)}\left\{-\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)+q(x)\right\}$, then it is linear and

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0 \quad\longleftrightarrow\quad Ly=Ey,\quad y(0)=y(a)=0$$

4 Green's identity: $\langle\phi\,|\,L\psi\rangle_W-\overline{\langle\psi\,|\,L\phi\rangle}_W=pW\left(\psi,\phi^*\right)|_{x=0}^{x=a}$

$$\langle\phi\,|\,L\psi\rangle_W=\int_0^a\phi^*L\psi w\,dx=\int_0^a\phi^*\left\{-\frac{d}{dx}\left(p(x)\frac{d\psi}{dx}\right)+q(x)\psi\right\}dx=-p\phi^*\frac{d\psi}{dx}|_0^a\;+\;\boxed{\int_0^a\left[p\frac{d\phi^*}{dx}\frac{d\psi}{dx}+q(x)\phi^*\psi\right]dx}$$

$$\langle\psi\,|\,L\phi\rangle_W=-p\psi^*\frac{d\phi}{dx}|_0^a+\int_0^a\left[p\frac{d\psi^*}{dx}\frac{d\phi}{dx}+q(x)\psi^*\phi\right]dx$$

$$\overline{\langle\psi\,|\,L\phi\rangle}_W=-p\psi\frac{d\phi^*}{dx}|_0^a\;+\;\boxed{\int_0^a\left[p\frac{d\phi^*}{dx}\frac{d\psi}{dx}+q(x)\phi^*\psi\right]dx}$$

The same

hence $\langle\phi\,|\,L\psi\rangle_W-\overline{\langle\psi\,|\,L\phi\rangle}_W=p\left[\psi\frac{d\phi^*}{dx}-\phi^*\frac{d\psi}{dx}\right]_0^a=pW\left(\psi,\phi^*\right)|_{x=0}^{x=a}$

Dirichlet boundary condition:

$$\phi(0)=\phi(a)=0$$

$$\psi(0)=\psi(a)=0$$

$$\langle\phi\,|\,L\psi\rangle_W-\overline{\langle\psi\,|\,L\phi\rangle}_W=0$$

Dirichlet eigenvalue problem [3]

5 *Definition*: operator ***L*** is called self-adjoint on inner-product space $L^2\left([0,a],w\right)=\left\{f:[0,a]\to C:\int_0^a |f|^2\, wdx<\infty\right\}$

If Green's identity is zero, say $\langle \phi \mid L\psi\rangle_W - \overline{\langle \psi \mid L\phi\rangle}_W = 0$

Matrix computation (finite dimension):

$$e_i A e_j = A_{ij}$$

$$e_j A e_i = A_{ji}$$

$$\xrightarrow[e_j \to \psi]{e_i \to \phi}$$

Functional analysis (infinite dimension):

$$\langle \phi \mid L\psi\rangle_W = L_{ij}$$

$$\overline{\langle \psi \mid L\phi\rangle}_W = L_{ji}^*$$

Matrix A is Hermitian (self-adjoint): $A_{ij} = A_{ji}^*$

operator ***L*** is self-adjoint: $\langle \phi \mid L\psi\rangle_W - \overline{\langle \psi \mid L\phi\rangle}_W = 0$

Matrix A is Hermitian, then

1 A is diagonalizable and has real eigenvalue

2 eigenvectors are orthogonal

$$AV = V\Lambda \longrightarrow A = V\Lambda V^H$$

$$\Lambda = diag\left(\lambda_1,\cdots,\lambda_n\right)$$

$V^H V = I$: orthonormal

$$\xrightarrow{?}$$

operator ***L*** is Hermitian, then

1 ***L*** is diagonalizable and has real eigenvalue

2 eigenvectors are orthogonal

Dirichlet eigenvalue problem [4]

Suppose (ϕ, E_1) and (ψ, E_2) are two eigen-pair of $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y = Ew(x)y,\quad y(0)=y(a)=0$

(ϕ, E_1) and (ψ, E_2) are two eigen-pair $\longrightarrow$ $\begin{array}{l} L\phi = E_1\phi \\ L\psi = E_2\psi \end{array}$

$$L\phi = E_1\phi \longrightarrow \langle \psi | L\phi \rangle_W = E_1 \langle \psi | \phi \rangle_W$$

$$L\psi = E_2\psi \longrightarrow \langle \phi | L\psi \rangle_W = E_2 \langle \phi | \psi \rangle_W$$

$$\langle \phi | L\psi \rangle_W - \overline{\langle \psi | L\phi \rangle}_W = \left(E_2 - E_1^*\right)\langle \phi | \psi \rangle_W \xrightarrow{\langle \phi | L\psi \rangle_W - \overline{\langle \psi | L\phi \rangle}_W = 0} \boxed{0 = \left(E_2 - E_1^*\right)\langle \phi | \psi \rangle_W}$$

Theorem 1: all eigenvalue of Sturm-Liouville Dirichlet problem are real

<proof>

$$L = \frac{1}{w(x)}\left\{-\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)+q(x)\right\} \xrightarrow{p,q,w:real} L = L^*$$

$$L\phi = E_1\phi \longrightarrow (L\phi)^* = E_1^*\phi^* \xrightarrow{L=L^*} L\phi^* = E_1^*\phi^*$$

Hence (ϕ, E_1) is eigen-pair if and only if $\left(\phi^*, E_1^*\right)$ is eigen-pair

$$0 = \left(E_2 - E_1^*\right)\langle \phi | \psi \rangle_W \xrightarrow{\text{choose } E_2 = E_1^*,\ \psi = \phi^*} 0 = \left(E_1 - E_1^*\right)\langle \phi | \phi \rangle_W \xrightarrow{\phi \neq 0} E_1 = E_1^* \Rightarrow E_1 \in R$$

Dirichlet eigenvalue problem [5]

Theorem 2: if (ϕ, E_1) and (ψ, E_2) are two eigen-pair of $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\ \ y(0)=y(a)=0$

If eigenvalue $E_1 \neq E_2$, then $\langle\phi\,|\,\psi\rangle_W=0$ $:\phi,\psi$ are orthogonal in $L^2([0,a],w)$

<proof> from Theorem 1, we know *E1* and *E2* are real

$$0=(E_2-E_1^*)\langle\phi\,|\,\psi\rangle_W \xrightarrow{E_1, E_2\ :\ real} 0=(E_2-E_1)\langle\phi\,|\,\psi\rangle_W \xrightarrow{E_1\neq E_2} 0=\langle\phi\,|\,\psi\rangle_W$$

Theorem 3 (unique eigen-function): eigenfunction of Sturm-Liouville Dirichlet problem is unique,
in other words, eignevalue is simple.

<proof>

Abel's formula

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y$$

$$\Big\downarrow\ z(x)=p(x)\frac{dy}{dx}$$

$$\frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix}=\begin{pmatrix} 0 & \frac{1}{p(x)} \\ q(x)-Ew(x) & 0 \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix}$$

$\det\Phi(x)=\det\Phi(0)\quad \forall x\in[0,a]$ since $trA=0$

suppose $L\phi=E\phi$, $L\psi=E\psi$ and $\phi(0)=\phi(a)=0$, $\psi(0)=\psi(a)=0$

Let $\Phi(x)=\begin{bmatrix} \phi & \psi \\ p\phi' & p\psi' \end{bmatrix}$, then

$$\det\Phi(0)=0 \longrightarrow \det\Phi(x)=0\quad \forall x\in[0,a]$$

$\longrightarrow$ $\phi=c\psi$ for some constant ***c***

Dirichlet eigenvalue problem [6]

Theorem 4 (eigen-function is real): eigenfunction of Sturm-Liouville Dirichlet problem can be chosen as real function.

<proof> suppose $\phi = u + \sqrt{-1}v$ is eigen-function with eigen-value E , satisfying

$$\begin{cases} L\phi = E\phi \quad \text{and} \\ \phi(0) = \phi(a) = 0 \end{cases} \xrightarrow[L = L^*]{\phi = u + \sqrt{-1}v} \begin{matrix} Lu = Eu \\ Lv = Ev \end{matrix} \quad \text{and} \quad \begin{matrix} u(0) = u(a) = 0 \\ v(0) = v(a) = 0 \end{matrix}$$

Hence $(u, E), (v, E)$ are both eigen-pair, from uniqueness of eigen-function, we have $v = cu$

$$\phi = u + \sqrt{-1}v \xrightarrow{v = cu} \phi = \left(1 + c\sqrt{-1}\right)u$$

we can choose real function ***u*** as eigenfunction

So far we have shown that Sturm-Liouville Dirichlet problem has following properties

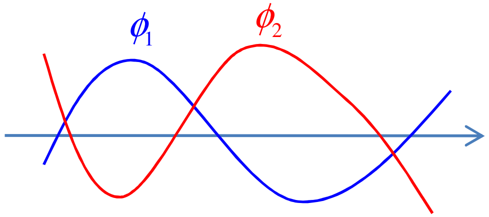
1. Eigenvalues are real and simple, ordered as $E_0 < E_1 < E_2 < \cdots$
2. Eigen-functions are orthogonal in $L^2([0,a], w)$ with inner-product $\langle \phi \mid \psi \rangle_W \triangleq \int_0^a \phi^*(x)\psi(x)w(x)\,dx$
3. Eigen-functions are real and twice differentiable

Exercise (failure of uniqueness): consider $\begin{cases} -\dfrac{d^2y}{dx^2} = Ey \\ y(-\pi) = y(\pi), \ \dfrac{d}{dx}y(-\pi) = \dfrac{d}{dx}y(\pi) \end{cases}$, find eigen-pair and show “eigenvalue is not simple”, can you explain this? (compare it with Theorem 3)

Dirichlet eigenvalue problem [7]

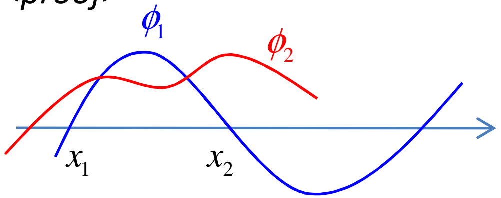
Theorem 5 (Sturm's Comparison theorem): let $(\phi_1, E_1), (\phi_2, E_2)$ be eigen-pair of Sturm-Liouville Dirichlet problem.

suppose $E_2 > E_1$, then ϕ_2 is more oscillatory than ϕ_1 . Precisely speaking



Between any consecutive two zeros of ϕ_1 , there is at least one zero of ϕ_2

<proof>



Let x_1, x_2 are consecutive zeros of ϕ_1 and $\phi_1 > 0$ on (x_1, x_2) as left figure

suppose $\phi_2 > 0$ on (x_1, x_2)

$(\phi_1, E_1), (\phi_2, E_2)$ are eigen-pair, then

$$\begin{cases} -\dfrac{d}{dx}\left(p(x)\dfrac{d\phi_1}{dx}\right) + q(x)\phi_1 = Ew(x)\phi_1, \quad \phi_1(0) = \phi_1(a) = 0 \\ -\dfrac{d}{dx}\left(p(x)\dfrac{d\phi_2}{dx}\right) + q(x)\phi_2 = Ew(x)\phi_2, \quad \phi_2(0) = \phi_2(a) = 0 \end{cases}$$

define $\det\Phi(x) = \det\begin{pmatrix} \phi_2 & \phi_1 \\ p\phi_2' & p\phi_1' \end{pmatrix} = pW(\phi_2, \phi_1)$

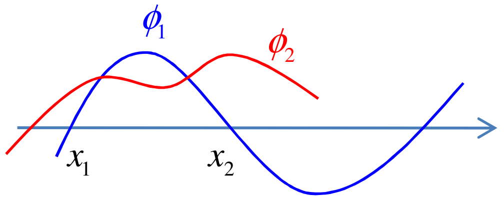
$$\det\Phi(x_1) = \phi_2(x_1)(p\phi_1')(x_1) - \overset{\phi_1(x_1)=0}{\cancel{\phi_1(x_1)}}\, p\phi_2'(x_1) = \phi_2(x_1)(p\phi_1')(x_1) > 0$$

$$\xrightarrow{\text{IVT}} \det\Phi(c) = 0, \quad c \in (x_1, x_2)$$

$$\det\Phi(x_2) = \phi_2(x_2)(p\phi_1')(x_2) - \overset{\phi_1(x_2)=0}{\cancel{\phi_1(x_2)}}(p\phi_2')(x_2) = \phi_2(x_2)(p\phi_1')(x_2) < 0$$

Dirichlet eigenvalue problem [8]

$$\frac{d}{dx}\det\Phi(x)=\cancel{\det\begin{pmatrix}\phi_2' & \phi_1'\\ p\phi_2' & p\phi_1'\end{pmatrix}}+\det\begin{pmatrix}\phi_2 & \phi_1\\ (p\phi_2')' & (p\phi_1')'\end{pmatrix}=\det\begin{pmatrix}\phi_2 & \phi_1\\ (p\phi_2')' & (p\phi_1')'\end{pmatrix}$$



$$-\frac{d}{dx}\left(p(x)\frac{d\phi_1}{dx}\right)+q(x)\phi_1=Ew(x)\phi_1$$

$$-\frac{d}{dx}\left(p(x)\frac{d\phi_2}{dx}\right)+q(x)\phi_2=Ew(x)\phi_2$$

$$\downarrow$$

$$\frac{d}{dx}\det\Phi(x)=\det\begin{pmatrix}\phi_2 & \phi_1\\ (q-E_2w)\phi_2 & (q-E_1w)\phi_1\end{pmatrix}=(E_2-E_1)w\phi_1\phi_2>0 \quad \text{on } (x_1,x_2)$$

$\det\Phi(x_1)>0$ and $\frac{d}{dx}\det\Phi(x)>0$ on (x_1,x_2) implies $\det\Phi(x)>0$ on (x_1,x_2) $—\!\!\times\!\!—$ $\det\Phi(c)=0,\ c\in(x_1,x_2)$

Question: why ϕ_2 is more oscillatory than ϕ_1 , any physical interpretation?

Sturm-Liouville equation $\longleftrightarrow$ Time-independent Schrodinger equation

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=E\,w(x)y \quad\longleftrightarrow\quad \left(-\frac{\hbar}{2}\nabla\cdot\frac{\hbar}{m_e}\nabla+V(\vec{x})\right)\psi(\vec{x})=E\psi(\vec{x})$$

Definition: average quantity of operator $\hat{O}$ over interval $I=(x_1,x_2)$ by

$$\langle\hat{O}\rangle_I=\int_I y\hat{O}ywdx\,/\int_I y^2wdx$$

Dirichlet eigenvalue problem [9]

Express operator ***L*** as $L = \frac{1}{w(x)}\left\{-\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)+q(x)\right\} = T + V$ where T : kinetic operator, V : potential operator

$$L\psi = E\psi \longrightarrow \langle \psi \mid L\psi \rangle_I = E\langle \psi \mid \psi \rangle_I$$

where $\langle \psi \mid L\psi \rangle_I = \cancel{-p\psi\frac{d\psi}{dx}\Big|_{x_1}^{x_2}} + \int_{x_1}^{x_2} p\left(\frac{d\psi}{dx}\right)^2 dx + \int_{x_1}^{x_2} q\psi^2 dx$

neglect boundary term

$\langle L \rangle_I = E \longrightarrow \langle T \rangle_I + \langle V \rangle_I = E$ where $\langle T \rangle_I = \dfrac{\int_{x_1}^{x_2} p\left(\frac{d\psi}{dx}\right)^2 dx}{\int_{x_1}^{x_2} \psi^2 w dx}$ and $\langle V \rangle_I = \dfrac{\int_{x_1}^{x_2} q\psi^2 dx}{\int_{x_1}^{x_2} \psi^2 w dx}$

Heuristic argument for Theorem 5

$$(\phi_1, E_1), (\phi_2, E_2) \longrightarrow \begin{matrix} \langle T \rangle_I(\phi_1) = E_1 - \langle V \rangle_I \\ \langle T \rangle_I(\phi_2) = E_2 - \langle V \rangle_I \end{matrix} \xrightarrow{E_2 > E_1} \langle T \rangle_I(\phi_2) > \langle T \rangle_I(\phi_2) \longrightarrow \int_{x_1}^{x_2} p\left(\frac{d\phi_2}{dx}\right)^2 dx > \int_{x_1}^{x_2} p\left(\frac{d\phi_1}{dx}\right)^2 dx$$

$\longrightarrow$ Average value of $\left|\frac{d\phi_2}{dx}\right| >$ Average value of $\left|\frac{d\phi_1}{dx}\right|$

$\longrightarrow$ ϕ_2 is more oscillatory than ϕ_1

Prufer method [1]

Sturm-Liouville Dirichlet eigenvalue problem: $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0$

Idea: introduce polar coordinate (ρ,θ) in the phase plane $(y, z=py')$

$$\begin{cases} y=\rho\sin\theta \\ z=py'=\rho\cos\theta \end{cases} \longleftrightarrow \begin{cases} \rho^2=y^2+z^2 \\ \tan\theta=\dfrac{y}{z} \end{cases}$$

$$\begin{pmatrix}\dfrac{dy}{dx}\\[2ex] \dfrac{dz}{dx}\end{pmatrix}=\begin{pmatrix}\sin\theta & \rho\cos\theta \\ \cos\theta & -\rho\sin\theta\end{pmatrix}\begin{pmatrix}\dfrac{d\rho}{dx}\\[2ex] \dfrac{d\theta}{dx}\end{pmatrix} \longleftrightarrow \begin{pmatrix}\dfrac{d\rho}{dx}\\[2ex] \dfrac{d\theta}{dx}\end{pmatrix}=\begin{pmatrix}\sin\theta & \cos\theta \\ \dfrac{\cos\theta}{\rho} & -\dfrac{\sin\theta}{\rho}\end{pmatrix}\begin{pmatrix}\dfrac{dy}{dx}\\[2ex] \dfrac{dz}{dx}\end{pmatrix}$$

$$\frac{d}{dx}\begin{pmatrix}y\\ z\end{pmatrix}=\begin{pmatrix}0 & \dfrac{1}{p(x)} \\ q(x)-Ew(x) & 0\end{pmatrix}\begin{pmatrix}y\\ z\end{pmatrix} \longleftrightarrow \begin{aligned} \frac{d\theta}{dx}&=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta \\ \frac{1}{\rho}\frac{d\rho}{dx}&=\left(\frac{1}{p}-(Ew-q)\right)\sin\theta\cos\theta \end{aligned}$$

Exercise: check it

Objective: find eigenvalue E such that $\longleftrightarrow$ ***Objective***: find eigenvalue E such that

$$y(0)=y(a)=0 \qquad\qquad \tan\theta(0)=\tan\theta(a)=0$$

Advantage of Prufer method: we only need to solve $\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta$

when solution $\theta(x;E)$ is found with condition $\tan\theta(0;E)=\tan\theta(a;E)=0$

then $\rho(x)=\rho(0)\exp\left[\int_0^x\left(\frac{1}{p(t)}-(Ew(t)-q(t))\right)\sin\theta(t;E)\cos\theta(t;E)\,dt\right]$

Prufer method [2]

Observation:

① $\rho^2 = y^2 + z^2 > 0$

Suppose $\rho(x_0) = 0, \ \ 0 < x_0 < a \longrightarrow y(x_0) = 0, \ z(x_0) = 0$

$$\longrightarrow \frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} 0 & \dfrac{1}{p(x)} \\ q(x) - Ew(x) & 0 \end{pmatrix}\begin{pmatrix} y \\ z \end{pmatrix}$$

has unique solution $y(x) \equiv 0, \ \ z(x) \equiv 0$ $\not\longrightarrow$

with initial condition $y(x_0) = 0, \ \ z(x_0) = 0$

② fixed $x > 0, \ \theta(x;E)$ is a strictly increasing function of variable E

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) + q(x)y = Ew(x)y \xrightarrow{p=1, q=0, w=1} -\frac{d^2y}{dx^2} = Ey$$

is Hook's law

$$\begin{cases} -\dfrac{d^2y}{dx^2} = Ey \\ y(0) = 0 \end{cases}$$

has general solution $y = \sin kx, \ k = \sqrt{E}, \ E > 0$

$$\frac{d\theta}{dx} = \frac{1}{p}\cos^2\theta + (Ew - q)\sin^2\theta \xrightarrow{p=1, q=0, w=1} \frac{d\theta}{dx} = \cos^2\theta + E\sin^2\theta$$

and $\tan\theta(x;E) = \dfrac{1}{k}\tan(kx)$

$$\begin{cases} \dfrac{d\theta(x;k_1)}{dx} = \cos^2\theta + k_1^2\sin^2\theta \\ \dfrac{d\theta(x;k_2)}{dx} = \cos^2\theta + k_2^2\sin^2\theta \end{cases} \xrightarrow{k_1 > k_2}$$

$slope: \cos^2\theta + k_1^2\sin^2\theta > \cos^2\theta + k_2^2\sin^2\theta$

implies $\theta(x;k_1) > \theta(x;k_2) \geq 0$

Prufer method [3]

Question: Given energy ***E***, how can we solve $\frac{d\theta}{dx} = \cos^2\theta + E\sin^2\theta, \quad \theta(0)=0$ numerically

Forward Euler method: consider first order ODE $\frac{dy}{dx} = f(x,y), \quad y(0)=y_0$

1 Uniformly partition domain $[0,a]$ as $0 = x_0 < x_1 < x_2 < \cdots < x_j = jh < \cdots < x_n = a$

2 Let $y^{(k)} = y(x_k)$ and approximate $\frac{dy}{dx}(x_k)$ by one-side finite difference $\frac{dy}{dx}(x) = \frac{y(x+h)-y(x)}{h} - \frac{h}{2}\frac{d^2y}{dx^2}(c)$

continuous equation: $\frac{dy}{dx} = f(x,y), \quad y(0)=y_0$

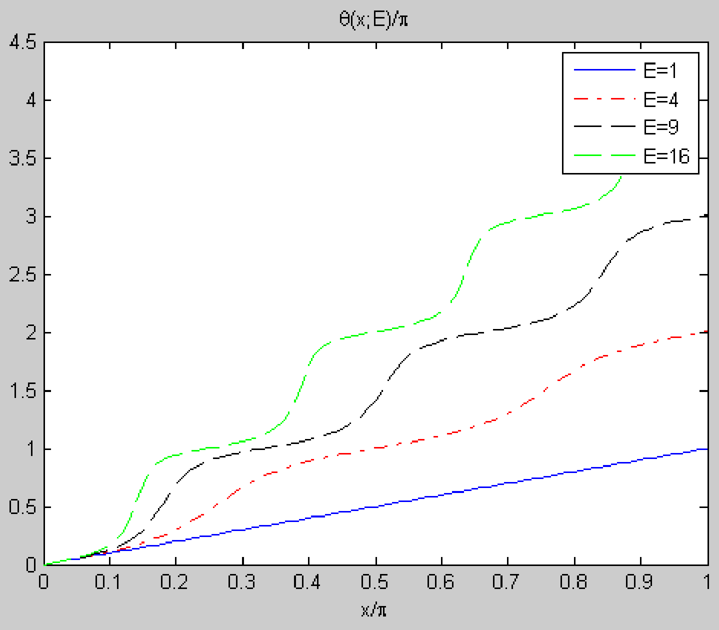
$$\Big\downarrow \; \frac{dy}{dx}(x) \approx \frac{y(x+h)-y(x)}{h}$$

discrete equation: $\frac{y^{(k+1)}-y^{(k)}}{h} = f\left(x_k, y^{(k)}\right), \quad y^{(0)} = y_0$

Exercise : use forward Euler method to solve angle equation

$$\frac{d\theta(x;E)}{dx} = \cos^2(\theta(x;E)) + E\sin^2(\theta(x;E)), \quad \theta(0;E)=0$$

for different E = 1, 4, 9, 16 as right figure



It is clear that $\theta(x;E)$ is a strictly increasing function of variable E

Prufer method [4]

③

$$\left\{\begin{array}{l} y=\rho\sin\theta \\ z=py'=\rho\cos\theta \end{array}\right. \longleftrightarrow \left\{\begin{array}{l} \rho^2=y^2+z^2 \\ \tan\theta=\dfrac{y}{z} \end{array}\right.$$

$$\begin{array}{l} -\dfrac{d}{dx}\left(p(x)\dfrac{dy}{dx}\right)+q(x)\,y=Ew(x)\,y \\ y(0)=y(a)=0 \end{array} \longleftrightarrow \begin{array}{l} \dfrac{d\theta}{dx}=\dfrac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta \\ \tan(\theta(0))=\tan(\theta(a))=0 \end{array}$$

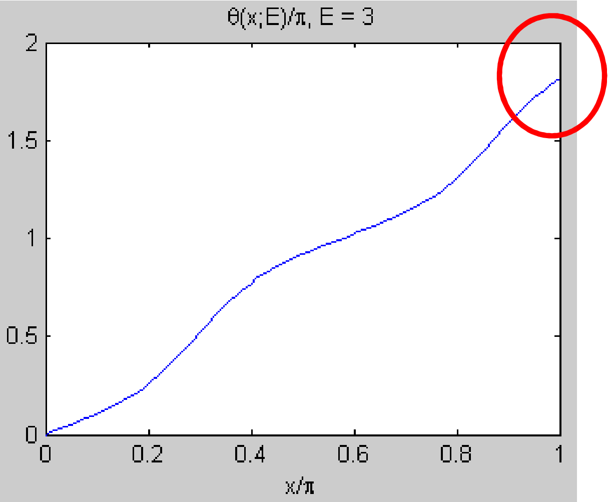
$$\boxed{y(x)=0 \xleftrightarrow[\rho>0]{y=\rho\sin\theta} \sin(\theta(x;E))=0 \longleftrightarrow \theta(x;E)=n\pi}$$

Although $\begin{array}{l} \dfrac{d\theta}{dx}=\dfrac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta \\ \theta(0)=0 \end{array}$ has a unique solution $\theta(x;E)$. But we want to find energy *E*

such that $\begin{array}{l} \dfrac{d\theta}{dx}=\dfrac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta \\ \theta(0)=0,\ \ \tan(\theta(a))=0 \end{array}$, that is $\theta(a;E)=n\pi$ is constraint.

Example: for model problem $\dfrac{d\theta}{dx}=\cos^2(\theta)+E\sin^2(\theta),\quad \theta(0)=0,\ E=3$

$$\theta(\pi)=1.817\pi\neq n\pi$$



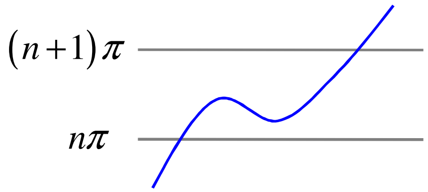
Prufer method [5]

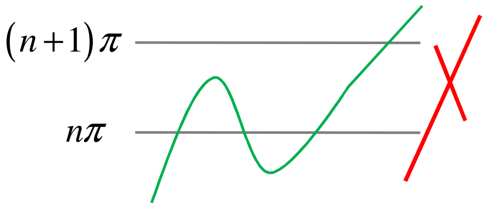
④ $$\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta \xrightarrow{\quad y(x_i)=0\Leftrightarrow\theta(x_i)=n\pi\quad} \frac{d\theta}{dx}(x_i)=\frac{1}{p(x_i)}>0$$

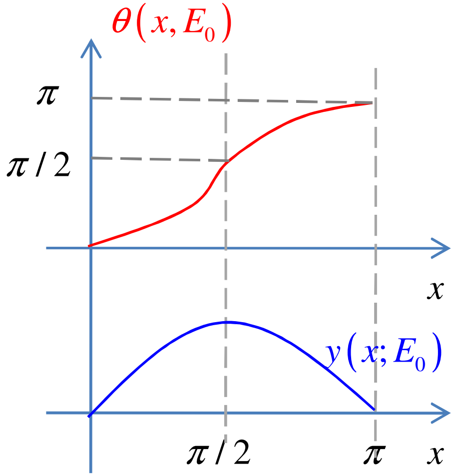
$$\boxed{y(x)=0 \xleftrightarrow[\rho>0]{\quad y=\rho\sin\theta\quad} \theta(x;E)=n\pi}$$

$\longrightarrow$ θ never decrease in a point where $\theta(x_i)=n\pi$

$\longrightarrow$ number of zeros of y in $(0,a)=$ number of multiples of π in $\left(\theta(0),\theta(a)\right)$







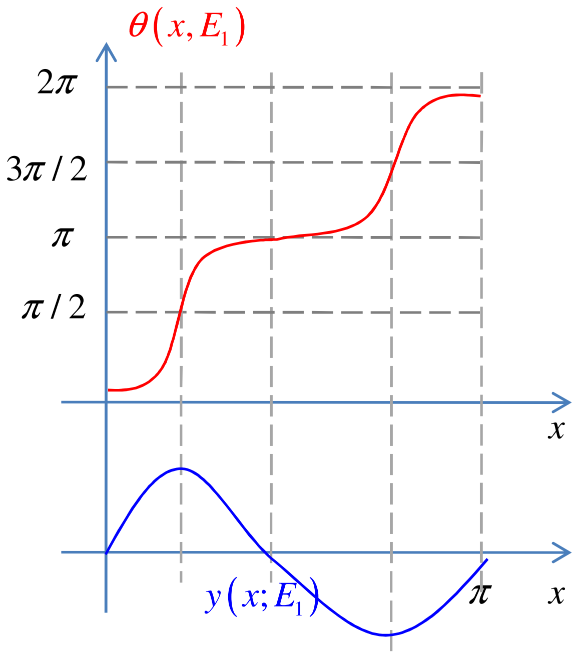
$$\tan\theta(x)=\frac{y(x)}{py'(x)}$$

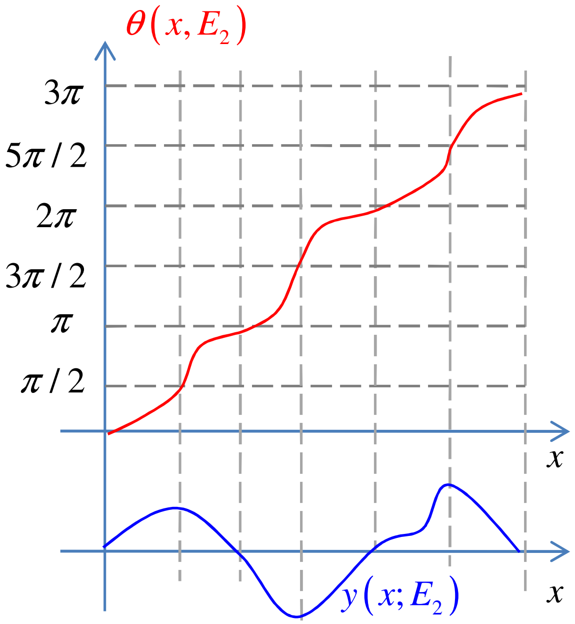
$$y(x)=0 \longleftrightarrow \tan\theta(x)=0 \longleftrightarrow \theta(x)=n\pi$$

$$y'(x)=0 \longleftrightarrow \tan\theta(x)=\pm\infty \longleftrightarrow \theta(x)=\left(n+\frac{1}{2}\right)\pi$$

Ground state $y(x;E_0)$ has no zeros except end points.

Prufer method [6]





First excited state $y(x;E_1)$ has one zero in $(0,\pi)$

$$\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta$$

$$\Big\downarrow \quad \theta(x_j)=\left(n+\frac{1}{2}\right)\pi \quad \Rightarrow \quad z=py'=\rho\cos\theta=0$$

$$\frac{d\theta}{dx}(x_j)=(Ew-q)$$

model problem: $\frac{d\theta}{dx}(x_j)=E>0$

second excited state $y(x;E_1)$ has two zeros in $(0,\pi)$

conjecture: k-th excited state $y(x;E_k)$ has k zeros in $(0,\pi)$

Prufer method [7]

Theorem 6 : consider Prufer equations of regular Sturm-Liouville Dirichlet problem

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0 \qquad p\in C^1[0,a],\ \ q,w\in C[0,a] \text{ and } \quad p>0,w>0$$

Let boundary values satisfy following normalization:

$$\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta$$

$$\theta(0)=0,\quad \theta(a)=\pi$$

Then the kth eigenvalue E_k satisfies $\theta(0,E_k)=0,\ \ \theta(a,E_k)=\pi+k\pi$

Moreover the kth eigen-function $y(x,E_k)=0$ has k zeros in $(0,a)$

Remark: for detailed description, see Theorem 2.1 in

Veerle Ledoux, Study of Special Algorithms for solving Sturm-Liouville and Schrodinger Equations.

Prufer method [8]

Scaled Prufer transformation: a generalization of simple Prufer method

$$\begin{cases} y = \dfrac{1}{\sqrt{S}}\rho\sin\theta \\ z = py' = \sqrt{S}\rho\cos\theta \end{cases}$$

where $S(x;E) > 0:$ scaling function, continuous differentiable

$$\frac{d}{dx}\begin{cases} y = \dfrac{1}{\sqrt{S}}\rho\sin\theta \\ z = py' = \sqrt{S}\rho\cos\theta \end{cases} \longrightarrow \frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} = \frac{S'\rho}{2\sqrt{S}}\begin{pmatrix} -\dfrac{1}{S}\sin\theta \\ \cos\theta \end{pmatrix} + \begin{pmatrix} \dfrac{\sin\theta}{\sqrt{S}} & \dfrac{\rho\cos\theta}{\sqrt{S}} \\ \sqrt{S}\cos\theta & -\sqrt{S}\rho\sin\theta \end{pmatrix}\frac{d}{dx}\begin{pmatrix} \rho \\ \theta \end{pmatrix}$$

1

$$A \triangleq \begin{pmatrix} \dfrac{\sin\theta}{\sqrt{S}} & \dfrac{\rho\cos\theta}{\sqrt{S}} \\ \sqrt{S}\cos\theta & -\sqrt{S}\rho\sin\theta \end{pmatrix} \longrightarrow A^{-1} = \begin{pmatrix} \sqrt{S}\sin\theta & \dfrac{\cos\theta}{\sqrt{S}} \\ \sqrt{S}\dfrac{\cos\theta}{\rho} & -\dfrac{\sin\theta}{\rho\sqrt{S}} \end{pmatrix}$$

2

$$\frac{d}{dx}\begin{pmatrix} \rho \\ \theta \end{pmatrix} = A^{-1}\left\{ \frac{d}{dx}\begin{pmatrix} y \\ z \end{pmatrix} - \frac{S'\rho}{2\sqrt{S}}\begin{pmatrix} -\dfrac{1}{S}\sin\theta \\ \cos\theta \end{pmatrix} \right\}$$

$$\Big\downarrow \quad \frac{dy}{dx} = \frac{z}{p(x)}, \quad \frac{dz}{dx} = \left(q(x) - Ew(x)\right)z$$

$$\frac{d\theta}{dx} = \frac{S}{p}\cos^2\theta + \frac{Ew-q}{S}\sin^2\theta + \frac{S'}{S}\sin\theta\cos\theta$$

$$\frac{2}{\rho}\frac{d\rho}{dx} = \left(\frac{S}{p} - \frac{Ew-q}{S}\right)\sin 2\theta - \frac{S'}{S}\cos 2\theta$$

Theorem 6 holds for scaled Prufer equations

Exercise: use Symbolic toolbox in MATLAB to check scaled Prufer transformation.

Prufer method [9]

Scaled Prufer transformation

$$\frac{d\theta}{dx}=\frac{S}{p}\cos^2\theta+\frac{Ew-q}{S}\sin^2\theta+\frac{S'}{S}\sin\theta\cos\theta$$

$$\frac{2}{\rho}\frac{d\rho}{dx}=\left(\frac{S}{p}-\frac{Ew-q}{S}\right)\sin 2\theta-\frac{S'}{S}\cos 2\theta$$

$$\xrightarrow{S=1}$$

Simple Prufer transformation

$$\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta$$

$$\frac{1}{\rho}\frac{d\rho}{dx}=\left(\frac{1}{p}-(Ew-q)\right)\sin\theta\cos\theta$$

Recall time-independent Schrodinger's equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+V\psi(x)=E\psi(x)$$

$\hbar=1.0542\times10^{-34}J\cdot s$

$m_e\,(\text{mass of electron})=9.1\times10^{-31}kg$

dimensionless form

$$\Big\downarrow$$

$\vec{x}=a\vec{y},$ or say $[\vec{x}]=a$

$E=\varepsilon\tilde{E},$ or say $[E]=\varepsilon$ $\quad[V]=[E]$

$$\left(-\frac{1}{2}\Delta_y+\frac{ma^2}{\hbar^2}V(a\tilde{y})\right)\psi(a\tilde{y})=\frac{ma^2\varepsilon}{\hbar^2}\tilde{E}\psi(a\tilde{y})$$

$$\varepsilon=\frac{\hbar^2}{ma^2}$$

$$\Big\downarrow$$

reduce to 1D Dirichlet problem

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x)$$

$$\psi(0)=\psi(\pi)=0$$

$$\xleftarrow{p=\frac{1}{2},q=V,w=1}$$

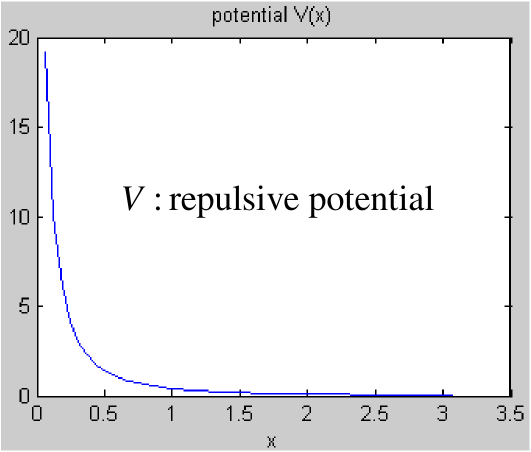
$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0$$

Exercise 1 [1]

Consider 1D Schrodinger equation with Dirichlet boundary condition

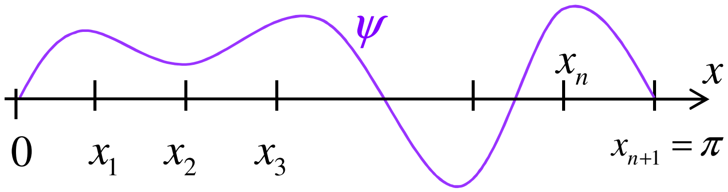
$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x) \qquad V(x)=\frac{1}{2(x+0.1)^2}$$

$$\psi(0)=\psi(\pi)=0$$

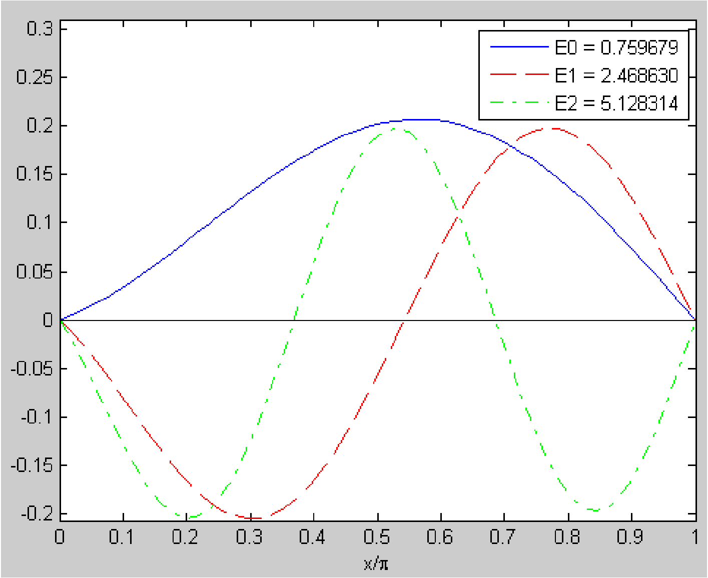


① use standard 3-poiint centered difference method to find eigenvalue

$$\left\{-\frac{1}{2h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}+diag(V)\right\}\vec{\psi}=E\vec{\psi}$$



number of grids = 50, (n = 50)



1 $0<E_0=0.7597<E_1<\cdots$

all eigenvalues ae positive, can you explain this?

2 Ground state $\psi(x;E_0)\equiv\psi_0$ has no zeros in $(0,\pi)$

1st excited state $\psi(x;E_1)\equiv\psi_1$ has 1 zero in $(0,\pi)$

2nd excited state $\psi(x;E_2)\equiv\psi_2$ has 2 zero in $(0,\pi)$

Check if ***k-th*** eigen-function has ***k*** zeros in $(0,\pi)$

Exercise 1 [2]

② solve simple Prufer equation for first 10 eigenvalues

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x),\quad \psi(0)=\psi(\pi)=0$$

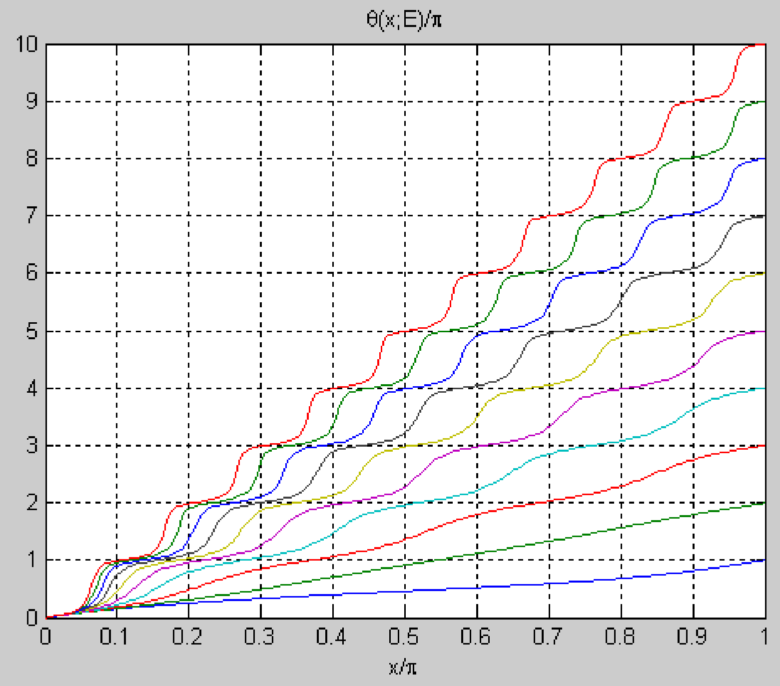
$$E(0:9)=\begin{array}{r} 0.7597 \\ 2.4686 \\ 5.1283 \\ 8.7374 \\ 13.2895 \\ 18.7736 \\ 25.1734 \\ 32.4683 \\ 40.6337 \\ 49.6406 \end{array}$$

$$\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta \qquad \xrightarrow{p=\frac{1}{2},q=V,w=1} \qquad \frac{d\theta}{dx}=2\cos^2\theta+(E-V)\sin^2\theta$$

$$\theta(0;E)=0 \qquad\qquad \theta(0;E)=0$$

Forward Euler method: N = 200

$$\frac{dy}{dx}=f(x,y),\quad y(0)=y_0 \longrightarrow \frac{y^{(k+1)}-y^{(k)}}{h}=f\left(x_k,y^{(k)}\right),\quad y^{(0)}=y_0$$



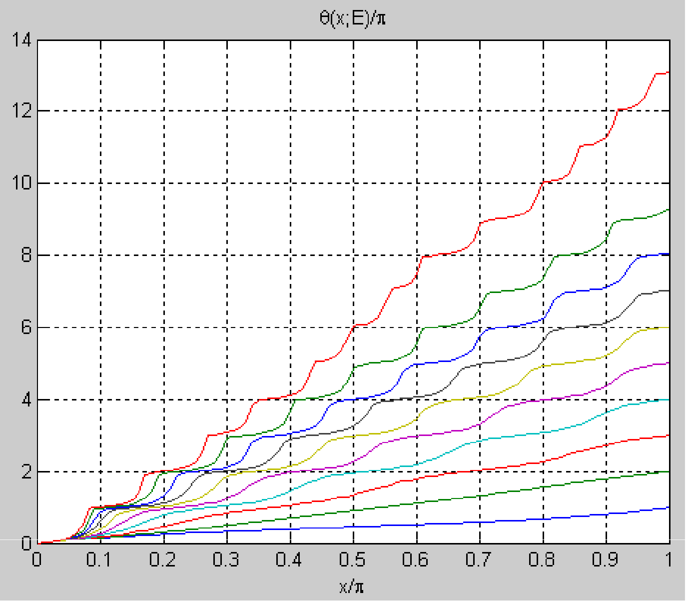
1. $\theta(\pi,E_k)=k\pi+\pi$ is consistent with that in ***theorem 6***

2. $\theta(\pi,E_k)$ increases gradually "staircase" shape with "plateaus" at $\theta(\pi,E_k)=j\pi$ and steep slope around $\theta(\pi,E_k)=\left(j-\frac{1}{2}\right)\pi$

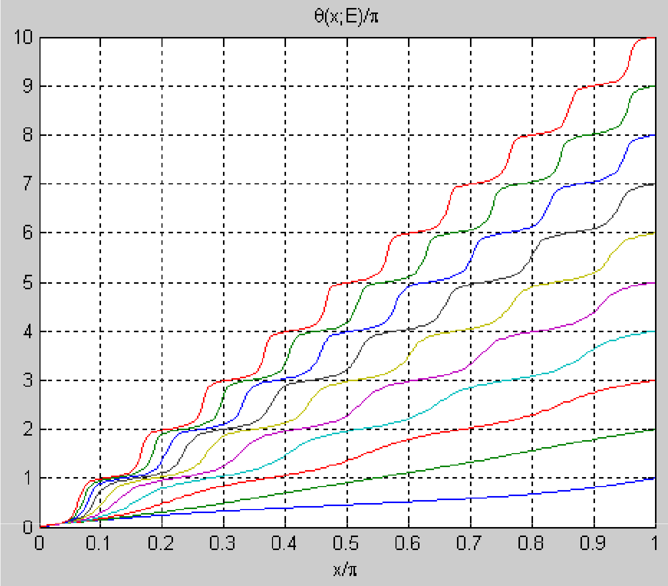
Question: what is disadvantage of this "staircase" shape?

Exercise 1 [3]

Forward Euler method: N = 100



Forward Euler method: N = 200



$\theta(\pi, E_9) = 12\pi + \pi$ under Forward Euler method with number of grids, N = 100, this is wrong!

Question: Can you explain why $\theta(x, E_9)$ is not good?

hint: see page 21 in reference

Veerle Ledoux, Study of Special Algorithms for solving Sturm-Liouville and Schrodinger Equations.

Exercise 2 [1]

Scaled Prufer transformation

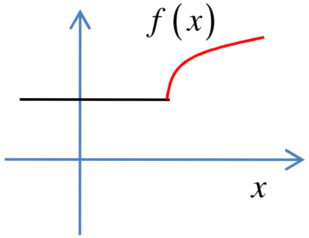
$$\frac{d\theta}{dx}=\frac{S}{p}\cos^2\theta+\frac{Ew-q}{S}\sin^2\theta+\frac{S'}{S}\sin\theta\cos\theta \longrightarrow \frac{d\theta}{dx}=\frac{1}{2}\left[\left(\frac{S}{p}+\frac{Ew-q}{S}\right)+\left(\frac{S}{p}-\frac{Ew-q}{S}\right)\cos 2\theta+\frac{S'}{S}\sin 2\theta\right]$$

$$=A(x)+B(x)\cos 2\theta+C(x)\sin 2\theta$$

1D Schrodinger: $\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x),\quad \psi(0)=\psi(\pi)=0$

$$\frac{d\theta}{dx}=A(x)+B(x)\cos 2\theta+C(x)\sin 2\theta \qquad \theta(0;E)=0 \xrightarrow{p=\frac{1}{2},q=V,w=1} \frac{d\theta}{dx}=\frac{1}{2}\left[\left(2S+\frac{E-V}{S}\right)+\left(2S-\frac{E-V}{S}\right)\cos 2\theta+\frac{S'}{S}\sin 2\theta\right] \qquad \theta(0;E)=0$$

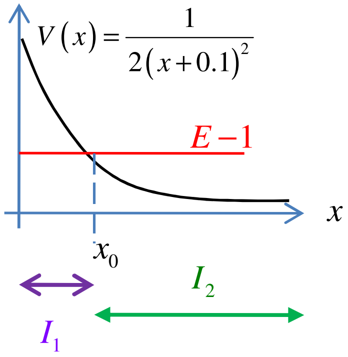
Suppose we choose $S(x)=\begin{cases}1 & \text{if } E-V(x)\le 1\\ \sqrt{E-V(x)} & \text{if } E-V(x)>1\end{cases}=f(E-V(x))$ where $f(x)=\begin{cases}1 & \text{if } x\le 1\\ \sqrt{x} & \text{if } x>1\end{cases}$ is continuous



Question: function ***f*** is continuous but not differentiable at ***x = 1.*** How can we obtain $\frac{dS}{dx}$

Although we have known $\frac{dS}{dx}(x)=0$ on open set $I_1=\{x:E-V(x)<1\}$ and

$\frac{dS}{dx}(x)=\frac{-1}{2S}\frac{dV}{dx}$ on open set $I_2=\{x:E-V(x)>1\}$



$$V(x_0)=\frac{1}{2(x_0+0.1)^2}=E-1 \longrightarrow x_0=\frac{1}{\sqrt{2(E-1)}}-0.1$$

Exercise 2 [2]

solve simple Prufer equation for first 10 eigenvalues

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x),\quad \psi(0)=\psi(\pi)=0$$

$$E(0:9)=\begin{matrix}0.7597\\2.4686\\5.1283\\8.7374\\13.2895\\18.7736\\25.1734\\32.4683\\40.6337\\49.6406\end{matrix}$$

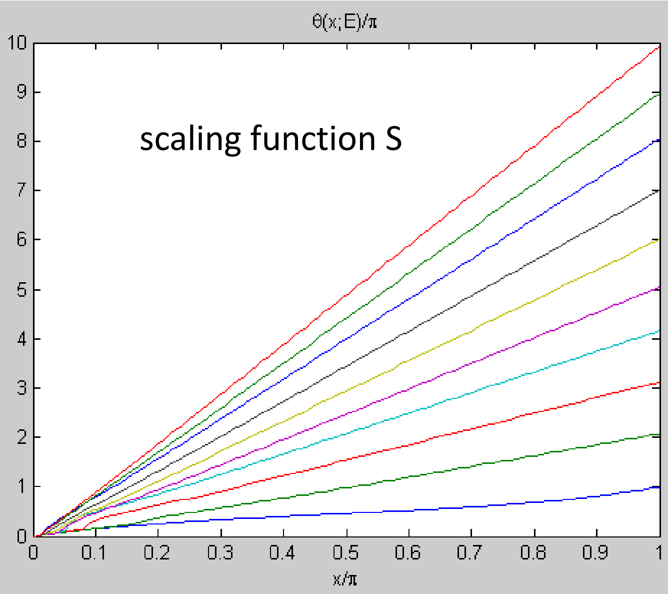
$$\frac{d\theta}{dx}=\frac{S}{p}\cos^2\theta+\frac{Ew-q}{S}\sin^2\theta+\frac{S'}{S}\sin\theta\cos\theta \qquad \theta(0;E)=0$$

$$\xrightarrow{p=\frac{1}{2},q=V,w=1}$$

$$\frac{d\theta}{dx}=2S\cos^2\theta+\frac{E-V}{S}\sin^2\theta+\frac{S'}{S}\sin\theta\cos\theta \qquad \theta(0;E)=0$$

Choose scaling function $S(x)=\begin{cases}\sqrt{0.5} & \text{if } E-V(x)\le 1\\ \sqrt{0.5(E-V(x))} & \text{if } E-V(x)>1\end{cases}$

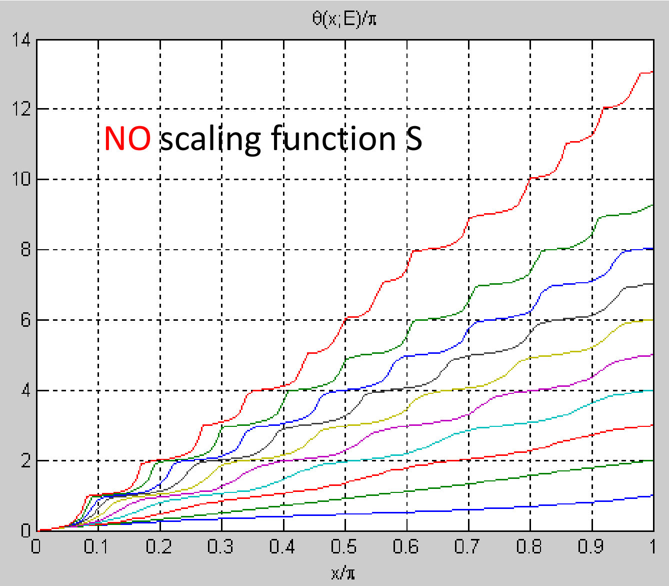
Forward Euler method: N = 100



scaling function S

Compare both figures and interpret why “staircase” disappear when using scaling function

Forward Euler method: N = 100



NO scaling function S