

"TRICK" SHOOTING

①

EIGENVALUE PROBLEMS

WE POSED THE SHOOTING PROBLEM INITIALLY AS A BOUNDARY VALUE PROBLEM:

$$\frac{d}{dt} \vec{x} = \vec{f}(\vec{x}), \quad \vec{x} \in \mathbb{R}^N$$

WITH $M < N$ CONDITIONS AT t_0 , AND $N - M$ CONDITIONS AT t_1 .

THE BASKETBALL PROBLEM VARIED THIS THEME SLIGHTLY BY REPLACING THE B.C. AT t_1 WITH A REQUIREMENT THAT THE PHASE SPACE TRAJECTORY INTERSECT THE BASKET AT SOME UNSPECIFIED TIME.

IN PHYSICS, WE COMMONLY ENCOUNTER A WIDE RANGE OF VARIATIONS ON THE BASIC SHOOTING PROBLEM. ONE ESPECIALLY COMMON VARIETY IS THE EIGENVALUE PROBLEM, IN WHICH THE ODE CONTAINS AN ADJUSTABLE PARAMETER λ . FOR EXAMPLE:

$$\mathcal{D} \vec{q} = \lambda \vec{q}, \quad \vec{q} \in \mathbb{R}^N$$

↑ ADJUSTABLE PARAMETER

↑ STATE VARIABLE

↑ DIFFERENTIAL OPERATOR (NOT NECESSARILY LINEAR!)

IF WE ARE GIVEN $N+1$ BC'S, THE PROBLEM WOULD BE OVERDETERMINED — EXCEPT FOR THE ADDED DEGREE OF FREEDOM PROVIDED BY LAMBDA. A VALUE OF λ THAT ALLOWS US TO SATISFY ALL BC'S IS CALLED THE EIGENVALUE, AND WE CAN SOLVE FOR THE EIGENVALUE BY SHOOTING.

IN GENERAL, NOTE THAT THERE MAY BE $m \geq 1$ ADJUSTABLE PARAMETERS, AND $N+m$ BOUNDARY CONDITIONS.

SCHRÖDINGER'S EQUATION

GOAL: FIND BOUND STATES FOR AN ARBITRARY POTENTIAL.

DIMENSIONLESS VERSION OF THE ODE:

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

VARIABLE	UNITS
x	λ
V, E	$\hbar^2/2m\lambda^2$

A SIMPLE ANALYTICAL EXAMPLE — SQUARE WELL:

$$V(x) = \begin{cases} -V_0, & |x| \leq 1 \\ 0, & |x| \geq 1 \end{cases}$$

FOR CONSTANT POTENTIAL V , (1) BECOMES:

$$\psi'' = -(E-V)\psi, \quad \underline{\underline{-V_0 < E < 0}} \quad (\text{BOUND STATES})$$

$$\Rightarrow \psi = A e^{kx}, \quad k^2 = E - V$$

SO FOR OUR POTENTIAL, SINCE $\psi \rightarrow 0$ AS $|x| \rightarrow \infty$, (BOUND STATES)

$$(2) \quad \psi(x) = \begin{cases} A e^{kx}, & x \leq -1 \\ B \cos(kx) + C \sin(kx), & |x| \leq 1 \\ D e^{-kx}, & x \geq 1 \end{cases}$$

WHERE $K \equiv \sqrt{-E}$, $k \equiv \sqrt{V_0 + E}$; $K, k > 0 \in \mathbb{R}$



(3)

SINCE (1) IS A 2nd ORDER EQN, REQUIRE BOTH ψ' AND ψ'' TO BE FINITE (PROVIDED V IS FINITE!). THEREFORE ψ AND ψ' ARE CONTINUOUS.

$$(3) \quad \psi'(x) = \begin{cases} A k e^{kx}, & x \leq -1 \\ -B k \sin(kx) + C k \cos(kx), & |x| \leq 1 \\ -D k e^{-kx}, & x \geq 1. \end{cases}$$

CONTINUITY AT $x = -1$:

$$(4a) \quad \psi: A e^{-k} = B \cos(k) - C \sin(k)$$

$$(4b) \quad \psi': A k e^{-k} = +B k \sin(k) + C k \cos(k)$$

$$(4c) \quad \Rightarrow \left(B \frac{k}{k} + C\right) \sin k + \left(C \frac{k}{k} - B\right) \cos k = 0$$

CONTINUITY AT $x = +1$:

$$(5a) \quad \psi: D e^{-k} = B \cos k + C \sin k$$

$$(5b) \quad \psi': -D k e^{-k} = -B k \sin k + C k \cos k$$

$$(5c) \quad \Rightarrow \left(C - \frac{B k}{k}\right) \sin k + \left(B + \frac{C k}{k}\right) \cos k = 0$$

NOW, ADD (4c + 5c):

$$(6) \quad C \sin k + C \frac{k}{k} \cos k = 0 \\ \Rightarrow C = 0 \quad \underline{\text{OR}} \quad k = -k \cot k$$

AND SUBTRACT (4c - 5c):

$$(7) \quad B \frac{k}{k} \sin k - B \cos k = 0 \\ \Rightarrow B = 0 \quad \underline{\text{OR}} \quad k = k \tan k$$

(4)

IN TERMS OF THE ENERGIES, (6) AND (7) MEAN

$$(8) \quad C = 0 \quad \underline{\text{OR}} \quad \sqrt{-E} = -\sqrt{V_0 + E} \cot \sqrt{V_0 + E}$$

$$(9) \quad B = 0 \quad \underline{\text{OR}} \quad \sqrt{-E} = \sqrt{V_0 + E} \tan \sqrt{V_0 + E}$$

TWO THINGS TO NOTE:

- WE CANNOT HAVE BOTH $B = 0$ AND $C = 0$.
(THIS WOULD ALSO $\Rightarrow A = D = 0$).
- THE SECOND OPTIONS CANNOT BOTH BE TRUE EITHER; THERE IS NO REAL SOLN. FOR

$$\sqrt{-E} = \sqrt{V_0 + E} \tan \sqrt{V_0 + E} = -\sqrt{V_0 + E} \cot \sqrt{V_0 + E}.$$

TWO POSSIBILITIES REMAIN:

$$(10) \quad C = 0 \quad \underline{\text{AND}} \quad 0 = \sqrt{V_0 + E} \tan \sqrt{V_0 + E} - \sqrt{-E}$$

OR

$$(11) \quad B = 0 \quad \underline{\text{AND}} \quad 0 = \sqrt{V_0 + E} \cot \sqrt{V_0 + E} + \sqrt{-E}$$

SOLUTION (10) CORRESPONDS TO THE EVEN EIGENSTATES, INCLUDING THE GROUND STATE, WHILE (11) CORRESPONDS TO THE ODD EIGENSTATES.

4.5

graph.gcf

Energy eigenvalues of the finite square well, in units of $\hbar^2/(mw)$, where w is the width of the well. The depth of the well is given by V (defined to be positive):

$$V = -n$$

$$E = x$$

FOR $V_1 = -100$, THERE ARE 7 LEVELS.

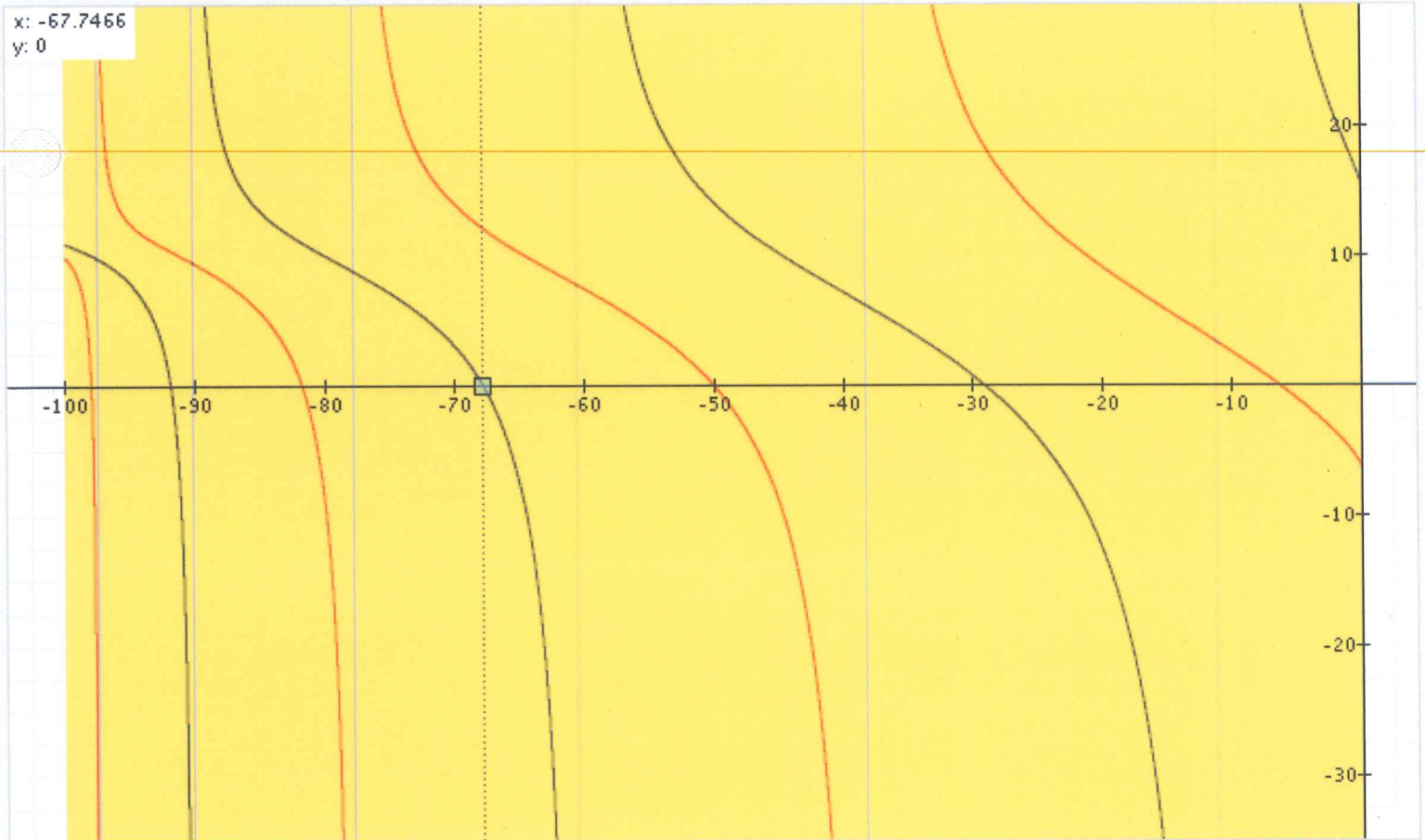
$V < E < 0$

Even eigenfunctions are roots of:

$-\sqrt{E - V} \cdot \tan(\sqrt{E - V}) + \sqrt{-E}$

Odd eigenfunctions are roots of:

$\sqrt{E - V} \cdot \cot(\sqrt{E - V}) + \sqrt{-E}$

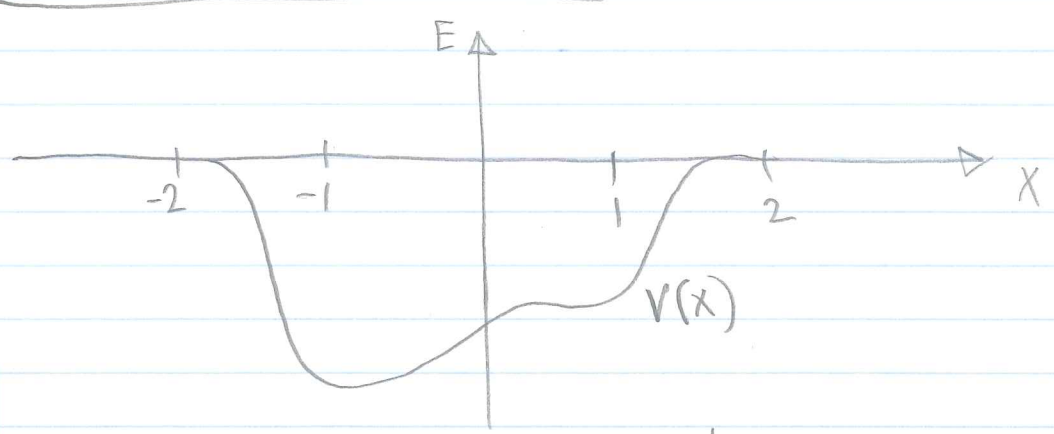


x: -67.7466
y: 0

n

Graph

THE ARBITRARY POTENTIAL



$$V(x) = \begin{cases} V_1(x), & |x| < \frac{w}{2} \\ 0, & |x| > \frac{w}{2} \end{cases}$$

(w is DIMENSIONLESS WIDTH OF THE POTENTIAL)
 SCHRÖDINGER EQUATION REDUCED TO FIRST ORDER:

$$\frac{d\psi}{dx} = \psi'$$

$$\frac{d\psi'}{dx} = [V(x) - E] \psi$$

Q: WHAT ARE THE BOUNDARY CONDITIONS?

6

NOTE THAT, FOR $|x| > \frac{W}{2}$, LIKE THE FINITE SQUARE WELL,

$$\psi(x) = A e^{+\sqrt{-E} x} + D e^{-\sqrt{-E} x}.$$

WE REQUIRE $\psi \rightarrow 0$ AS $|x| \rightarrow \infty$, SO

$$\psi(x) = \begin{cases} A e^{\sqrt{-E} x}, & x < \frac{W}{2}, \\ D e^{-\sqrt{-E} x}, & x > \frac{W}{2}. \end{cases}$$

CONSEQUENTLY, THE RIGHT B.C.'S ARE:

$$\begin{aligned} \psi'(-\frac{W}{2}) &= \sqrt{-E} \psi(-\frac{W}{2}), \\ \psi'(\frac{W}{2}) &= -\sqrt{-E} \psi(\frac{W}{2}). \end{aligned}$$

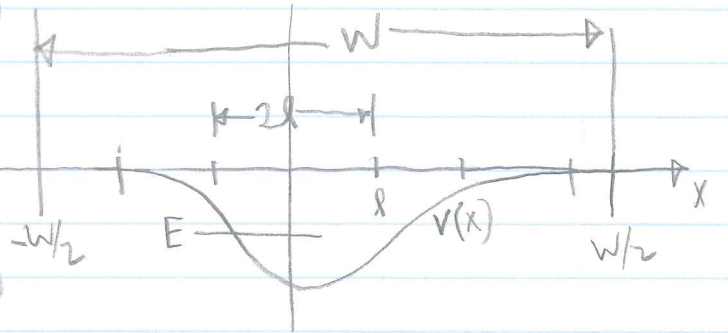
THERE IS NO VALUE IN SETTING ψ AT THE BOUNDARIES, AS THIS WOULD AFFECT ONLY THE NORMALIZATION.

Q: SINCE THERE WILL NORMALLY BE MORE THAN ONE EIGENVALUE, HOW DO WE FIND ALL OF THEM?

(7)

APPROACH FOR oneshot.m

- BOUNDARY CONDITIONS:
 $\psi(-w/2) = 1$ (ARBITRARY)
 $\psi'(-w/2) = \sqrt{-E}$
 $\psi'(w/2) = -\psi(w/2)\sqrt{-E}$



- INTEGRATE FROM LEFT BOUNDARY, SHOOTING TO $x = w/2$.
- DEFINE "ERROR"

$$\epsilon(E) = \psi'(w/2) + \psi(w/2)\sqrt{-E}$$

- NOTE THAT $\psi(w/2)$ AND $\psi'(w/2)$ DEPEND ON E.
- ROOTS OF $\epsilon(E)$ ARE EIGENVALUES.
- $\epsilon(0) = 0$, BUT $E = 0$ IS NOT AN EIGENVALUE!

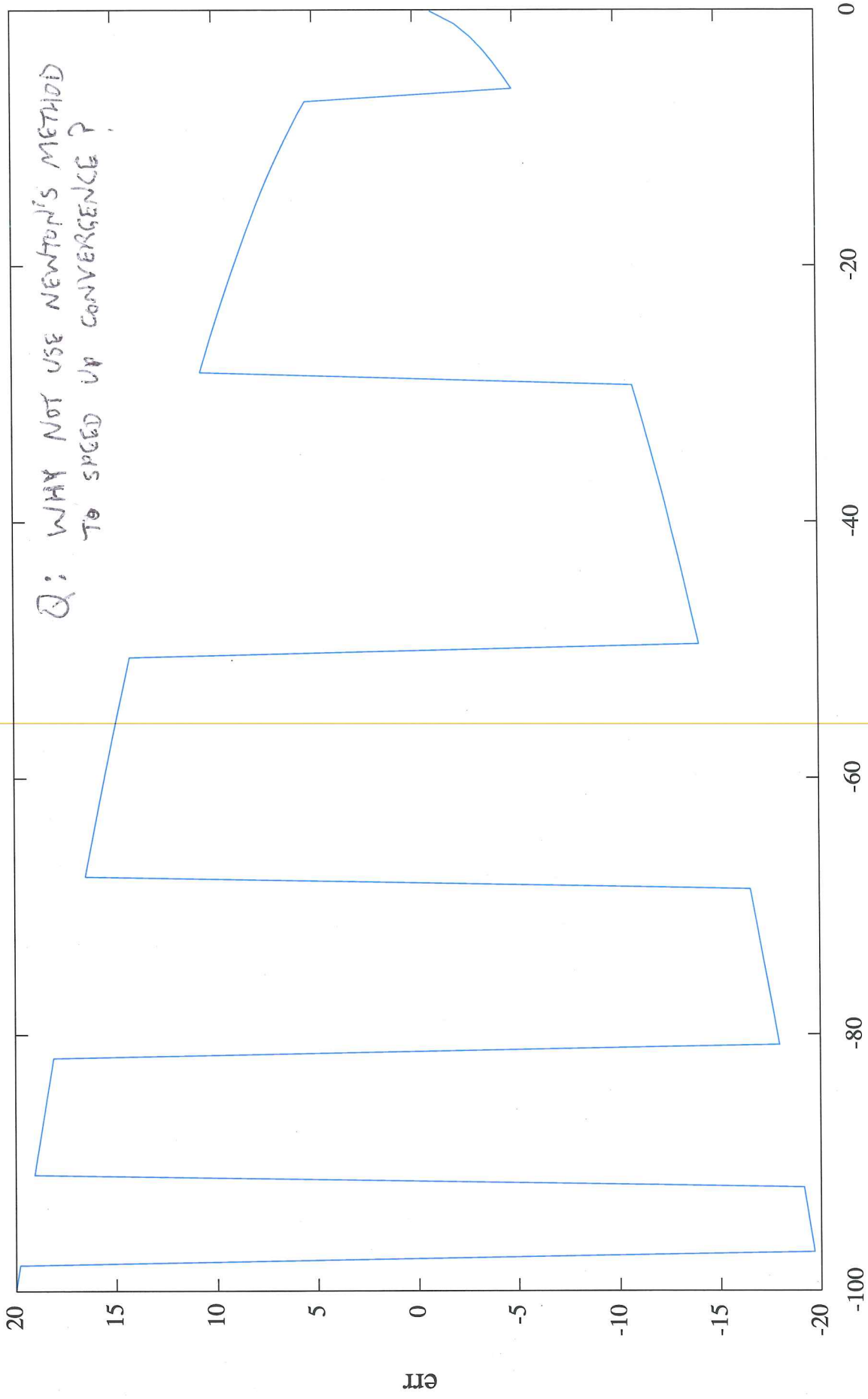
APPROACH FOR eigenstates.m

- TABULATE $\epsilon(E)$ ON $V_{\min} < E < 0$ WITH SUFFICIENT RESOLUTION TO IDENTIFY ALL ROOTS.
- EACH CHANGE IN SIGN ($E_i E_{i-1} < 0$) BRACKETS A ROOT.
- REFINE ROOTS BY BISECTION (GUARANTEED CONVERGENCE)

→ Q: WHY NOT NEWTON'S METHOD?

oneshotTest.m: Eigenvalues are the roots.

Q: WHY NOT USE NEWTON'S METHOD TO SPEED UP CONVERGENCE?



1 · schrodinger.m · 2009-04-06 13:34 · Charles Kankelborg

```
% Implementation of the time-independent Schrodinger equation for an
% assumed energy eigenvalue E and arbitrary 1D potential, V(x).
function dqdx = schrodinger(q, x, E, V)

% Interpret state of the system
psi = q(1);
dpsi_dx = q(2);

% Schrodinger equation
d2psi_dx2 = ( V(x) - E ) * psi;

% Return derivative of state vector
dqdx = [dpsi_dx; d2psi_dx2];

% Note that the output is a column vector. This makes the ODEs compatible
% with lsode rather than my lsode2 hack.
```

1 · vlsquare.m · 2009-04-06 13:34 · Charles Kankelborg

```
% square well potential. Width is 1, depth is 100.
function v1 = vlsquare(x)

inside = ( abs(x) < 1 );
v1(inside) = -100;
v1(!inside) = 0;
```

9.1

1 · vlskewed.m · 2009-04-06 14:33 · Charles Kankelborg

```
% Skewed potential well. FWHM is 1, depth is 100.  
% All of the nonzero potential is contained within -2.5 < x < 2.5,  
% and the integral of the potential equals -2 (same as vlsquare).  
function v1 = vlskewed(x)
```

```
steep = (x >= -1.5) & (x <= -0.5);  
v1(steep) = 50 * ( - 1 - sin( (1+x(steep)) * pi) );
```

```
gradual = (x >= -0.5) & (x <= 2.5);  
v1(gradual) = 50 * ( - 1 - sin( (1-x(gradual)) * pi/3) );
```

```
v1( (x <= -1.5) | (x >= 2.5) ) = 0;
```

1 · vlrounded.m · 2009-04-06 14:33 · Charles Kankelborg

```
% Rounded-off square well potential. FWHM is 1, depth is 100.  
% All of the nonzero potential is contained within -2 < x < 2,  
% and the integral of the potential equals -2 (same as vlsquare).  
function v1 = vlrounded(x)
```

```
inside = ( abs(x) < 2 );  
v1(inside) = 50 * ( - 1 - cos(x(inside)) * pi/2 );  
v1(!inside) = 0;
```


9.2

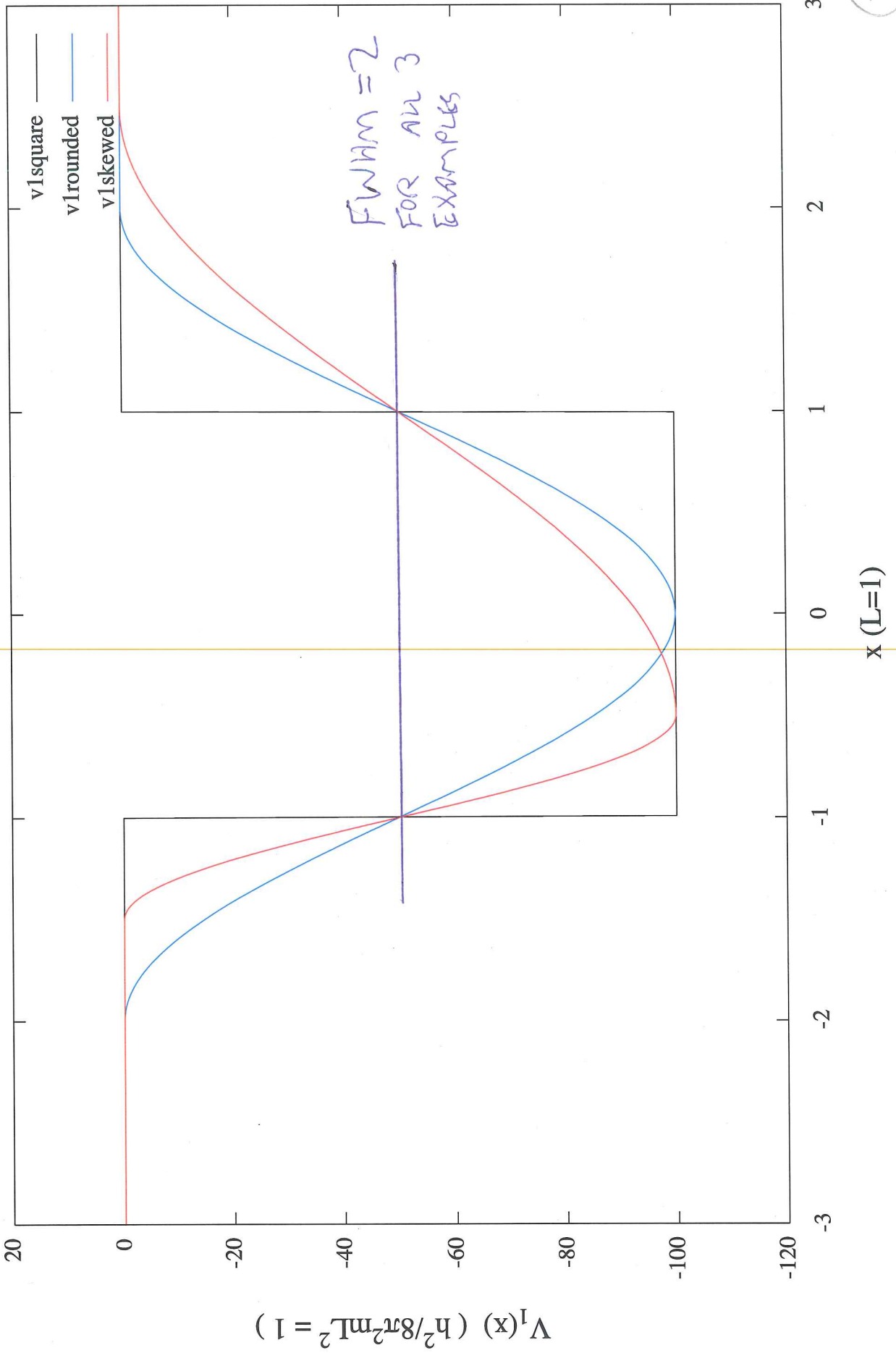
1 · vlpotentialsTest.m · 2009-04-06 14:35 · Charles Kankelborg

```
% Plot several of the potentials for handy comparison.
function vlpotentialsTest

x = linspace(-3, 3, 1000);

plot(x, vlsquare(x), 'k', x, vlrounded(x), 'b', x, vlskewed(x), 'r')
axis([-3,3,-120,20])
title('Potential Wells','fontsize',20)
xlabel('{x} (L=1)','fontsize',18)
ylabel('V_1(x) ( h^2/8\pi^2mL^2 = 1 )','fontsize',18)
legend('vlsquare','vlrounded','vlskewed')
```

Potential Wells



1 · oneshot.m · 2009-04-06 13:34 · Charles Kankelborg

```
% Integrate Schrodinger's equation once for a particular potential V, given
% as a function handle, a domain width w (centered at x=0), and an assumed
% (possibly incorrect) eigenvalue E. The procedure is:
% - Start with a V=0 boundary condition at x = -w/2.
% - Integrate to find psi(x) on -w/2 < x < w/2.
% - Normalize psi, dpsi/dx so that max(psi) = 1 (nice for plotting).
% - Evaluate deviation from V=0 boundary condition at x = w/2.
% - Return this deviation as the error, 'err'.
% The roots of err as a function of E are the correct energy eigenvalues.
% The returned q is an array of psi and d/dx(psi)
% CCK 2009-Apr-05
function [err, q, x] = oneshot(E, V, w, Npoints)

if !exist('Npoints','var')
    Npoints = 1000; % default value
end

x = linspace(-w/2, w/2, Npoints);

% boundary conditions
psi_0 = 1; % completely arbitrary
dpsi_dx_0 = psi_0 * sqrt(-E);
    % consistent with psi --> 0 as x --> -infinity, if V=0.
q_0 = [psi_0, dpsi_dx_0];

% integrate the ODE
q = lsode(@(q,x) schrodinger(q,x,E,V), q_0, x);

% Normalize the wave function to a maximum of 1.
normalization = max( abs(q(:,1)) );
q = q/normalization;

% evaluate the error
psi_final = q(Npoints,1);
dpsi_dx_final = q(Npoints,2);
err = dpsi_dx_final + sqrt(-E) * psi_final;
    % err == 0 is equivalent to psi --> 0 as x --> infinity with V=0.
```



```
% Test of oneshot.m
function oneshotTest

N_energies = 100;
E_lowest = -100;
E = linspace(E_lowest, 0, N_energies);
width = 6; % This means -3 < x < 3.
for i=1:N_energies
    i
    err(i) = oneshot(E(i), @vlsquare, width);
end

plot(E, err)
% plot(E, sign(err).*abs(err).^(1/7) )
xlabel('{E}', 'fontsize', 18);
ylabel('{err}', 'fontsize', 18);
title('oneshotTest.m: Eigenvalues are the roots.', 'fontsize', 20)

% Note that the root at E=0 is an artifact!

% err(E) is sometimes almost discontinuous near the roots. Unless E
% is very close to an eigenvalue, the result of the shooting is a wave
% function psi(x) that grows exponentially when the potential is near zero,
% resulting in a large error compared to the boundary condition.
Normalization
% of psi scales this large error down, so that all the wildly erroneous
results
% are of similar order. The typical error in dpsi/dx is of order sqrt(-E),
so
% the "err" as defined in oneshot.m tends to look like a square wave
multiplied
% by +/- sqrt(E).
```

Q: HOW CAN WE KNOW HOW FINELY TO GRID OUR SEARCH FOR EIGENVALUES?


IF WE COULD PREDICT THE NUMBER OF EIGENVALUES FOR ANY GIVEN $V_1(x)$, IT WOULD SOLVE THIS PROBLEM AND ALSO PERHAPS LEND THEORETICAL INSIGHT TO THE PROBLEM OF SOLVING GENERAL POTENTIALS.

START WITH THE SQUARE WELL, WIDTH w ($=2$ IN OUR UNITS), DEPTH V_0 . ($V_1(x) > -V_0, V_0 > 0$)

DE BROGLIE "MATTER WAVES" TRAPPED IN THE WELL:

(1) $(n-1)\lambda/2 \approx w, n \in (1, 2, \dots, n_{max}), (n-1) = \# \text{ NODES}$

$p = \hbar/\lambda \approx \frac{\hbar}{2w}(n-1)$



ENERGY OF BOUND STATE:

(2) $E = T + V = \frac{p^2}{2m} - V_0 < 0$

$\Rightarrow \frac{p^2}{2m} \leq V_0$

HIGHEST E_n WILL HAVE SMALL K .

COMBINE (1) & (2):

$$\frac{\hbar^2(n-1)^2}{8mw^2} < V_0 \Rightarrow n \leq 1 + \sqrt{\frac{8V_0w^2m}{\hbar^2}}$$

PUTTING V IN UNITS OF $\hbar^2/2ml^2$, AND $l \equiv 1$ (UNITS),

(3) $n \leq 1 + \frac{w}{\pi} \sqrt{V_0}$ (SQUARE WELL - EXACT)

$V_0 = 100 \Rightarrow n \leq 7.4$ CORRECT!

Q: HOW DO WE GENERALIZE TO SOME OTHER $V_1(x)$?

OUR DIMENSIONLESS SCHRÖDINGER EQUATION IS UNCHANGED UNDER THE TRANSFORMATION

$$(4) \quad \left\{ \begin{array}{l} \lambda \rightarrow \alpha \lambda \\ V \rightarrow V/\alpha^2 \\ E \rightarrow E/\alpha^2 \end{array} \right.$$

WHICH IMPLIES THAT THE LEVEL STRUCTURE IS INVARIANT UNDER THIS TRANSFORMATION.

LOOKING BACK AT (3) FOR INSPIRATION, I PREDICT

(5)

$$N_{\text{STATES}} \approx 1 + \frac{1}{\pi} \int_{-w/2}^{w/2} \sqrt{-V_1(x)} dx$$

THIS EXPRESSION

- IS INVARIANT UNDER TRANSFORMATION (4), LIKE SCHRÖDINGER'S EQUATION.
- REDUCES TO THE EXACT RESULT (3) FOR THE SQUARE WELL.
- ASSUMES $V_1(x) = 0$ FOR $|x| > w/2$.

FOR V_1 SKEWED, THE INTEGRAL PREDICTS $N_{\text{STATES}} \approx$ THERE ARE ACTUALLY 8 EIGENVALUES FOR THAT POTENTIAL.

I WANT `eigenvalues.m` TO WORK FOR ANY $V(x)$.

- WROTE IT AS THOUGHTFULLY AS I COULD
- TRIED ON SOME NEW POTENTIALS. IT FAILED!
- MADE IT MORE ROBUST, ADDED OPTIONAL PARAMETERS.
- TRIED ON MORE POTENTIALS. MORE PROBLEMS!

→ THIS IS HOW THINGS NORMALLY ARE, EVEN FOR THE BEST NUMERICISTS. CODES ARE RARELY MUCH MORE GENERAL THAN THE TEST CASES USED TO DEVELOP THEM.

→ THE CODE AS YOU WILL SEE IT HAS BENEFITTED FROM SEVERAL ITERATIONS OF TEST-FAIL-IMPROVE.

→ I'LL SHOW YOU WHAT MY CODE CAN DO, BUT I WILL ALSO EMPHASIZE ITS SHORTCOMINGS.

EXAMPLES ON WEB!