PHYSICS 410

SOLVING BVPs WITH THE ode45 INTEGRATOR AND SHOOTING

Introduction

- Recall: Two pt. boundary value problem (BVP); b.c.'s supplied at two points—typically end points of soln domain—rather than at some single pt as in the case of an IVP
- In idealized physical problems, one of the points will often be $x = \infty$
- 2-pt. BVPs often (but not always) eigenvalue problems
  - Problem characterized by parameter (the eigenvalue), and solutions satisfying b.c.'s only exist for certain values of that parameter
  - Often a countable infinity of solutions (eigenfunctions) and parameters

Example

- Second order linear ODE:

$$u''(x) = -\omega^2 u(x) \qquad \text{on} \qquad 0 \leq x \leq 1$$

with b.c.'s

$$u(0) = u(1) = 0$$

- Countable infinity of solutions, $u_n(x)$

$$u_n(x) = \sin(\omega_n x)$$

$$\omega_n = \pi n, \;\; n = 0, 1, 2, \ldots$$

- $u_n(x)$ are the eigenfunctions, ω_n are the eigenvalues

Example: Toy model for deuteron (proton-neutron) from Arfken, Ex. 9.1.2

- Potential

$$V = V_0,\ V_0 < 0 \qquad \text{for} \qquad 0 \le r \le a$$
$$V = 0 \qquad \text{for} \qquad r > a$$

Time Independent Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{1}$$

where m is the "deuteron" mass

- Assume spherical symmetry, then $\psi(x, y, z) \to \psi(r)$

$$\nabla^2\psi(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right)$$

- Define $u(r) \equiv r\psi(r)$, then (verify)

$$\nabla^2\psi(r) \to \frac{1}{r}\frac{d^2u(r)}{dr^2}$$

- so (1) can be written

$$\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}(E - V)\,u = 0 \qquad (2)$$

- Now, as discussed in Arfken, progress can be made in solving (2) by writing down the general solutions in the domains $0 \le r \le a$ and $r > a$ and matching u and du/dr at $r = a$ subject to normalizability of ψ:

$$\int \psi\psi^* dV = 1 \to 4\pi \int r^2 |\psi(r)|^2 = 1$$

  which effectively means $\psi(r) \to 0$ as $r \to \infty$.

- Further, for given a and other problem parameters (m, V_0) fixed, normalizable soln will only exist for specific (i.e. discrete) values of E

- I.e. E is an eigenvalue and the corresponding wave function $u(r) = r\psi(r)$ is an eigenfunction

- Let us now consider solving (2) directly using shooting; first rewrite (2) in an non-dimensional form

- Let $x \equiv (2m)^{1/2} r$ so that
$$\frac{d^2u}{dr^2} \to 2m \frac{d^2u}{dx^2}$$
and choose units such that $\hbar = 1$ and $V_0 = -1$ (should establish that this is possible if it isn't clear to you)

- Problem left with one free parameter, a, equivalently
$$x_0 \equiv (2m)^{1/2} a$$
and (2) becomes
$$\frac{d^2u}{dx^2} + (E - V)u = 0 \tag{3}$$
$$V(x) = \begin{cases} -1 & 0 \le x < x_0 \\ 0 & x > x_0 \end{cases}$$

- Again, note that E is an eigenvalue in (3). For specified x_0, expect specific E to result in normalizable $u(r)$ (eigenfunction)

- Boundary conditions are derived from demands that

  1. $\psi(r)$ is *regular* at $r = 0$
  2. $\lim_{r\to\infty} \psi(r) = 0$

- Regularity at $r = 0$

$$\lim_{r\to 0} \psi(r) = \psi_0 + r^2\psi_2 + O(r^4)$$
$$\lim_{r\to 0} u(r) = r\psi(r) = r\psi_0 + r^3\psi_2 + O(r^5)$$

- Thus

$$u(0) = 0$$
$$\frac{du}{dr}(0) = \psi(0)$$

- Now, note that eqn (1), like all Schrödinger equations, is *linear*; given any soln $\psi(r)$, $c\psi(r), c \in \Re$ is also a soln; the particular soln we seek is fixed by normalization
$$\int \psi\psi^* dV = 1$$
so we can choose $\psi(0)$ arbitrarily (say $\psi(0) = 1$ for convenience) then (for specific x_0) vary E until we find a soln which satisfies $\lim_{r\to\infty} \psi(r) = 0$

- This process of varying a parameter and then integrating a set of ODEs outwards (or inwards) to achieve a bundary condition at the outer (inner) limit of ihtegration is known as **shooting**

- Once we have such a solution, we can then normalize it (upcoming tutorial)

- Note that since both of the b.c.'s on the ODE have been set at $r = 0$, we can use an initial value solver, such as `ode45` to solve this problem

- To that end we rewrite (3) in canonical form by introducing $w \equiv du/dx$, then

$$\frac{du}{dx} = w \tag{4}$$

$$\frac{dw}{dx} = (V - E)u \tag{5}$$

- We can view the task of determining the eigenvalue, E, for specified x_0 as finding a root of a non-linear equation (consider $f(E; x_0) = \lim_{x \to \infty} u(x; E, x_0)$ for example)

- Provided we have an initial bracket of the eigenvalue $[E_{\mathrm{LO}}, E_{\mathrm{HI}}]$ such that $E_{\mathrm{LO}} \leq E \leq E_{\mathrm{HI}}$, we can use bisection to systematically refine our estimate of E (tutorial)

Deuteron Model Recap

- Differential equation

$$\frac{d^2u}{dx^2} + (E - V)u = 0$$

where the potential $V(x)$ is given by

$$V(x) = \begin{cases} -1 & 0 \leq x < x_0 \\ 0 & x > x_0 \end{cases}$$

and the boundary conditions at $x = 0$ are

$$u(0) = 0 \qquad \frac{du}{dr}(0) = \psi(0) = 1$$

- E is an eigenvalue and, in the solution of the ODE, must be adjusted using bisection, for example, until the true boundary condition

$$\lim_{x \to \infty} u(x) = 0$$

is achieved

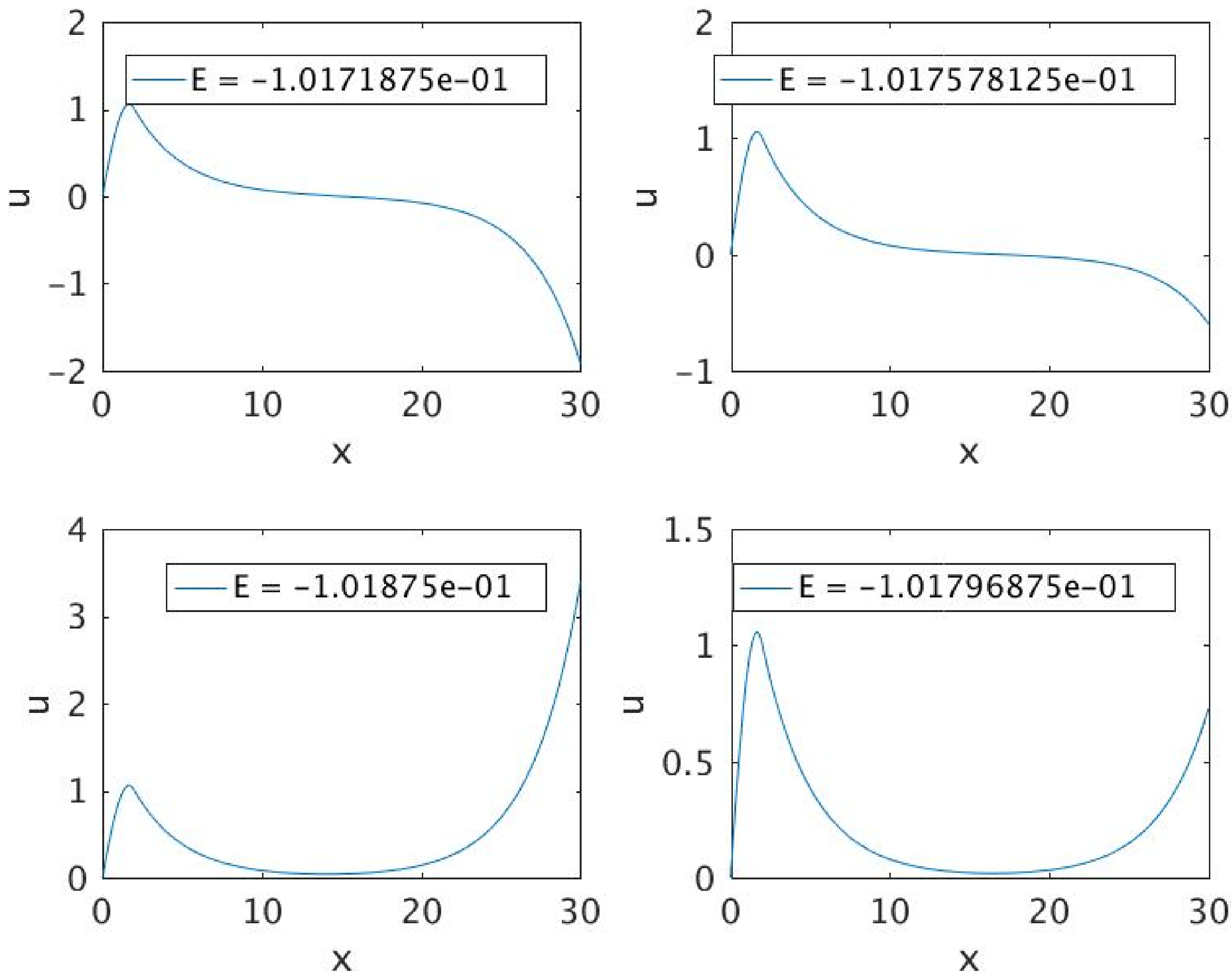
Script deut.m

```
% deut: Solves ODE for toy deuteron problem.
global x0  E;
% Domain outer boundary ...
xmax = 60.0;
% Tolerance parameters ...
abstol = 1.0e-8;
reltol = 1.0e-8;
options = odeset('AbsTol', abstol * [1 1]', 'RelTol', reltol);
% Parameters ...
x0 = 6.0;
E = -0.80067
% Integrate ODE ...
[xout yout] = ode45(@fcn_deut, [0.0 xmax], [0.0 1.0]', options);
% Make plot and output as JPEG ...
figure(1);
clf;
hold on;
axis square;
xlabel('x');
ylabel('u');
plot(xout, yout(:, 1));
print('deut.jpg','-djpeg');
```

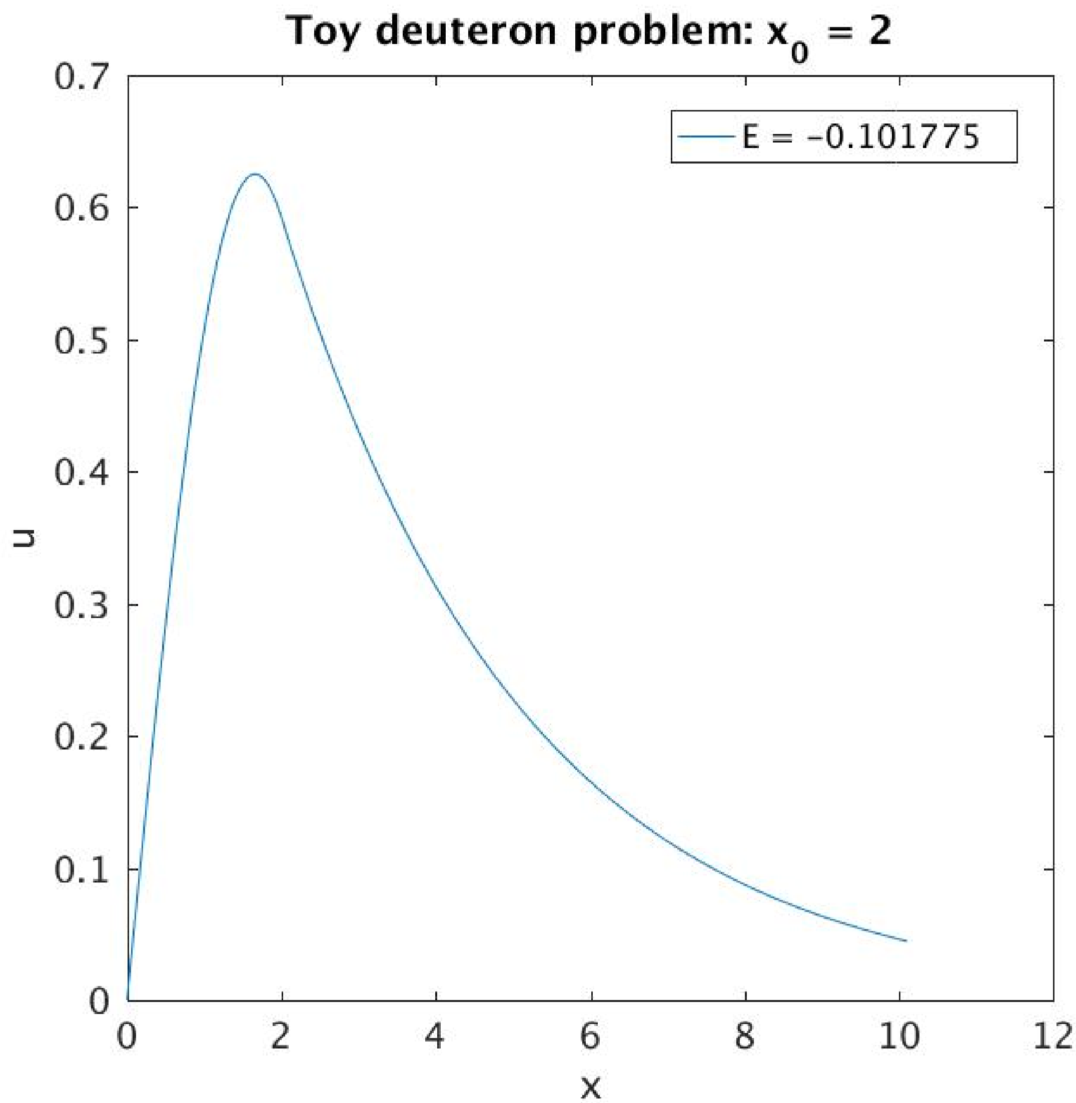
Function `fcn_deut`

```
function dydx = fcn_deut(x, y)
% Function fcn_deut evaluates derivatives for toy deuteron problem.
   global x0  E;

   dydx = ones(2,1);

   dydx(1,1) = y(2);
   if x <= x0
      dydx(2,1) = (-1 - E) * y(1);
   else
      dydx(2,1) = -E * y(1);
   end
end
```

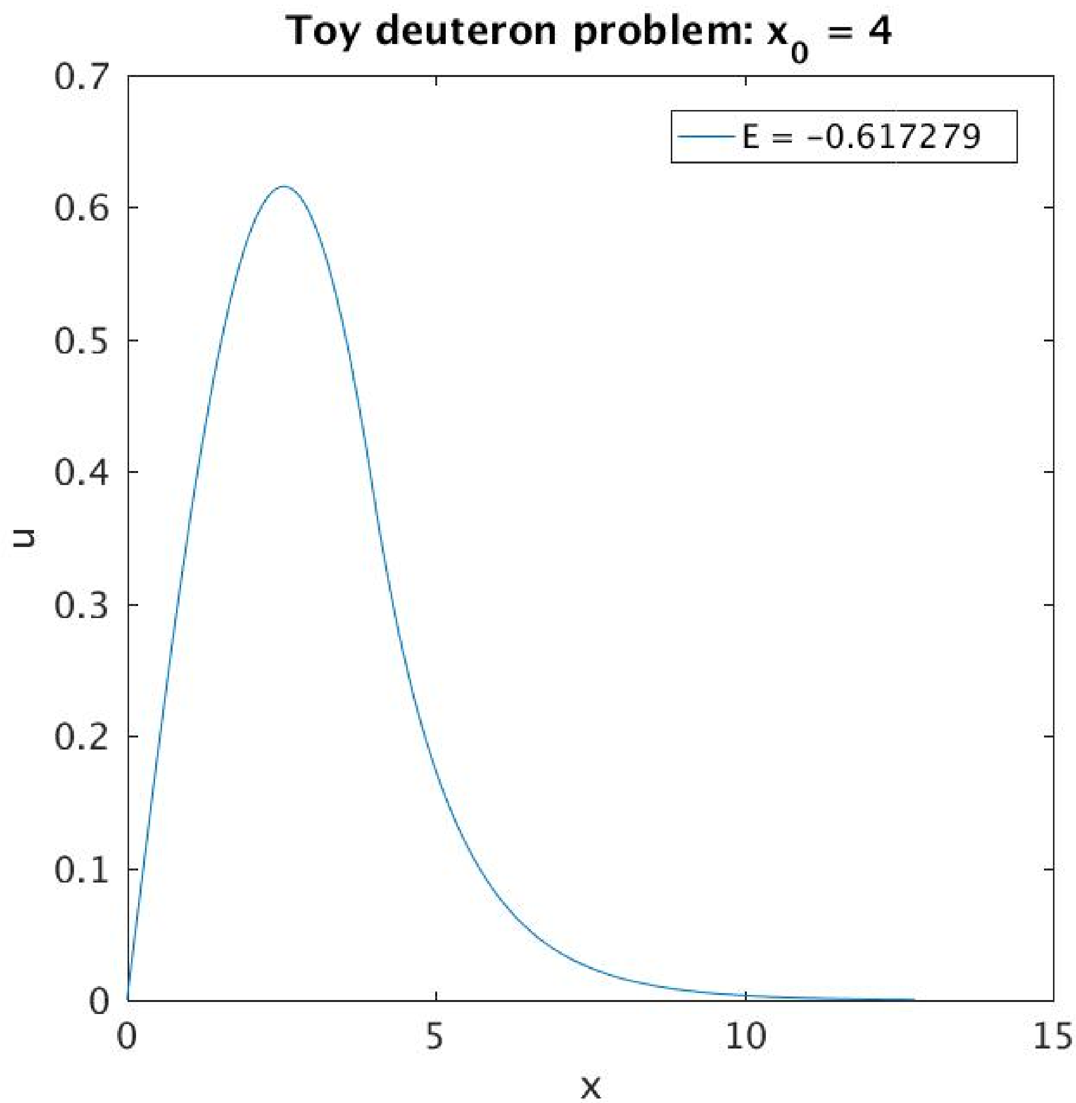
- Sample output during bisection procedure (shooting) for $x_0 = 2.0$



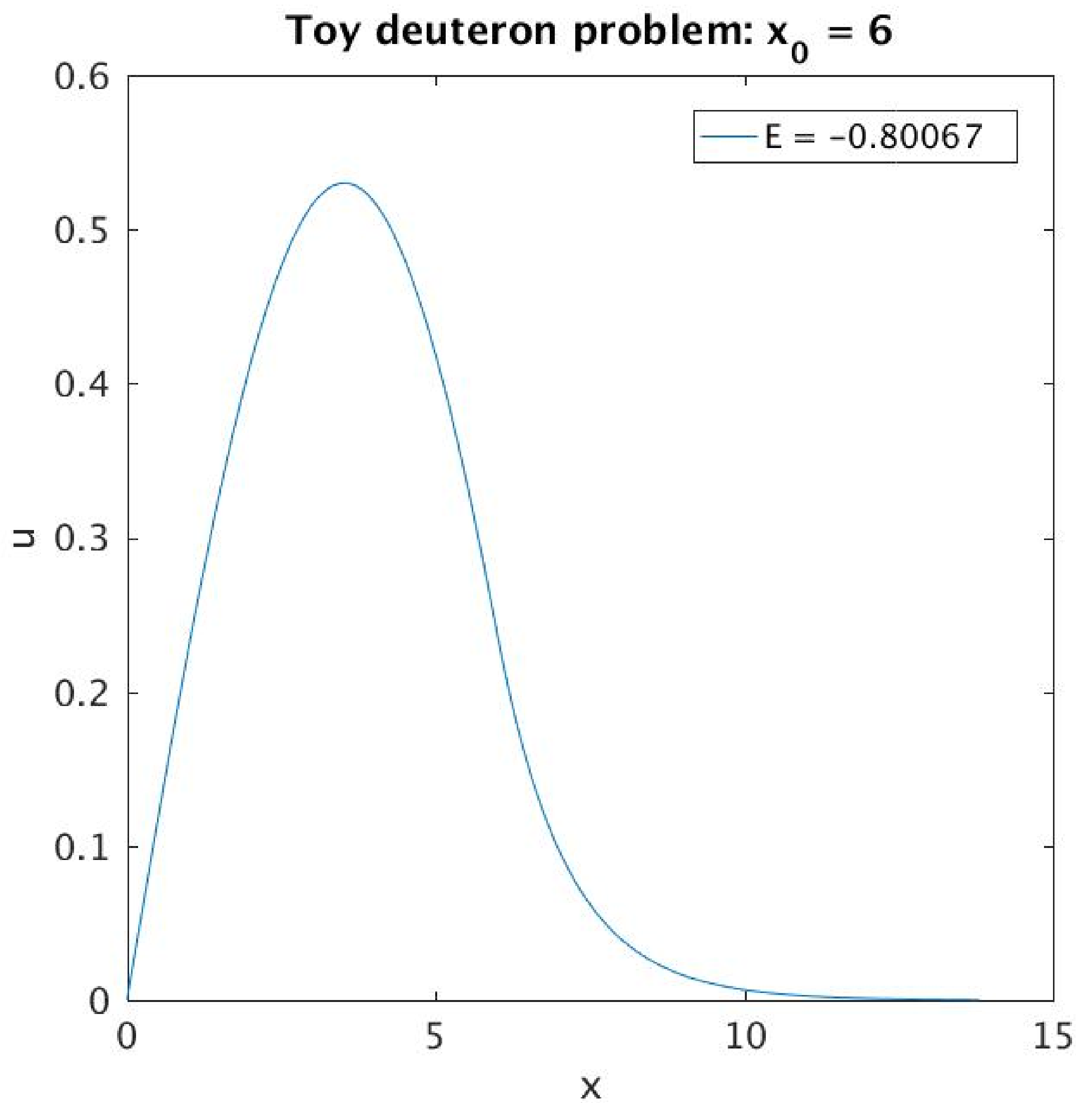
- Normalized wave function for $x_0 = 2.0$



- Normalized wave function for $x_0 = 4.0$



- Normalized wave function for $x_0 = 6.0$



- Normalized wave function for $x_0 = 8.0$