Assigned: Friday Mar. 19, 2010
Due: Friday Apr. 2, 2010

MATH 442: Homework 7
Spring 2010

NOTE: For each homework assignment observe the following guidelines:

- Include a cover page.
- At the beginning of each problem, clear state the problem (with assumptions) and what method or approach you intend to use to solve the problem.
- Clear mark your answer.
- Always clearly label all plots (title, x-label, y-label, and legend).
- Use the `subplot` command from MATLAB when comparing 2 or more plots to make comparisons easier and to save paper.

1. If $\mathcal{L}$ is the following first-order linear differential operator:
$$\mathcal{L} = p(x)\frac{d}{dx},$$
then determine the adjoint operator $\mathcal{L}^*$ such that
$$\int_a^b \left[u\mathcal{L}^*(v) - v\mathcal{L}(u)\right]\, dx = B(x)\Big|_a^b.$$
What is $B(x)$?

2. Consider the eigenvalue problem
$$\frac{d^2\phi}{dx^2} + \left(\lambda - x^2\right)\phi = 0.$$
subject to $\phi'(0) = \phi'(1) = 0$.
   (a) Show that $\lambda > 0$. **NOTE:** showing that $\lambda \geq 0$ is relatively straightforward, but showing that $\lambda \neq 0$ will take a little bit of work (you need to solve a <u>FIRST-ORDER ODE</u> and apply the appropriate BCs).
   (b) Use the trial function $u_T(x) = (x - x^2)^2 + \alpha$, where α is a constant, to obtain an estimate for λ_1. Find the optimal α that gives the sharpest upper bound. (**NOTE:** Be careful, remember that the trial function to estimate λ_1 must satisfy the BCs and is not allowed to have any roots in $0 < x < 1$.)

3. Schrödinger's equation from quantum mechanics can be written as
$$\begin{aligned} \frac{\hbar}{2m}\Psi_{xx} - U(x)\Psi &= -i\hbar\Psi_t \quad 0 < x < 1, \quad t > 0 \\ \Psi(0,t) &= \Psi(1,t) = 0 \\ \Psi(x,0) &= f(x), \end{aligned}$$
where $\Psi(x,t)$ is the particle's *wavefunction*, $\hbar$ is Planck's constant, m is the particle's mass (also constant), $U(x)$ potential energy function, and $i = \sqrt{-1}$.

(a) Separate variables and derive a space and a time ODE.

(b) Explicitly the solve the time ODE.

(c) Verify that the space ODE is a Sturm-Liouville eigenvalue problem by writing down what $p(x)$, $q(x)$, and $\sigma(x)$ are for this problem.

(d) Assuming that all the eigenvalues and eigenfunctions for this problem are known, write down the solution to Schrödinger's equation. Give formulas for any coefficients that have been introduced.

4. Consider Schrödinger's equations with the following potential energy function:

$$U(x) = (1+x)^2.$$

(a) Use the Rayleigh Quotient to show that $\lambda > 0$.

(b) Use the trial function $u_T(x) = \sin(\pi x)$ to approximate the smallest eigenvalue.

5. In a previous homework assignment we showed that

$$\mathcal{L}\left(\sum_{n=1}^{M} a_n \phi_n(x)\right) = \sum_{n=1}^{M} a_n \mathcal{L}(\phi_n(x)),$$

where $M \geq 1$ is a *finite* integer and $\mathcal{L}$ is a linear operator. In the proof of the *Minimization Principle* for the Rayleigh quotient we made use of the following theorem.

> **Theorem.**
> If $\mathcal{L}$ is a linear and self-adjoint operator that satisfies the eigenvalue problem
>
> $\mathcal{L}\left(\phi_n(x)\right) = -\lambda_n \sigma(x) \phi_n(x),$
>
> then
>
> $\mathcal{L}\left(u\right) = \sum_{n=1}^{\infty} a_n \mathcal{L}(\phi_n(x)), \quad \text{where} \quad u = \sum_{n=1}^{\infty} a_n \phi_n(x).$

Prove this theorem by assuming that $\mathcal{L}(u)/\sigma$ is piecewise smooth, which means that

$$\mathcal{L}(u)/\sigma = \sum_{n=1}^{\infty} b_n \phi_n(x),$$

and determining the coefficients b_n.

6. For a matrix A whose entries are complex numbers, the complex conjugate of the tranpose is denote by A^H – [this means first transpose A, then replace all of the entries in A^T by their complex conjugates]. For matrices in which $A^H = A$, or in component form $a_{ij} = \bar{a}_{ji}$, (called **Hermitian** matrices):

(a) Prove the following identity (u and v are any two vectors):

$$\bar{u} \cdot \left(Av\right) - \left(\bar{A}\bar{u}\right) \cdot v = 0.$$

(b) Prove that the eigenvalues are real. (**HINT:** use the identity from part (a).)

(c) Prove that eigenvectors corresponding to different eigenvalues are orthogonal. (**HINT:** again use the identity from part (a).)