M454 - Boundary Value Problems - Winter 2008

Assignment # 8.
Due: Tuesday, March 25, 2008.

1. 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 $\lambda > 0$.

   (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: Remember that the trial function to estimate λ_1 must satisfy the BCs and is not allowed to have any roots in $0 < x < 1$.)

2. Schrödinger's equation from quantum mechanics can be written as

$$\frac{\hbar}{2m}\Psi_{xx} - U(x)\Psi = -i\hbar\Psi_t \quad 0 < x < 1, \quad t > 0$$

$$\Psi(0,t) = \Psi(1,t) = 0$$
$$\Psi(x,0) = f(x),$$

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.

3. 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.

4. In a previous homework assignment we used mathematical induction to show 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:

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.

5. Consider heat flow in a 1D rod without sources and non-constant thermal properties. Assume that the temperature is zero at $x = 0$ and $x = L$. Suppose that $c\rho_{\text{min}} \leq c(x)\rho(x) \leq c\rho_{\text{max}}$ and $K_{\text{min}} \leq K_0(x) \leq K_{\text{max}}$. Obtain an upper and (nonzero) lower bound on the slowest exponential rate of decay of the temperature.

6. Consider the boundary value problem

$$\begin{aligned}
&\phi'' + \lambda\phi = 0 \\
&\phi(0) - \phi'(0) = 0 \\
&\phi(1) + \phi'(1) = 0.
\end{aligned}$$

   (a) Using the Rayleigh quotient, show that $\lambda > 0$.

   (b) Show that

$$\tan\sqrt{\lambda} = \frac{2\sqrt{\lambda}}{\lambda - 1}.$$

   Determine the eigenvalues graphically. Estimate the large eigenvalues.