HW 8 Solution
PHZ 5156, Computational Physics
October 25, 2005

1. The operator $\mathcal{L} = i\, d/dx$ has as its domain the set of all differentiable functions on the interval $0 \le x \le L$ with periodic boundary conditions $f(0) = f(L)$. Derive the adjoint operator $\mathcal{L}^\dagger$ and its domain.

   Solution:

$$\begin{aligned}
\langle g|\mathcal{L}f\rangle &= \int_0^L dx\, g^*(x) i \frac{df}{dx} \\
&= i\left[g^*(L)f(L) - g^*(0)f(0)\right] - i\int_0^L dx\, \frac{dg^*}{dx} f \\
&= i f(0)\left[g(L) - g(0)\right]^* + \int_0^L dx\, \left(i\frac{dg}{dx}\right)^* f.
\end{aligned}$$

   If $g(L) = g(0)$ the boundary term vanishes. This defines the domain of the adjoint operator. For such functions g the above becomes

$$\langle g|\mathcal{L}f\rangle = \langle \mathcal{L}^\dagger g|f\rangle$$

   with $\mathcal{L}^\dagger = i\, d/dx$. Since $\mathcal{L}^\dagger = \mathcal{L}$ and the domains are identical, $\mathcal{L}$ is self-adjoint.

2. The operator $\mathcal{L} = i\, d/dx$ has as its domain the set of all differentiable functions on the interval $0 \le x \le L$ with boundary conditions $f'(0) = 0 = f'(L)$ (notice the two derivatives). Derive the adjoint operator $\mathcal{L}^\dagger$ and its domain.

   Solution:

$$\begin{aligned}
\langle g|\mathcal{L}f\rangle &= \int_0^L dx\, g^*(x) i \frac{df}{dx} \\
&= i\left[g^*(L)f(L) - g^*(0)f(0)\right] - i\int_0^L dx\, \frac{dg^*}{dx} f.
\end{aligned}$$

   Since $f(L)$ and $f(0)$ can be anything, the boundary term only vanishes if $g(L) = 0 = g(0)$. This defines the domain of the adjoint operator. For such functions g the above becomes

$$\langle g|\mathcal{L}f\rangle = \langle \mathcal{L}^\dagger g|f\rangle$$

   with $\mathcal{L}^\dagger = i\, d/dx$. We have $\mathcal{L}^\dagger = \mathcal{L}$; but because the domains are different, $\mathcal{L}$ is *not* self-adjoint. (In fact it is not even Hermitian: the boundary term does not vanish for all functions g in the original domain.)

3. The operator $\mathcal{L} = d^2/dx^2$ has as its domain the set of all twice-differentiable functions on the interval $0 \le x \le L$ with boundary conditions $f'(0) = 0 = f(L)$ (notice the one derivative). Derive the adjoint operator $\mathcal{L}^\dagger$ and its domain.

   Solution:

$$\begin{aligned}
\langle g|\mathcal{L}f\rangle &= \int_0^L dx\, g^*(x)\frac{d^2 f}{dx^2} \\
&= \left[g^*(L)\,\frac{df}{dx}\bigg|_{x=L} - g^*(0)\,\frac{df}{dx}\bigg|_{x=0}\right] - \int_0^L dx\,\frac{dg^*}{dx}\frac{df}{dx} \\
&= g^*(L)\,\frac{df}{dx}\bigg|_{x=L} - \int_0^L dx\,\frac{dg^*}{dx}\frac{df}{dx}.
\end{aligned}$$

   Here part of the boundary term vanishes because of the boundary condition $f'(0) = 0$. Integrating by parts again gives

$$\begin{aligned}
\langle g|\mathcal{L}f\rangle &= g^*(L)\,\frac{df}{dx}\bigg|_{x=L} - \left[\frac{dg^*}{dx}\bigg|_{x=L} f(L) - \frac{dg^*}{dx}\bigg|_{x=0} f(0)\right] + \int_0^L dx\,\frac{d^2g^*}{dx^2} f \\
&= g^*(L)\,\frac{df}{dx}\bigg|_{x=L} + \frac{dg^*}{dx}\bigg|_{x=0} f(0) + \int_0^L dx\,\left(\frac{d^2 g}{dx^2}\right)^* f,
\end{aligned}$$

   where I have used $f(L) = 0$. The boundary term vanishes if $g'(0) = 0 = g(L)$. This defines the domain of the adjoint operator. For such functions g the above becomes

$$\langle g|\mathcal{L}f\rangle = \langle \mathcal{L}^\dagger g|f\rangle$$

   with $\mathcal{L}^\dagger = d^2/dx^2$. Since $\mathcal{L}^\dagger = \mathcal{L}$ and the domains are identical, $\mathcal{L}$ is self-adjoint.

4. Find the eigenfunctions and eigenvalues of the operator $\mathcal{L} = i\,d/dx$ on the interval [0,L] with periodic boundary conditions $y(L) = y(0)$. Show that, properly normalized, the eigenfunctions form an infinite orthonormal set.

   Solution: The eigenfunction ODE

$$i\frac{dy}{dx} = \lambda y$$

   has the general solution $y(x) = Ce^{-i\lambda x}$. Imposing $y(L) = y(0)$ yields $e^{-i\lambda L} = 1$. This is solved by $\lambda L = 2n\pi$ with $n = 0, \pm 1, \pm 2, \ldots$. Thus the eigenvalues are

$$\lambda_n = 2n\pi/L, \quad n = 0, \pm 1, \pm 2, \ldots.$$

The eigenfunctions are $y_n(x) = Ce^{-i2n\pi x/L}$. These are normalized by setting

$$\langle y_n | y_n \rangle = 1 = \int_0^L dx\, y_n^*(x) y_n(x) = \int_0^L dx\, |C|^2 = |C|^2 L,$$

which is solved by $C = 1/\sqrt{L}$. Thus the normalized eigenfunctions are

$$y_n(x) = \frac{1}{\sqrt{L}} e^{-i2n\pi x/L}.$$

Orthogonality is checked by examining

$$\langle y_n | y_m \rangle = \frac{1}{L} \int_0^L dx\, e^{i2\pi(n-m)/L}.$$

When $m = n$ this produces unity, as above. When $m \neq n$ it gives

$$\frac{1}{L} \frac{L}{i2\pi(n-m)} \left. e^{i2\pi(n-m)x/L} \right|_0^L = \frac{1}{i2\pi(n-m)} \left[e^{i2\pi(n-m)} - 1 \right] = 0.$$

The last step follows because $e^{i2\pi k} = 1$ for any integer k.

5. Find the eigenfunctions and eigenvalues of the operator $\mathcal{L} = i\, d/dx$ on the interval [0,L] with boundary conditions $y'(0) = 0 = y'(L)$ (notice the two derivatives).

   Solution: The eigenfunction ODE

   $$i \frac{dy}{dx} = \lambda y$$

   has the general solution $y(x) = Ce^{-i\lambda x}$. Imposing $y'(0) = 0$ yields

   $$-iC\lambda = 0.$$

   Choosing $C = 0$ gives the trivial solution $y(x) \equiv 0$. The other choice $\lambda = 0$ gives $y(x) = C$. In that case the other boundary condition $y'(L) = 0$ is also satisfied. Thus we have managed to find only one eigenstate:

   $$\lambda = 0, \quad y(x) = const.$$

   We did not find an infinite set because the operator is not self-adjoint; briefly, because the boundary conditions are unsuitable.

6. Find the eigenfunctions and eigenvalues of the operator $\mathcal{L} = d^2/dx^2$ on the interval [0,L] with boundary conditions $y'(0) = 0 = y(L)$ (notice the one derivative). Show that, properly normalized, the eigenfunctions form an infinite orthonormal set.

Solution: The eigenfunction ODE

$$\frac{d^2y}{dx^2} = \lambda y$$

has the general solution

$$y(x) = A\sinh(\lambda^{\frac{1}{2}}x) + B\cosh(\lambda^{\frac{1}{2}}x).$$

Taking one derivative gives

$$y'(x) = A\lambda^{\frac{1}{2}}\cosh(\lambda^{\frac{1}{2}}x) + B\lambda^{\frac{1}{2}}\sinh(\lambda^{\frac{1}{2}}x).$$

Imposing $y'(0) = 0$ yields $A\lambda^{\frac{1}{2}} = 0$. Thus either $A = 0$ or $\lambda = 0$. Try the latter first. In that case $y(x) = B$; imposing the other condition $y(L) = 0$ then forces $B = 0$, which produces the trivial solution $y(x) \equiv 0$. So instead we must have $A = 0$ and thus $y(x) = B\cosh(\lambda^{\frac{1}{2}}x)$. Now imposing $y(L) = 0$ gives $\cosh(\lambda^{\frac{1}{2}}L) = 0$, which is solved by $\lambda^{\frac{1}{2}}L = i(n+1/2)\pi$ with $n = 0, 1, 2, 3, \ldots$. Since $\lambda^{\frac{1}{2}}$ is imaginary, the eigenfunction becomes

$$y_n(x) = B_n\cos((n+1/2)\pi x/L).$$

By choosing $B_n = \sqrt{2/L}$ the solutions are normalized. The final answer is thus

$$\lambda = -\left(\frac{(n+1/2)\pi}{L}\right)^2, \quad y_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{(n+1/2)\pi x}{L}\right), \quad n = 1, 2, 3, \ldots.$$

It is easy to show (for instance by checking an integral table) that these are orthonormal:

$$\langle y_n|y_m\rangle = \frac{2}{L}\int_0^L dx\, \sin\left(\frac{(n+1/2)\pi x}{L}\right)\sin\left(\frac{(m+1/2)\pi x}{L}\right) = \delta_{nm}.$$

It would have been easier to solve this by realizing from the beginning that the solutions had to be sinusoidal rather than hyperbolic. That means λ must be negative. Thus we could write $\lambda = -k^2$. The ODE becomes

$$\frac{d^2y}{dx^2} = -k^2y,$$

which is solved by

$$y(x) = A\sin(kx) + B\cos(kx).$$

The boundary condition $y'(0) = 0$ forces $A = 0$, so the eigenfunction becomes

$$y(x) = B\cos(kx).$$

Now imposing the other boundary condition $y(L) = 0$ forces

$$\cos(kL) = 0 \text{ or } kL = (n + 1/2)\pi.$$

Then the above solution follows easily.