Chemistry 542

Fall, 2002

Problem Set 2

Due Friday, September 13

Read the handout on boundary value problems (especially pp 206-221).

1. Consider the following vectors:

$$|u\rangle = 2|1\rangle + 5|2\rangle + \alpha|3\rangle$$
$$|v\rangle = |1\rangle + 2|2\rangle - 3|3\rangle$$

   A. Find the value of a such that the two vectors are orthogonal.
   B. Next, multiply each vector by a suitable constant to normalize it.

2. Consider the expansion:

$$f(x) = \sum_n a_n \phi_n(x), \quad \text{a § x § b}$$

A. Show that

$$\int_a^b [f(x)]^2 r(x)dx = \sum_n a_n^2$$

where r(x) is the Sturm-Liouville weighting factor.

B. Suppose that f(x) = x , r(x) = 1, 0 § x § L, and

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

In class we derived the expansion coefficients. Use them to show that $\frac{\pi^2}{6} = \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \ldots$

3. Expand the function f(x)=1 in a Fourier sine series over the interval [0,L]. Show that

$$\frac{\pi^2}{8} = \frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + \ldots$$

4. Express the function f(x) = x^2 in a Fourier sine series, for 0 § x § L

5. Hermite's differential equation is given by

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2ny = 0, \quad \text{- ¶ § x § ¶}$$

A. Write this equation in Sturm-Liouville form, and identify p(x), q(x), and r(x).

B. The solutions are a set of polynomials, which may be obtained from a generating function as follows:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^2} e^{-x^2}$$

(There are other ways of getting these polynomials, but this is an especially pretty one.) Determine the first four polynomials (n = 0, 1, 2, 3). The answer is found in Levine, problem 4.19.

C. Show that these functions satisfy the recursion relation

$$xH_n(x) = nH_{n-1}(x) + \frac{1}{2}H_{n+1}(x)$$

D. Show that H_2(x) and H_3(x) are orthogonal. Don't forget the weighting function.

This problem is typical of many of the differential equations common in quantum mechanics, such as the Legendre and LaGuerre equations.

6. Suppose the following eigenvalue equation is satisfied:

‹ *n, = n^2 *n,,

where ‹ is the operator for observable L.

Consider the following function:

*f, = $6^{!½}$ *1, + $3^{!½}$ *2, + $2^{!½}$ *3,.

A. Suppose a measurement of L is performed. What is the probability that the system will be found in state *1, after the measurement is performed?

B. What is the expectation value of L?