Chem 212
Problem 2. (Due Tuesday, September 16, 2008)

Two terms that you will often hear in quantum mechanics are "vector space" and "basis". A vector space is a collection of objects that can be scaled and added. The most familiar vector spaces are the 2 dimensional and 3 dimensional Euclidian spaces, where vectors are represented as ordered pairs or triples of real numbers. A basis is a set of vectors that can be used to form every other vector in the vector space, without any of those elements being able to form the others. For instance, the x and y unit vectors form a basis for 2-d Euclidean space because they can be used to form every vector in 2-d by simply scaling and adding them, but one cannot be used to form the other (i.e. x and y are linearly independent).

The pioneering work of the mathematician David Hilbert extended the concept of a vector space to include functions, rather than discrete numbers, in what is known as "Hilbert space". For instance, we can consider the vector space consisting of all the real continuous functions of x. The various powers of x (1, x, $x^2$…) form a basis for this vector space, but not an orthonormal basis. In this problem we'll utilize the Gram-Schmidt process to form an orthonormal basis over two different intervals, and see that some well-known polynomials are generated.

The Gram-Schmidt process is a multi-step algorithm that generates a series of orthonormal vectors ($e_0$, $e_1$, $e_2$, …$e_n$) from a set of independent vectors ($v_0$, $v_1$, $v_2$, …$v_n$). It follows the general process of:

1) Pick your first vector, $v_0$.
2) Normalize your first vector, $v_0$. This is $e_0$.
3) Pick your second vector, $v_1$.
4) Subtract the projection of $e_0$ on $v_1$ from $v_1$.
5) Normalize $v_1$. This becomes $e_1$.
6) Pick your third vector, $v_2$.
7) Subtract the projection of $e_0$ and $e_1$ on $v_2$ from $v_2$.
8) Normalize $v_2$. This becomes $e_2$.
9) Repeat ad nauseum.

<u>Part 1</u>

We will first work over the interval -1 ≤ x ≤ 1. To utilize the Gram-Schmidt process, we need to define the inner product. In Euclidean space, this is simply the dot product. However, in Hilbert space it's a little more complicated. Over the interval we are interested in, the inner product between vectors $v_n$ and $v_m$ is:

$$v_n \bullet v_m = \frac{2n+1}{2}\int_{-1}^{1} v_n v_m dx$$

Once the inner product is defined, we can the projection operator. The projection of vector $v_n$ onto vector $v_m$ is:

$$v_n(v_n \bullet v_m)$$

Now that we have all the tools to find the orthonormal vectors for this vector space, let's begin:

a) What are the first four starting vectors for our vector space ($v_0$, $v_1$, $v_2$, and $v_3$)?
b) Normalize $v_0$. This is our new vector $e_0$. (Remember, to normalize a vector, divide the vector by the square root of the inner product of the vector with itself, i.e. $e_0 = \frac{v_0}{\sqrt{v_0 \bullet v_0}}$).
c) What is the projection of $e_0$ onto $v_1$?
d) Subtract the projection of $e_0$ onto $v_1$ from $v_1$, and then normalize. Call this $e_1$.
e) Find $e_2$.

Congratulations, you have just derived the first three Legendre polynomials. The Legendre polynomials are found quite often in classical E&M, and are related to the spherical harmonics we will see while discussing the hydrogen atom in chapter 3.

<u>Part 2</u>

Now let's use the same vector basis (1, x, $x_2$…), but over a different interval, this time the entire real line. In this case the inner product is given by:

$$v_n \bullet v_m = \frac{1}{2^n \pi^{\frac{1}{2}} n!} \int_{-\infty}^{\infty} v_n v_m e^{-x^2} dx$$

Find the first three orthonormal vectors for this space (You may need to integrate by parts). You'll notice that they are the first three Hermite polynomials.