# Homework Assignment #10

## Math Methods

*Due: Wednesday, December 1st*

Instructions:

Below is the a list of questions and problems from the texbook. It is not sufficient to simply obtain the correct answer. You must also explain your calculation, and each step so that it is clear that you understand the material.

Homework should be written legibly, on standard size paper. Do not write your homework up on scrap paper. If your work is illegible, it will be given a zero.

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1. Byron & Fuller, Chapter 5, problem 2.

2. Use MATHEMATICA or some other symbolic calculational software to calculate the expansion of the following functions by the first eight Legendre polynomials, and plot the expansion and the original function in the interval $-1 < x < 1$.

   (a) $f(x) = |x|$

   (b) $f(x) = \Theta(x)$, (the Heaviside step function).

   Which function is better approximated by the expansion you calculated?

3. Use MATHEMATICA or any similar symbolic manipulation program to Gram-Schmidt orthonormalize the first five polynomials, $\{1, x, x^2, x^3, x^4\}$ is the interval $-\infty < x < \infty$, where the inner product is:

$$(f(x), g(x)) \equiv \int_{-\infty}^{\infty} f(x)\, g(x)\, e^{-x^2}\, dx$$

   How do your results compare to the Hermite polynomials?

   *Hint:* You might look at the MATHEMATICA command **Orthogonalize**.

4. **Fourier Analysis:**

   (a) Calculate the discrete Fourier transform of the following functions on the interval $[-\pi, \pi]$, using the sine and cosine basis described on p.241 of the text.

   *(i)*
$$f(x) = \begin{cases} -1 & \text{for } x < 0 \\ 0 & \text{for } x = 0 \\ 1 & \text{for } x > 0 \end{cases}$$

   *(ii)*
$$f(x) = \frac{|x|}{\pi}$$

   You may do this by hand or by computer.

(b) For both (i) and (ii) use a computer to sum the series:

$$f_n(x) = \frac{a_0}{2} + \sum_{n=1}^{N} (a_n \cos nx + b_n \sin nx)$$

numerically for $N$ =5, 10, 100, and 200, for $-\pi/10 < x < \pi/10$, plotting the results.

(c) Comment on how well the Fourier series can reproduce a discontinuous function, or a function with a discontinuous derivative. How well would you expect it to work on the function:

$$f(x) = \frac{x|x|}{\pi^2}$$

(Parts (a) and (b) worth 10 points, part (c) worth 5 points.)

5. **Simple Fourier Application:** Suppose we have a fourth order differential equation

$$\mathcal{L}\, y(x) = y'''' + \alpha\, y'' + \beta y = x^2 - x$$

defined in the interval $0 \le x \le 1$ with the boundary conditions:

$$\begin{aligned} y(0) = &\quad y(1) = 0 \\ y''(0) = &\quad y''(1) = 0 \end{aligned} \tag{1}$$

We may write $y(x)$ in sine series:

$$y(x) = \sum_{n=1}^{\infty} a_n \sin(n\pi x)$$

(a) The standard fourier expansion differs from the above expression - we have only the sine terms. Why?

(b) Insert the above expression for $y(x)$ into the differential equation, and then take the inner product with $\sin(m\pi x)$, obtaining an algebraic equation for $a_m$.

(c) Write down the full solution for $y(x)$ in terms of the Fourier sum.

(d) Use the solvability condition to state when the problem will have a solution. Give an example of values for $\alpha$ and $\beta$ for which the problem will not have a solution.

(Entire problem worth 15 points.)

6. Consider an electron in a box of width $L$, so that $\psi(0) = \psi(L) = 0$. The time-independent Schrodinger equation is given by

$$\left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - e\mathcal{E}\, x \right\} \psi(x) = E\psi(x) \tag{2}$$

(a) Make the change to dimensionless variables. Determine what it means for the electric field to be a "small" perturbation.

(b) In the limit that $\mathcal{E} = 0$, what are the eigenenergies and normalized eigenstates?

(c) In the limit that $\mathcal{E}$ is "small", what is the first order correction to the groundstate energy?

(d) In the limit that $\mathcal{E}$ is "small", what is the second order correction to the groundstate energy?

B&F Chapter 5, #2.

Find the potential inside a sphere of radius R if the potential on the boundary is

$$V(R,\theta) = \begin{cases} +V & \text{for } 0 \le \theta \le \frac{\pi}{2} \\ -V & \text{for } \frac{\pi}{2} < \theta \le \pi . \end{cases}$$

The general solution to the Poisson equ in a charge free region is

$$V(r,\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[ A_\ell r^\ell + B_\ell r^{-(\ell+1)} \right]$$

$$\times \left[ C_{\ell m} Y_{\ell m}(\theta,\varphi) + D_{\ell m} Q_{\ell m}(\theta,\varphi) \right]$$

We may set $B_\ell = 0$ since the answer must be finite as $r \to 0$

We may set $D_{\ell m} = 0$ since the answer must be finite as $\theta \to 0$ or $\pi$.

We may set $m = 0$ since there is no $\varphi$ dependence in our problem

$$\overset{\delta}{=} \quad V(r,\theta) = \sum_{\ell=0}^{\infty} A_\ell \, r^\ell \, C_{\ell 0} \, P_\ell(\cos\theta)$$

Set $a_\ell = A_\ell C_{\ell 0}$

$x = \cos\theta$

Then $V(R,x) = \sum_{\ell=0}^{\infty} a_\ell R^\ell P_\ell(x) = V(R,x)$.

where $V(R,x) = \begin{cases} V & 0 \le x \le 1 \\ -V & -1 \le x \le 0 \end{cases}$

Then $\left(P_{\ell'}(x), V(R,x)\right) = \sum_{\ell=0}^{\infty} a_\ell R^\ell (P_{\ell'}, P_\ell)$

$$= \int_{-1}^{1} P_{\ell'}(x) \, V(R,x) \, dx$$

The $P_\ell$'s are orthogonal.

$$a_{\ell'} R^{\ell'} \frac{2}{2\ell'+1} = \int_{-1}^{1} P_{\ell'} V(R,x) \, dx$$

$V(x)$ is an odd fxn of $x$ so this is zero if $\ell'$ is even. Set $\ell' = 2p+1$

$$a_{2p+1} = \frac{1}{R^{2p+1}} \frac{2}{2(2p+1)+1} \, 2 \int_0^1 P_{2p+1}(x)\,dx$$

The integral is a mess - looking it up I find -

$$\int_0^1 P_n(x)\,dx = \frac{\sqrt{\pi}}{2\,\Gamma\left(\frac{1}{2}-n\right)\Gamma\left(\frac{n+3}{2}\right)}$$

So that
$$\int_0^1 P_{2p+1}(x)\,dx = \frac{\sqrt{\pi}}{2\,\Gamma\left(-\left(2p+\frac{1}{2}\right)\right)\Gamma(p+2)}$$

$$a_{2p+1} = \frac{1}{R^{2p+1}} \frac{2}{4p+3} \frac{\sqrt{\pi}}{\Gamma(p+2)\,\Gamma\left(-2p-\frac{1}{2}\right)}$$

Since $\Gamma(n) = (n-1)!$

$$V(r,\theta) = \sum' \left(\frac{r}{R}\right)^{2p+1} \frac{2}{4p+3} \frac{1}{(n+1)!} \frac{\sqrt{\pi}}{\Gamma\left(-\left(2p+\frac{1}{2}\right)\right)}$$

$$\times P_\ell(\cos\theta).$$

# Homework 12, Problem 4

Make the basis:

```
basis = Table[x^n, {n, 0, 4}]
```

$\{1, x, x^2, x^3, x^4\}$

Copying directly from the Mathematica help file on **Orthogonalize**:

```
orthbasis =
 Orthogonalize[basis, Integrate[#1 #2 Exp[-x^2], {x, -Infinity, Infinity}] &]
```

$$\left\{\frac{1}{\pi^{1/4}}, \frac{\sqrt{2}\, x}{\pi^{1/4}}, \frac{\sqrt{2}\left(-\frac{1}{2}+x^2\right)}{\pi^{1/4}}, \frac{2\left(-\frac{3x}{2}+x^3\right)}{\sqrt{3}\,\pi^{1/4}}, \frac{\sqrt{\frac{2}{3}}\left(-\frac{3}{4}+x^4-3\left(-\frac{1}{2}+x^2\right)\right)}{\pi^{1/4}}\right\}$$

The first five Hermite polynomials are:

```
hPoly = Table[HermiteH[n, x], {n, 0, 4}]
```

$\{1, 2x, -2+4x^2, -12x+8x^3, 12-48x^2+16x^4\}$

Looking at the ratios of each element in the table, we see that they are proportional:

```
Simplify[Table[orthbasis[[i]] / hPoly[[i]], {i, 1, 5}]]
```

$$\left\{\frac{1}{\pi^{1/4}}, \frac{1}{\sqrt{2}\,\pi^{1/4}}, \frac{1}{2\sqrt{2}\,\pi^{1/4}}, \frac{1}{4\sqrt{3}\,\pi^{1/4}}, \frac{1}{8\sqrt{6}\,\pi^{1/4}}\right\}$$

That's because our functions are normalized and the Hermite polynomials aren't. Let's normalize them:

```
hPolyNorm = Table[fxn = hPoly[[i]];
  c0 = Integrate[fxn^2 Exp[-x^2], {x, -Infinity, Infinity}];
  fxn/Sqrt[c0], {i, 1, 5}]
```

$$\left\{\frac{1}{\pi^{1/4}}, \frac{\sqrt{2}\, x}{\pi^{1/4}}, \frac{-2+4x^2}{2\sqrt{2}\,\pi^{1/4}}, \frac{-12x+8x^3}{4\sqrt{3}\,\pi^{1/4}}, \frac{12-48x^2+16x^4}{8\sqrt{6}\,\pi^{1/4}}\right\}$$

Now we can check if they are the same:

```
Simplify[Table[orthbasis[[i]] / hPolyNorm[[i]], {i, 1, 5}]]
```

$\{1, 1, 1, 1, 1\}$

(3) (i) $f(x) = \begin{cases} -1 & \text{for } x < 0 \\ 0 & \text{for } x = 0 \\ 1 & \text{for } x > 0 \end{cases}$

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx \, dx = 0 \quad \text{(by symmetry)}$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx \, dx$$

$$= \frac{2}{\pi} \int_{0}^{\pi} \sin nx \, dx$$

$$= \frac{2}{\pi n} \left. -\cos nx \right|_{0}^{\pi} = -\frac{2}{n\pi} \left[ (-1)^n - 1 \right]$$

$$= -\frac{4}{n\pi} \quad \text{for } n \text{ odd}$$

$$= 0 \quad \text{for } n \text{ even}$$

<u>Or</u> $$f(x) = \sum_{m=0} \frac{-4}{(2m+1)\pi} \sin((2m+1)x)$$

(ii) $$f(x) = x|x|/\pi$$

Note this function is just $1/2\pi$ the integral of the step function in (i). Thus

$$f(x) = \sum_{m=0}^{1} \frac{-4}{\pi^2(2m+1)^2} \cos((2m+1)x) +$$

Alternatively one can do the tedious algebra:

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x) \sin nx \, dx = 0 \quad \text{(by symmetry)}$$

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x) \cos nx \, dx$$

$$= \frac{2}{\pi}\int_0^{\pi} \frac{x}{\pi} \cos nx \, dx$$

$$= \frac{2}{\pi^2}\left\{ \frac{x \sin nx}{n}\Big|_0^{\pi} - \int \frac{1}{n} \sin nx \, dx \right\}$$

$$= -\frac{2}{n\pi^2}\Big[ -\cos nx \Big]_0^{\pi} = \frac{2}{n\pi^2}\left[(-1)^n - 1\right]$$

$$= \begin{cases} 0 & \text{for } n \text{ even.} \\ \dfrac{-4}{n\pi^2} & \text{for } n \text{ odd.} \end{cases}$$

For $n = 0$ $\quad a_0 = \frac{2}{\pi}\int_0^{\pi} \frac{x}{\pi} \, dx = \frac{1}{\pi^2} x^2 \Big|_0^{\pi} = 1$

$$f(x) = \frac{1}{2} + \sum_{m=0}^{\infty} \frac{-4}{(2m+1)^2\pi^2} \cos nx$$

(b) Plots are attached.

(c) The function $\frac{x|x|}{\pi^2}$ has a higher order discontinuity (i.e. in second derivative). We are effectively integrating over the wiggles in the Gibbs phenomena $\rightarrow$ smoother approximation near $x = 0$.

However, the function is <u>discontinuous</u> at $x = \pm \pi$. We should see Gibbs phenomena at the edges.

# Problem 4

Define our functions

```
In[314]:= fxn1 = If[x ≤ 0, -1, 1];
          fxn2 = Abs[x]/π;
```

## Part (a) Fourier Expansion

### Step function:

We can break the integral into two parts, for x<0 and x>0. The cosine terms are all zero:

```
In[326]:= Integrate[-Cos[n x] , {x, -π, 0}] + Integrate[Cos[n x], {x, 0, π}]
```

Out[326]= 0

The sine terms are either zero or 4/n.

```
In[327]:= Integrate[-Sin[n x] , {x, -π, 0}] + Integrate[Sin[n x], {x, 0, π}]
```

Out[327]= $\frac{2\,(1-\mathrm{Cos}[n\,\pi])}{n}$

### Absolute value function:

Again, we can break the integral into two parts, for x<0 and x>0. The cosine terms are all zero:

```
In[331]:= aout = Integrate[-x Cos[n x] , {x, -π, 0}] + Integrate[x Cos[n x], {x, 0, π}]
```

Out[331]= $\frac{2\left(-1+\mathrm{Cos}[n\,\pi]+n\,\pi\,\mathrm{Sin}[n\,\pi]\right)}{n^2}$

```
In[332]:= Simplify[aout, Assumptions → Element[n, Integers] ]
```

Out[332]= $\frac{2\left(-1+(-1)^n\right)}{n^2}$

The sine terms are all zero:

```
In[335]:= bout = Integrate[-x Sin[n x] , {x, -π, 0}] + Integrate[x Sin[n x], {x, 0, π}]
```

Out[335]= $\frac{n\,\pi\,\mathrm{Cos}[n\,\pi]-\mathrm{Sin}[n\,\pi]}{n^2}+\frac{-n\,\pi\,\mathrm{Cos}[n\,\pi]+\mathrm{Sin}[n\,\pi]}{n^2}$

```
In[336]:= Simplify[bout, Assumptions → Element[n, Integers] ]
```

Out[336]= 0

## Part (b)

### The step function:

In[340]:=
```
nmax = 5;
cosList = Join[{1/Sqrt[2]}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
```

Let's check the normalization:

In[343]:=
```
Table[Integrate[cosList[[i]]^2, {x, -π, π}], {i, 1, Length[cosList]}]
Table[Integrate[sinList[[i]]^2, {x, -π, π}], {i, 1, Length[sinList]}]
```

Out[343]= $\{\pi, \pi, \pi, \pi, \pi, \pi\}$

Out[344]= $\{\pi, \pi, \pi, \pi, \pi\}$

Okay, we have a factor of $\pi$ to divide by at the end. First the coefficients:

In[323]:=
```
alist = Table[-Integrate[ cosList[[i]] , {x, -π, 0}] +
   Integrate[ cosList[[i]] , {x, 0, π}], {i, 1, Length[cosList]}]
```

Out[323]= $\{0, 0, 0, 0, 0, 0\}$

In[322]:=
```
blist = Table[-Integrate[ sinList[[i]] , {x, -π, 0}] +
   Integrate[ sinList[[i]] , {x, 0, π}], {i, 1, Length[sinList]}]
```

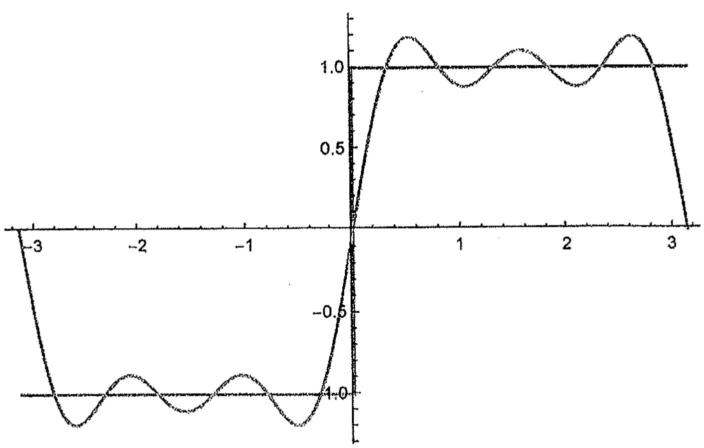
Out[322]= $\left\{4, 0, \frac{4}{3}, 0, \frac{4}{5}\right\}$

In[345]:=
```
appStep5 = (alist.cosList + blist.sinList)/π
```

Out[345]= $\dfrac{4\,\mathrm{Sin}[x] + \frac{4}{3}\mathrm{Sin}[3\,x] + \frac{4}{5}\mathrm{Sin}[5\,x]}{\pi}$

In[346]:=
```
Plot[{fxn1, appStep5}, {x, -π, π}]
```

Out[346]=




There is a more clever way to do this with functions at lists, but I'll do it by brute force.

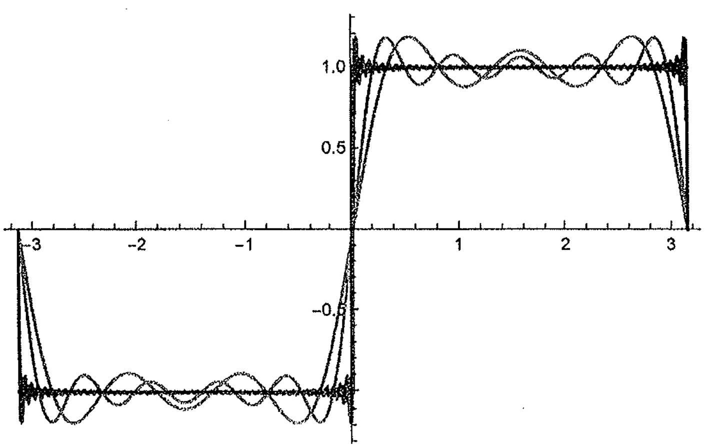
```
nmax = 10;
cosList = Join[{1/√2}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
alist = Table[-Integrate[ cosList[[i]] , {x, -π, 0}] +
    Integrate[ cosList[[i]] , {x, 0, π}], {i, 1, Length[cosList]}];
blist = Table[-Integrate[ sinList[[i]] , {x, -π, 0}] +
    Integrate[ sinList[[i]] , {x, 0, π}], {i, 1, Length[sinList]}];
appStep10 = (alist.cosList + blist.sinList)/π;
```

```
In[353]:= nmax = 100;
cosList = Join[{1/√2}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
alist = Table[-Integrate[ cosList[[i]] , {x, -π, 0}] +
    Integrate[ cosList[[i]] , {x, 0, π}], {i, 1, Length[cosList]}];
blist = Table[-Integrate[ sinList[[i]] , {x, -π, 0}] +
    Integrate[ sinList[[i]] , {x, 0, π}], {i, 1, Length[sinList]}];
appStep100 = (alist.cosList + blist.sinList)/π;
```

```
In[359]:= nmax = 200;
cosList = Join[{1/√2}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
alist = Table[-Integrate[ cosList[[i]] , {x, -π, 0}] +
    Integrate[ cosList[[i]] , {x, 0, π}], {i, 1, Length[cosList]}];
blist = Table[-Integrate[ sinList[[i]] , {x, -π, 0}] +
    Integrate[ sinList[[i]] , {x, 0, π}], {i, 1, Length[sinList]}];
appStep200 = (alist.cosList + blist.sinList)/π;
```

```
In[365]:= Plot[{fxn1, appStep5, appStep10, appStep100, appStep200}, {x, -π, π}]
```

Out[365]=




Note the "Gibb's ears" at the edges of the discontinuities.

The absolute value function:

In[390]:=
```
nmax = 5;
cosList = Join[{1/Sqrt[2]}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
```

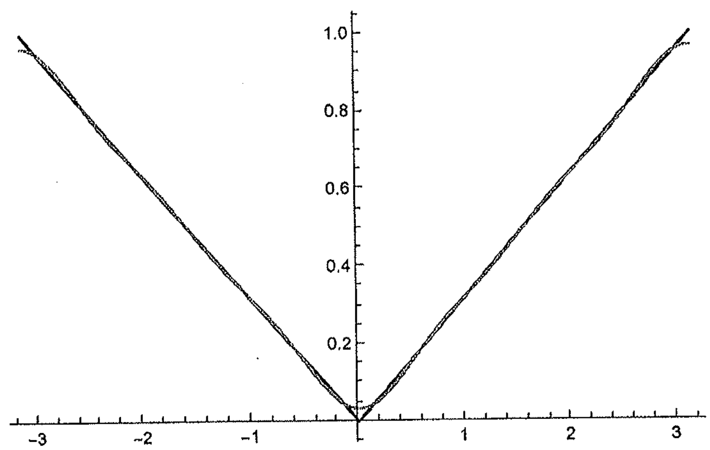
In[393]:=
```
alist = ParallelTable[
   (-Integrate[ x cosList[[i]] , {x, -π, 0}] + Integrate[x cosList[[i]] , {x, 0, π}]) / π,
   {i, 1, Length[cosList]}]
```

Out[393]= $\left\{\frac{\pi}{\sqrt{2}}, -\frac{4}{\pi}, 0, -\frac{4}{9\pi}, 0, -\frac{4}{25\pi}\right\}$

In[394]:=
```
appAbs5 = (alist.cosList)/π;
```

In[395]:=
```
Plot[{fxn2, appAbs5}, {x, -π, π}]
```

Out[395]=




There is a more clever way to do this with functions at lists, but I'll do it by brute force.

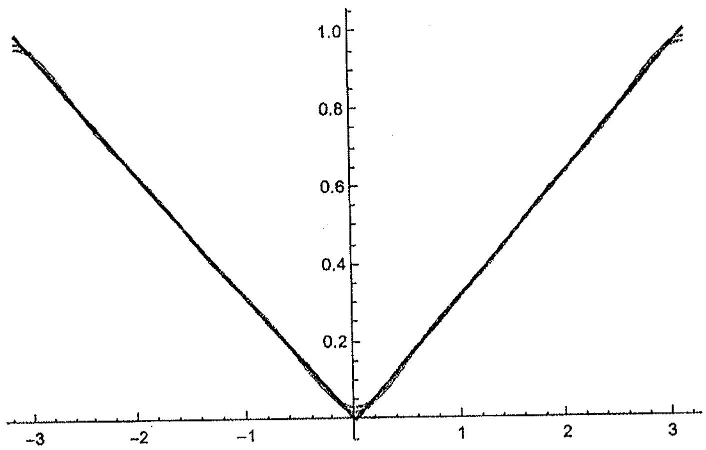
In[396]:=
```
nmax = 10;
cosList = Join[{1/Sqrt[2]}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
alist = ParallelTable[
   (-Integrate[ x cosList[[i]] , {x, -π, 0}] + Integrate[x cosList[[i]] , {x, 0, π}]) /
    π, {i, 1, Length[cosList]}];
appAbs10 = (alist.cosList)/π;
```

In[401]:=
```
nmax = 100;
cosList = Join[{1/Sqrt[2]}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
alist = ParallelTable[
   (-Integrate[ x cosList[[i]] , {x, -π, 0}] + Integrate[x cosList[[i]] , {x, 0, π}]) /
    π, {i, 1, Length[cosList]}];
appAbs100 = (alist.cosList)/π;
```

In[406]:=
```
nmax = 200;
cosList = Join[{1/Sqrt[2]}, Table[Cos[n x], {n, 1, nmax}]];
sinList = Table[Sin[n x] , {n, 1, nmax}];
alist = ParallelTable[
   (-Integrate[ x cosList[[i]] , {x, -π, 0}] + Integrate[x cosList[[i]] , {x, 0, π}]) /
    π, {i, 1, Length[cosList]}];
appAbs200 = (alist.cosList)/π;
```

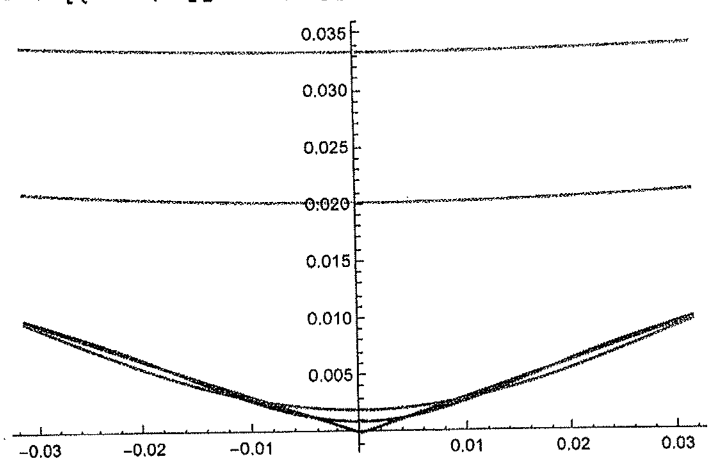
In[411]:=
```
Plot[{fxn2, appAbs5, appAbs10, appAbs100, appAbs200}, {x, -π, π}]
```

Out[411]=




In[413]:=
```
Plot[{fxn2, appAbs5, appAbs10, appAbs100, appAbs200}, {x, -π / 100, π / 100}]
```

Out[413]=



Even the 5 term expansion looks pretty good! The 100 term and 200 term expansions are probably not worth the extra effort unless you are very close to the discontinuity.

4 (a) Only the sine terms are required because the cosine terms cannot obey the boundary conditions.

(b) Let $y(x) = \sum_{n=1}^{\infty} a_n \sin n$. Then.

$$L y(x) = \sum' a_n \left( (n\pi)^4 - \alpha (n\pi)^2 + \beta \right) \sin n\pi x$$

$$= x^2 - x$$

Taking the inner product with $\sin m\pi x$ yields.

$$\sum' a_n \left( (n\pi)^4 - \alpha (n\pi)^2 + \beta \right) \left( \tfrac{1}{2} \right) \delta_{mn}$$

$$= \int_0^1 (\sin m\pi x)(x^2 - x)\, dx$$

Note that:

$$\int_0^1 x \sin n\pi x\, dx = \left[ \frac{\sin n\pi x}{(n\pi)^2} - \frac{x \cos n\pi x}{n\pi} \right]_0^1$$

$$= - \frac{(-1)^n}{n\pi}$$

$$\int_0^1 x^2 \sin n\pi x\, dx = \left[ \frac{2x}{(n\pi)^2} \sin n\pi x + \left\{ \frac{2}{(n\pi)^3} - \frac{x^2}{n\pi} \right\} \cos n\pi x \right]_0^1$$

$$= \left[ \frac{2}{(n\pi)^3} - \frac{1}{n\pi} \right] (-1)^n - \frac{2}{(n\pi)^3}$$

Or

$$\frac{a_m}{2}\left((m\pi)^4 - \alpha(m\pi)^2 + \beta\right) = \frac{2}{(m\pi)^3}\left[(-1)^m - 1\right]$$

(c) $$y(x) = \sum_m{}' \frac{4}{(m\pi)^3} \frac{\left[(-1)^m - 1\right]}{(m\pi)^4 - \alpha(m\pi)^2 + \beta}$$

(d) There is no solution if the denominator is zero & the numerator is not zero. Thus if

$$(m\pi)^4 - \alpha(m\pi)^2 + \beta = 0$$

for $n$ even, there is no solution. For example, if $\beta = 0$ and $\alpha = 2\pi$, there is no solution.

If $(m\pi)^4 - \alpha(m\pi)^2 + \beta = 0$ then for that value of $m$,

$$L \sin m\pi x = 0$$

and $\sin m\pi x$ is a null vector. It must be orthogonal to the inhomogeneous term if there is to be a solution.

#5

Give

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} - e\mathcal{E} x \quad \psi$$

where $0 \leq x < L$

(a) Eigen states of unperturbed problem.

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

with eigenvalues

$$E_n = n^2\pi^2 E_0$$

with

$$E_0 = \frac{\hbar^2}{2mL^2}$$

(b) What are first order corrections to

$E_1$ an $E_2$ ?

$$E_1^{(1)} = -\langle \varphi_1 | e\mathcal{E}x | \varphi_1 \rangle$$

$$= \int_0^L -\frac{2}{L} e\mathcal{E}x \sin^2 \frac{\pi x}{L}\, dx$$

$$= -e\mathcal{E}L$$

$$E_2^{(1)} = -\langle \varphi_2 | e\mathcal{E}x | \varphi_2 \rangle$$

$$= \int_0^L -\frac{2}{L} e\mathcal{E}x \sin^2 \frac{2\pi x}{L}\, dx = -\frac{e\mathcal{E}L}{2}$$

Below in part (d) we need to compare with numerics. To do so it is handy to move to dimensionless units. I choose

$$s = \frac{x}{L}$$

So that

$$H\psi = \left\{ \frac{-\hbar^2}{2mL^2} \frac{\partial^2}{\partial s^2} + e\mathcal{E}L\, s \right\} \psi = E\psi$$

Then define $\epsilon = E/E_0$ so that

$$h\psi = \frac{H}{E_0}\psi = \left\{ -\frac{\partial^2}{\partial s^2} + \delta\, s \right\} \psi = \epsilon \psi.$$

where $\delta = \dfrac{e\mathcal{E}L}{\frac{\hbar^2}{2mL^2}}$

Then

$$\phi_n(s) = \sqrt{2}\, \sin n\pi s$$

with eigenvalues

$$\epsilon = n^2\pi^2$$

So

$$\epsilon_1^{(1)} = -\frac{\delta}{2}$$

$$\epsilon_2^{(1)} = -\frac{\delta}{2}.$$

(c) Second order correction to energy.

If $H_1 = -e\mathcal{E}x$ then.

$$E_1^{(2)} = \sum_{n=2}^{\infty} \frac{|\langle\varphi_n|H_1|\varphi_1\rangle|^2}{\pi^2(1-n^2)E_0}$$

Focussing on the matrix element

$$\langle\varphi_n|H_1|\varphi_1\rangle = -\frac{2}{L}\frac{e\mathcal{E}}{E_0}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right) x\,dx$$

Then. $\sin a \sin b = \frac{1}{2}(\cos(a-b) - \cos(a+b))$

So the integral is

$$\langle\varphi_n|H_1|\varphi_1\rangle = -\frac{e\mathcal{E}}{L}\int_0^L \left(\cos(n-1)\frac{\pi x}{L} - \cos(n+1)\frac{\pi x}{L}\right) x\,dx$$

$$= -e\mathcal{E}L\left\{\frac{(\cos(n-1)\pi - 1)}{(n-1)^2\pi^2} - \frac{(\cos(n+1)\pi - 1)}{(n+1)^2\pi^2}\right\}$$

$$= -\frac{e\mathcal{E}L}{\pi^2}\left\{\frac{((-1)^{n-1} - 1)}{(n-1)^2} - \frac{((-1)^{n+1} - 1)}{(n+1)^2}\right\}.$$

$$= -\frac{e\mathcal{E}L}{\pi^2} \times \frac{4n((-1)^n + 1)}{(n^2-1)^2}$$

So

$$E_1^{(2)} = \sum_{n=2}^{\infty} \frac{1}{E_0\pi^2(1-n^2)}\left(\frac{e\mathcal{E}L}{\pi^2}\right)^2 \left(\frac{16n^2((-1)^n+1)}{(n^2-1)^4}\right)^2$$

or

$$\epsilon_1^{(2)} = \sum_{n=2} \frac{1}{\pi^2(1-n^2)}\left(\frac{\delta}{\pi^2}\right)^2 \frac{16n^2((-1)^n+1)^2}{(n^2-1)^4}$$

Similarly

$$\langle \varphi_n | H_1 | \varphi_2 \rangle = -\frac{2e\mathcal{E}}{L} \int_0^L \sin\frac{n\pi x}{L} \sin\frac{2\pi x}{L}\, x\, dx$$

$$= -\frac{e\mathcal{E}}{L} \int_0^L \left\{ \cos\frac{(n-2)\pi x}{L} - \cos\frac{(n+2)\pi x}{L} \right\} x\, dx$$

$$= -e\mathcal{E}L \left\{ \frac{\cos(n-2)\pi - 1}{(n-2)^2\pi^2} - \frac{\cos(n+2)\pi - 1}{(n+2)^2\pi^2} \right\}$$

$$= -\frac{e\mathcal{E}L}{\pi^2} \left\{ \frac{(-1)^{n-2} - 1}{(n-2)^2} - \frac{(-1)^{n+2} - 1}{(n+2)^2} \right\}$$

$$= -\frac{e\mathcal{E}L}{\pi^2}\, 8\, \frac{n\left((-1)^{n+1} + 1\right)}{(n^2-4)^2}$$

So

$$E_2^{(2)} = \sum_{\substack{n=1 \\ n\neq 2}}^{\infty} \frac{1}{\mathcal{E}_0 \pi^2 (4-n^2)} \left(\frac{e\mathcal{E}L}{\pi^2}\right)^2 64n^2 \left[\frac{\left((-1)^{n+1}+1\right)}{(n^2-4)^2}\right]^2$$

or

$$\mathcal{E}_2^{(2)} = \sum_{\substack{n=1 \\ n\neq 2}}^{\infty} \frac{1}{\pi^2(4-n^2)} \left(\frac{\delta}{\pi^2}\right)^2 \frac{\left((-1)^n+1\right)^2}{(n^2-4)^2}\, 64n^2$$

# Homework 10, problem 5

## Various pieces of algebra

This section isn't necessary, it's just to show that the work I did by hand is correct. For example, the first matrix element is:

$$\text{matelem1} = \text{Integrate}\left[x\left(\sqrt{\frac{2}{L}}\,\text{Sin}[\pi\,x/L]\right)\left(\sqrt{\frac{2}{L}}\,\text{Sin}[n\,\pi\,x/L]\right),\ \{x, 0, L\}\right]$$

$$\left(-4\,L\,n\,(1+\text{Cos}[n\,\pi]) - 2\,L\,(-1+n^2)\,\pi\,\text{Sin}[n\,\pi]\right) \Big/ \left((-1+n^2)^2\,\pi^2\right)$$

I wrote this in the simplifed version:

$$\text{FullSimplify}\left[\left((-1)^{n+1}-1\right)\left(\frac{1}{(n-1)^2}-\frac{1}{(n+1)^2}\right)\right]$$

$$-\frac{4\,(1+(-1)^n)\,n}{(-1+n^2)^2}$$

Let's show that these are the same:

$$\text{Table}[\text{matelem1}, \{n, 2, 9\}]$$

$$\left\{-\frac{16\,L}{9\,\pi^2},\ 0,\ -\frac{32\,L}{225\,\pi^2},\ 0,\ -\frac{48\,L}{1225\,\pi^2},\ 0,\ -\frac{64\,L}{3969\,\pi^2},\ 0\right\}$$

$$\text{Table}\left[\left((-1)^{n+1}-1\right)\left(\frac{1}{(n-1)^2}-\frac{1}{(n+1)^2}\right),\ \{n, 2, 9\}\right]$$

$$\left\{-\frac{16}{9},\ 0,\ -\frac{32}{225},\ 0,\ -\frac{48}{1225},\ 0,\ -\frac{64}{3969},\ 0\right\}$$

Similarly, the second matrix elements was:

$$\text{matelem2} = \text{Integrate}\left[x\left(\sqrt{\frac{2}{L}}\,\text{Sin}[2\,\pi\,x/L]\right)\left(\sqrt{\frac{2}{L}}\,\text{Sin}[n\,\pi\,x/L]\right),\ \{x, 0, L\}\right]$$

$$\left(8\,L\,n\,(-1+\text{Cos}[n\,\pi]) + 4\,L\,(-4+n^2)\,\pi\,\text{Sin}[n\,\pi]\right) \Big/ \left((-4+n^2)^2\,\pi^2\right)$$

Which I wrote as:

$$\text{FullSimplify}\left[\left((-1)^{n+2}-1\right)\left(\frac{1}{(n-2)^2}-\frac{1}{(n+2)^2}\right)\right]$$

$$\frac{8\,(-1+(-1)^n)\,n}{(-4+n^2)^2}$$

And we can verify their equivalence:

```
Table[matelem2, {n, 3, 9}]
```

$$\left\{-\frac{48\,L}{25\,\pi^2},\ 0,\ -\frac{80\,L}{441\,\pi^2},\ 0,\ -\frac{112\,L}{2025\,\pi^2},\ 0,\ -\frac{144\,L}{5929\,\pi^2}\right\}$$

$$\text{Table}\left[\left((-1)^{n+2}-1\right)\left(\frac{1}{(n-2)^2}-\frac{1}{(n+2)^2}\right),\ \{n,\ 3,\ 9\}\right]$$

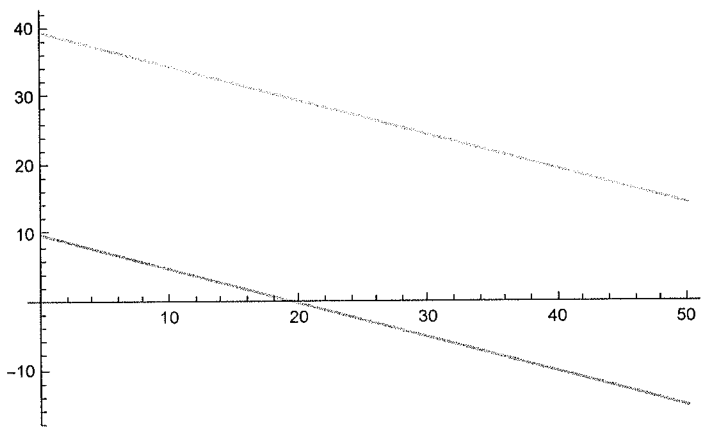
$$\left\{-\frac{48}{25},\ 0,\ -\frac{80}{441},\ 0,\ -\frac{112}{2025},\ 0,\ -\frac{144}{5929}\right\}$$

# Perturbation Results

## First order results

Here's the zeroth plus first order approximation, plotted in dimensionless units:

$$\text{appPlot1} = \text{Plot}\left[\left\{\pi^2-\frac{\delta}{2},\ 4\,\pi^2-\frac{\delta}{2}\right\},\ \{\delta,\ 0,\ 50\}\right]$$




## Second order results:

It's easy to ask Mathematica to sum from n=2 to Infinity in the correction to the ground state energy:

$$\text{appE12} = \text{Sum}\left[\frac{\delta^2}{\pi^6\,(1-n^2)}\,16\,n^2\,\frac{\left((-1)^n+1\right)^2}{\left(n^2-1\right)^4},\ \{n,\ 2,\ \text{Infinity}\}\right];$$

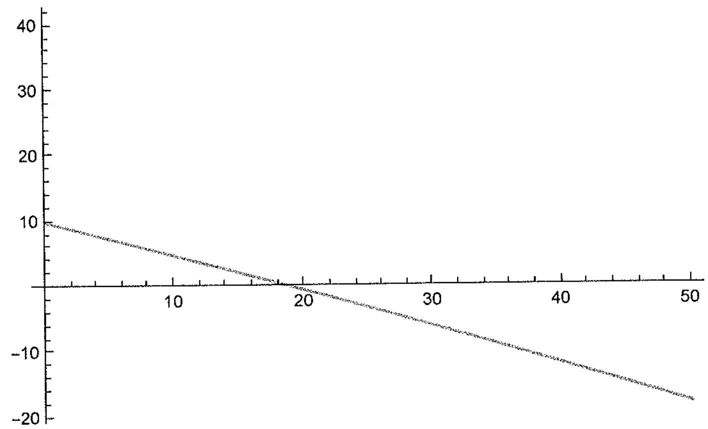
The first excited state is a bit more awkward since we need the n=1 term and then n=3 to Infinity.

$$\text{e12term} = \frac{\delta^2}{\pi^6\,(4-n^2)}\,64\,n^2\,\frac{\left((-1)^{n+1}+1\right)^2}{\left(n^2-4\right)^4};$$

```
appE22 = (e12term /. n → 1) + Sum[e12term, {n, 3, Infinity}];
```

We can plot the energies up to second order in $\delta$:

```
appPlot2 = Plot[{π² - δ/2 + appE12, 4 π² - δ/2 + appE22}, {δ, 0, 50}, PlotStyle → {Red, Green}]
```




As you can see, the second order correction is very small.

# Numerical solution

Here's a numerical solution with zero value boundary conditions. I chose a small value of dx because we're going to have pretty accurate analytic results.

```
ndx = 1000;
dx = 1.0/ndx;
npts = ndx - 1;

hmat = Table[c1 = If[i == j, 2/dx² - δ (i) dx, 0];
   c2 = If[Abs[i - j] == 1, - 1/dx², 0];
   c1 + c2
   , {i, 1, npts}, {j, 1, npts}];
```

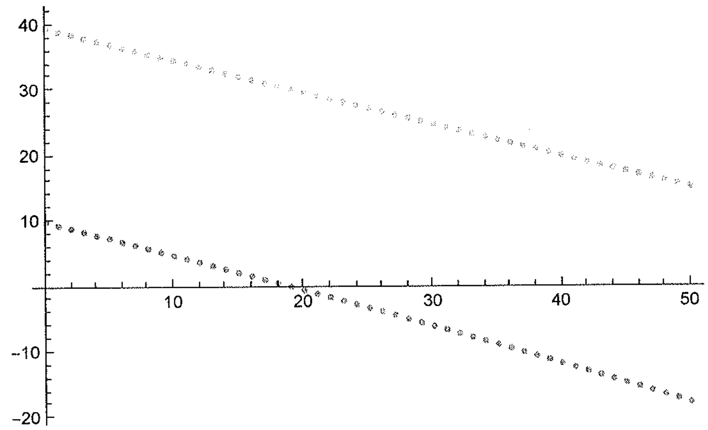
Let's check to see that if $\delta$=0 the energies are $n^2 \pi^2$

```
hval = hmat /. δ → 0;

Eigenvalues[hval, -4] / π²

{15.9998, 8.99993, 3.99999, 0.999999}
```

Yes, it seems that we are ok. Now lets solve the problem for varies values of $\delta$. The code below is very inefficient, but easy to read: I calculate the four smallest *in magnitude*, sort them by actual value, and then chose the first or second ones in the sorted list.

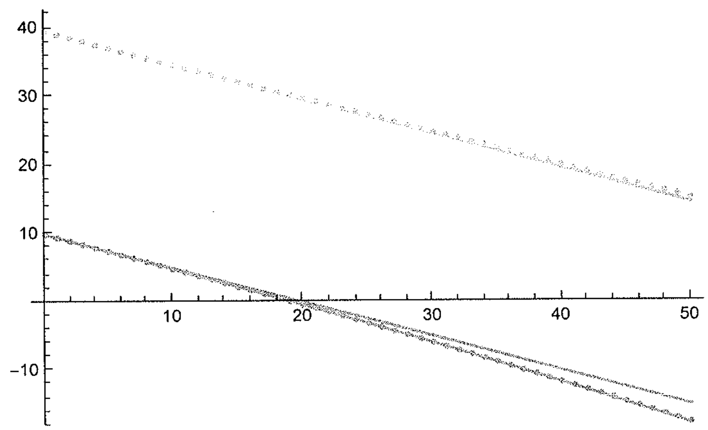
```
enum1 = Table[hval = hmat /. δ → dval;
   {dval, Sort[Eigenvalues[hval, -4]][[1]]}, {dval, 0, 50.0, 1}];
enum2 = Table[hval = hmat /. δ → dval;
   {dval, Sort[Eigenvalues[hval, -4]][[2]]}, {dval, 0, 50.0, 1}];
```

```
numPlot = ListPlot[{enum1, enum2}]
```




We can plot these "exact numerical" results along with the perturbative ones from above:

```
Show[appPlot1, appPlot2, numPlot]
```

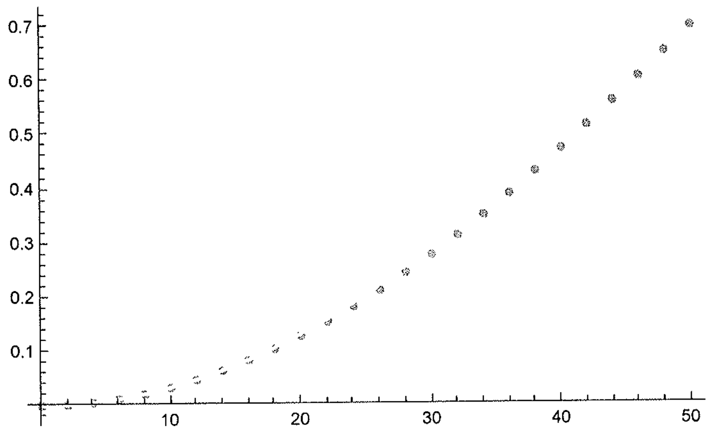



The results for the ground state look very good. However, it's hard to see the second order correction to the first excited state. Let's subtract the first order result from the numerical answer and plot the residual. We can compare that with the second order term alone. First, calculate the residual:

```
enum2a = Table[hval = hmat /. δ → dval;
   {dval, (Sort[Eigenvalues[hval, -20]][[2]] - 4 π^2 + dval/2)}, {dval, 0, 50.0, 2}];
```

We plot (silently) the numerical residual and the second order term separately, and then have Mathematica show the two plots together:

```
foo = ListPlot[enum2a];
quux = Plot[appE22, {δ, 0, 50}, PlotStyle → {Red, Green}];
Show[foo, quux]
```




I'd say that looks pretty good!