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Math Methods in Physics

PHYS 5013 Homework Assignment #10

Problems: {5.2, 2, 3, 4, 5, 6}

Due: December 1, 2021 By 11:59 PM

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Problem 1: 5.2

A metal spherical shell of radius R with its center at $x = y = z = 0$ is cut in half along its intersection with the plane $z = 0$. The two halves are separated by an infinitesimal gap and the upper and lower hemispheres are brought to voltages $+V$ and $-V$ respectively. Show that the potential inside the sphere is

$$\phi(r,\theta) = V\sum_{l=0}^{\infty}(-1)^l\left(\frac{r}{R}\right)^{2l+1}\frac{(2l)!}{(2^l l!)^2}\frac{4l+3}{2l+2}P_{2l+1}(\cos\theta),$$

where θ is the polar angle measured relative to the positive z-axis. *Hint:* $\nabla^2\phi = 0$ inside and on a spherical shell. ψ is clearly independent of ϕ. Following the usual procedure of separation of variables, we find that the solution is of the form

$$\psi(r,\theta) = \sum_{l=0}^{\infty}[A_l r^l + B_l r^{-l-1}][C_l P_l(\cos\theta) + D_l Q_l(\cos\theta)].$$

Immediately set $B_l = 0$ (all l) so $\psi(0,\theta)$ is finite and set $D_l = 0$ (all l) so $\psi(r,0)$ and $\psi(r,\pi)$ are finite. The problem is now one of mathematics-determining the constants $A_l C_l \equiv \alpha_l$ such that the boundary conditions are satisfied:

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

The general solution to our boundary-value problem in spherical co-ordinates is : $\varphi = 0$

$$\varphi(r,\theta) = \sum_{l=0}^{\infty}\left(A_l r^l + B_l r^{-(l+1)}\right)P_l\cos(\theta)$$

Applying the boundary conditions our solution simplifies to :

$$\varphi(r,\theta) = \sum_{l=0}^{\infty} A_l r^l P_l \cos(\theta)$$

we solve for A_l with

$$A_l = \frac{2l+1}{2r^l}\int_0^{\pi} V(\theta)P_l\cos(\theta)\sin(\theta)\,d\theta$$

Now applying the boundary conditions again

$$A_l = \frac{2l+1}{2r^l}\left[V\int_0^{\pi/2}P_l(\cos(\theta))\sin(\theta)\,d\theta - V\int_{\pi/2}^{\pi}P_l(\cos(\theta))\sin(\theta)\,d\theta\right]$$

we split the integral and evaluate each one , If l is even , $A_l = 0$ otherwise :

$$A_l = \left(-\frac{1}{2}\right)^{(l-1)/2}\frac{(2l+1)(l-2)!!}{2\left(\frac{l+1}{2}\right)!}\frac{V}{r^l} \quad \therefore \quad \varphi(r,\theta) = V\sum_{l=0}^{\infty}(-1)^l\left(\frac{r}{R}\right)^{2l+1}\frac{(2l)!}{(2^l l!)^2}\frac{4l+3}{2l+2}P_{2l+1}(\cos(\theta))$$

■

Problem 1: 5.2 Review

Procedure:

- Use the general solution for a boundary-value problem in spherical co-ordinates with $\phi = 0$
$$\phi(r,\theta) = \sum_{l=0}^{\infty}(A_l r^l + B_l r^{-(l+1)})P_l \cos\theta$$
and apply the boundary conditions.
- Then proceed to solve for A_l with
$$A_l = \frac{2l+1}{2r^l}\int_0^{\pi} V(\theta)P_l \cos\theta \sin\theta \, d\theta$$
and apply the boundary conditions again.
- Proceed to evaluate the integral and plug it into general solution.

Key Concepts:

- When we apply boundary conditions it simplifies our equation so that it is easier to solve.
- Using the rules of Calculus we can simplify the integrals and solve for A_l.

Variations:

- We can be given a different symmetry or potential.
  - This would change our general solution as well as our boundary condition. It would in turn create a completely different problem.

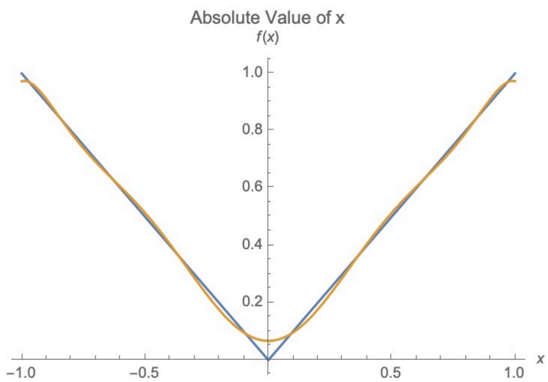
Problem 2:

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) $f(x) = |x|$

```
In[50]:= basis = Table[Sqrt[(2 n + 1)/2] LegendreP[n, x], {n, 0, 8}];
fxn = Abs[x];
coeffs = Integrate[fxn basis, {x, -1, 1}];
appFxn = coeffs.basis;
Plot[{fxn, appFxn}, {x, -1, 1}, PlotLabel → "Absolute Value of x", AxesLabel → {x, f[x]}]
```

Out[54]=

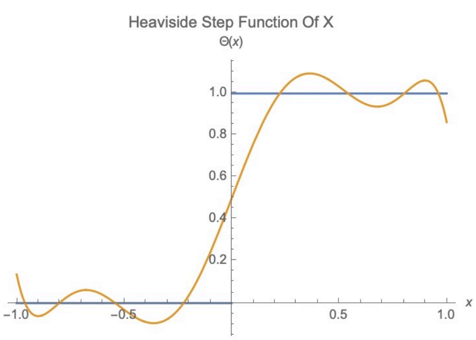


(b) $f(x) = \Theta(x)$, (the Heaviside step function).

What function is better approximated by the expansion you calculated?

```
In[80]:= Clear["Global`*"];
basis = Table[Sqrt[(2 n + 1)/2] LegendreP[n, x], {n, 0, 8}];
fxn = HeavisideTheta[x];
coeffs = Integrate[fxn basis, {x, -1, 1}];
appFxn = coeffs.basis;
Plot[{fxn, appFxn}, {x, -1, 1}, PlotLabel → "Heaviside Step Function Of X", AxesLabel → {x, θ[x]}]
```

Out[85]=



|x| is better approximated.

Problem 2: Review

Procedure:

- Use the *LegendreP* function in MATHEMATICA to calculate the Legendre polynomials.
- Proceed to integrate the Legendre polynomials against the function given in the problem statement.
- Then plot the answer.

Key Concepts:

- We can use numerical techniques in MATHEMATICA to plot the expansion of the original function in our given integral.
- Functions that are discontinuous at some point are harder to approximate than those that are not differentiable but still continuous.

Variations:

- We can be given different functions.
  - We would use the same procedure but with new functions.

Problem 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?

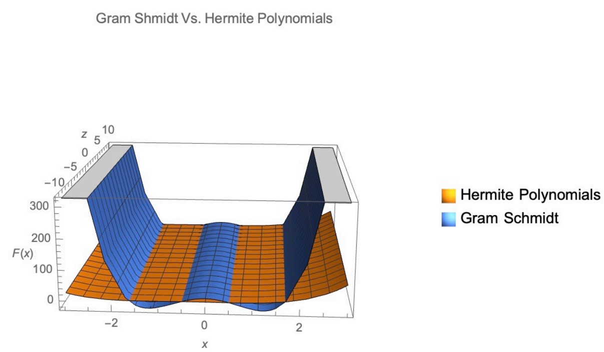
Hint: You might look at the MATHEMATICA command **Orthogonalize**.

```
In[117]:= ClearAll["Global`*"];
GramSchmidt = Orthogonalize[{1, x, x^2, x^3, x^4}, Integrate[#1 #2 Exp[-x^2], {x, -Infinity, Infinity}] &] // Simplify;
```

$$\texttt{GramSchmidtFxn} = \frac{1}{\pi^{1/4}} + \frac{\sqrt{2}\,x}{\pi^{1/4}} + \frac{\sqrt{2}\left(-\frac{1}{2}+x^2\right)}{\pi^{1/4}} + \frac{x\left(-3+2x^2\right)}{\sqrt{3}\,\pi^{1/4}} + \frac{3-12x^2+4x^4}{2\sqrt{6}\,\pi^{1/4}};$$

```
HermitePolyFxn = HermiteH[4, x];
Plot3D[{GramSchmidtFxn, HermitePolyFxn}, {x, -3, 3}, {y, -10, 10}, PlotLabel → "Gram Shmidt Vs. Hermite Polynomials", AxesLabel → {x, z, F[x]},
 PlotLegends → {"Hermite Polynomials", "Gram Schmidt"}]
```

Out[121]=



Hermite polynomials poorly approximate the Gram Schmidt process

Problem 3: Review

Procedure:

- Use the *Orthogonalize* function in mathematica to orthogonalize the polynomials given to us.
- Proceed to calculate the inner product.
- Use the *HermiteH* function to calculate the first 4 Hermite polynomials.
- Proceed to plot the inner product and Hermite polynomials against one another to see how they compare.

Key Concepts:

- We can use built in MATHEMATICA commands to do processes like the Gram Schmidt and write out the Hermite Polynomials.
- Hermite polynomials poorly approximate the Gram Schmidt process.

Variations:

- We could be given different functions or more polynomials.
  - We would use the same process but with different functions or polynomials.

Problem 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 Pg. 241 of the text.

(i)

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

```
In[147]:= ClearAll["Global`*"];
          fxn = Piecewise[{{-1, x < 0}, {0, x == 0}, {1, x > 0}}];
          an = 1/Pi * Integrate[fxn * Cos[n x], {x, -Pi, Pi}]
Out[149]= 0

In[150]:= bn = 1/Pi * Integrate[fxn*Sin[n x], {x, -Pi, Pi}]
Out[150]= -(2 (-1 + Cos[n π]))/(n π)
```

(ii)

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

You may do this by hand or by computer.

```
In[154]:= ClearAll["Global`*"];
          fxn = Abs[x] / (Pi);
          an = 1/Pi * Integrate[fxn * Cos[n x], {x, -Pi, Pi}]
Out[156]= (2 (-1 + Cos[n π] + n π Sin[n π]))/(n^2 π^2)

In[157]:= bn = 1/Pi * Integrate[fxn*Sin[n x], {x, -Pi, Pi}]
Out[157]= 0
```

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

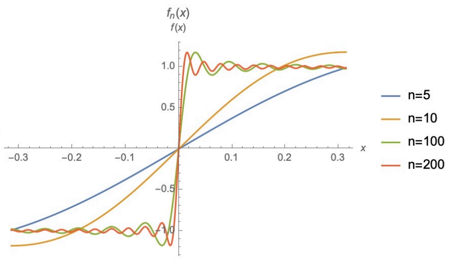
$$f_n(x) = \frac{a_0}{2} + \sum_{n=1}^{N} (a_n \cos(nx) + b_n \sin(nx))$$

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

Problem 4: Continued

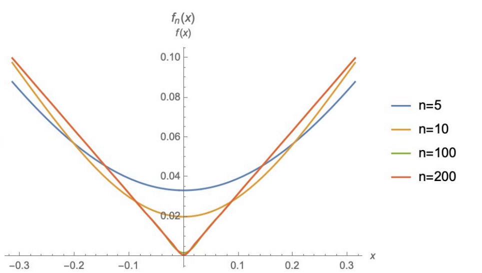
In[257]:=
```
ClearAll["Global`*"];
fxn = Piecewise[{{-1, x < 0}, {0, x == 0}, {1, x > 0}}];
a0 = 1/Pi * Integrate[fxn , {x, -Pi, Pi}];
an = 1/Pi * Integrate[fxn * Cos[n x], {x, -Pi, Pi}];
bn = 1/Pi * Integrate[fxn * Sin[n x], {x, -Pi, Pi}];
fxn5 = Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 5}]];
fxn10 = Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 10}]];
fxn100 = Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 100}]];
fxn200 = Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 200}]];
Plot[{fxn5, fxn10, fxn100, fxn200}, {x, -Pi / 10, Pi / 10}, PlotLabel → Subscript[f, n][x], AxesLabel → {x, f[x]}, PlotLegends → {"n=5", "n=10", "n=100", "n=200"}]
```

Out[266]=



In[247]:=
```
ClearAll["Global`*"];
fxn = Abs[x] / (Pi);
a0 = 1/Pi * Integrate[fxn , {x, -Pi, Pi}];
an = 1/Pi * Integrate[fxn * Cos[n x], {x, -Pi, Pi}];
bn = 1/Pi * Integrate[fxn * Sin[n x], {x, -Pi, Pi}];
fxn5 = a0/2 + Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 5}]];
fxn10 = a0/2 + Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 10}]];
fxn100 = a0/2 + Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 100}]];
fxn200 = a0/2 + Total[Table[an Cos[n x] + bn Sin[n x], {n, 1, 200}]];
Plot[{fxn5, fxn10, fxn100, fxn200}, {x, -Pi / 10, Pi / 10}, PlotLabel → Subscript[f, n][x], AxesLabel → {x, f[x]}, PlotLegends → {"n=5", "n=10", "n=100", "n=200"}]
```

Out[256]=



(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:

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

For functions that are discontinuous the Fourier series does not do a good job with reproducing functions. Since the above function is continuous we should expect the Fourier series to be a good reproduction.

Problem 4: Review

Procedure:

- Begin by calculating a_n and b_n with

$$a_n = \frac{1}{\pi}\int_{\pi}^{\pi} f(x)\cos(nx)\,dx \quad , \quad b_n = \frac{1}{\pi}\int_{\pi}^{\pi} f(x)\sin(nx)\,dx.$$

  Do the above for both both functions defined in (i) and (ii).

- Calculate the series with the function $f_n(x)$ definition.
- Calculate this series for the different values of N in MATHEMATICA.
- Define the functions in MATHEMATICA, calculate a_0, a_n, and b_n and then plot them on the same graph.

Key Concepts:

- We can calculate the Fourier coefficients by hand or with the use of MATHEMATICA.
- Fourier Series does not do a good job with reproducing functions that are continuous.

Variations:

- We can be given different functions to find the Fourier series and coefficients with.
  - This would result in doing the same process but with different functions.

Problem 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 $0 \leq x \leq 1$ with the boundary conditions:

$$y(0) = y(1) = 0$$
$$y''(0) = y''(1) = 0$$

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?

The interval in this problem is odd so even Functions (cosine), will not exist since the integral for these are zero.

(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.

$$y'(x) = a_n (n\pi)\cos(n\pi x) \ , \ y''(x) = -a_n (n\pi)^2 \sin(n\pi x)$$
$$y'''(x) = -a_n (n\pi)^3 \cos(n\pi x) \ , \ y''''(x) = a_n (n\pi)^4 \sin(n\pi x)$$

Inserting the above into the differential equation

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

The inner product is then

$$\langle \mathcal{L}y(x), a_m \sin(m\pi x)\rangle = \int_0^1 a_n \sin(n\pi x)\sin(m\pi x)\left((n\pi)^4 - \alpha(n\pi)^2 + \beta\right) dx \ , \ n = m \text{ or integral} = 0$$

Then we have

$$\langle \mathcal{L}y(x), a_m \sin(m\pi x)\rangle = \left((m\pi)^4 - \alpha(m\pi)^2 + \beta\right)\int_0^1 a_m \sin^2(m\pi x)\, dx = a_m\left((m\pi)^4 - \alpha(m\pi)^2 + \beta\right)\left(\frac{1}{2}\right)$$

we do this again

$$\langle \mathcal{L}y(x), a_m \sin(m\pi x)\rangle = \int_0^1 \sin(m\pi x)(x^2 - x)\, dx = \left(\frac{2\cos(m\pi) - 2}{(m\pi)^3}\right)$$

Equating both sides we have

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

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

Problem 5: Continued

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

The sine series is

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

This with part b.) is

$$\boxed{y(x) = \sum_{n=1}^{\infty} 4\left(\frac{\cos(n\pi) - 1}{(n\pi)^3\left((n\pi)^4 - \alpha(n\pi)^2 + \beta\right)}\right)\sin(n\pi x)}$$

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

The multiple of πx cannot be an integer value for this to have a solution.

For the values of α and β:

$$(n\pi)^4 - \alpha(n\pi)^2 + \beta = 0 \implies x^2 - \alpha x + \beta = 0 \quad \therefore \quad x = \frac{\alpha \pm \sqrt{\alpha^2 - 4\beta}}{2}$$

$$x + x = \frac{\alpha - \sqrt{\alpha^2 - 4\beta}}{2} + \frac{\alpha + \sqrt{\alpha^2 - 4\beta}}{2} = 2\alpha \quad \therefore \quad \alpha = x \quad \text{w/ } \alpha = (n\pi)^2$$

$$(n\pi)^2 = \frac{(n\pi)^2 \pm \sqrt{(n\pi)^4 - 4\beta}}{2} \quad \therefore \quad \beta = \frac{(n\pi)^4}{4}$$

We then say these values are

$$\boxed{\alpha = \frac{(n\pi)^2}{2}, \ \beta = \frac{(n\pi)^4}{4}}$$

Problem 5: Review

Procedure:

- Take the function for $y(x)$ and put it into the equation for $\mathcal{L}y(x)$.
- Proceed to take the inner product between $\mathcal{L}y(x)$ and $a_m \sin(m\pi x)$ and solve for a_m.
- Plug in this value for a_m into the equation for $y(x)$ for part (c).
- Solve for the values of α and β that make the denominator zero for a_m.

Key Concepts:

- This Fourier series only has sine terms because it is over an odd interval and that would result the even terms like cosine.
- There are values for α and β that produce a condition where a_m cannot exist.

Variations:

- We can be given a different differential equation $\mathcal{L}y(x)$.
  - This would result in a different answer for parts (b) through (d) but would use the same process.
- We can be given a different boundary condition.
  - This could in turn change the series for $y(x)$.

Problem 6:

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

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

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

we make the change:

$$s = x/\ell \ , \ E = E_0 \epsilon \ , \ \therefore \left\{ -\frac{\hbar^2}{2m\ell^2}\frac{\partial^2}{\partial s^2} - e\mathcal{E}s\ell \right\}\psi(s) = \epsilon E_0 \psi(s) \ , \ E_0 = \frac{\hbar^2}{2m\ell^2}$$

Simplify the equation

$$\left\{ -\frac{\partial^2}{\partial s^2} - \frac{2m\ell^3 e\mathcal{E}}{\hbar^2} s \right\}\psi(s) = \epsilon\psi(s) \ , \ w/ \ \delta = \frac{2m\ell^3 e\mathcal{E}}{\hbar^2}$$

we then have,

$$\boxed{\left\{ -\frac{\partial^2}{\partial s^2} - \delta s \right\}\psi(s) = \epsilon\psi(s)}$$

With a small perturbation this means there will be a small deviation from the original unperturbed solution.

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

The Schrödinger equation will go to

$$-\frac{\partial^2}{\partial s^2}\psi(s) = \epsilon\psi(s) \Rightarrow \psi(s) = A\cos(\sqrt{\epsilon}s) + B\sin(\sqrt{\epsilon}s)$$

If we apply the boundary conditions:

$$\psi(s) = B\sin(\sqrt{\epsilon}s)$$

If we normalize this we get

$$1 = \int_0^1 \psi^*(s)\psi(s)\, ds = \int_0^1 B^2\sin^2(\sqrt{\epsilon}s)\, ds \Big|_{\sqrt{\epsilon} = n\pi} = \int_0^1 B^2\sin^2(n\pi s)\, ds = \frac{B^2}{2} \quad \therefore \quad B = \sqrt{2}$$

$$\boxed{\psi(s) = \sqrt{2}\sin(n\pi s) \ , \ E_n = \frac{n^2\pi^2\hbar^2}{2m}}$$

Problem 6: Continued

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

```
In[126]:= ClearAll["Global`*"];
psi[n_, s_] = √2 * Sin[n Pi s];
FirstOrder = Refine[Integrate[psi[n, s] * δ s * psi[n, s], {s, 0, 1}], Element[n, Integers]]
Out[128]= δ/2
```

$$\boxed{E_n^{(1)} = \frac{\delta}{2}}$$

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

```
In[3]:= SecondOrder = N[Total[Table[If[m ≠ 1, (Integrate[√2 Sin[m Pi s] * δ s * √2 Sin[Pi s], {s, 0, 1}])^2 / (Pi^2 - m^2 Pi^2), 0], {m, 0, 10}]]]
Out[3]= -0.00109726 δ^2
```

$$\boxed{E_n^{(2)} = -0.00109726\ \delta^2}$$

Problem 6: Review

Procedure:

- Begin by making time-independent Schrödinger equation dimensionless.
- Solve the dimensionless time-independent Schrödinger equation and proceed to normalize it and solve for the eigenenergies.
- Use the first order correction formula for perturbation theory of functions for the groundstate energy

$$\lambda_1^1 = \langle \psi | \tilde{\mathbf{H}} | \psi \rangle \, .$$

- Proceed to calculate the second order correction using the second order perturbation theory of functions for the groundstate energy

$$\sum_{n \neq m}^{\infty} \frac{\langle \psi | \tilde{\mathbf{H}} | \psi \rangle}{E_n^2 - E_m^2} .$$

Key Concepts:

- We switch to dimensionless variables so that it is easy to tweak parameters within our system.
- We can evaluate an infinite sum in MATHEMATICA by finding out where the series converges to and only summing up to that value.

Variations:

- We can be given a different differential equation.
  - This would lead to a different dimensionless differential equation and potentially a different wave function.
- We can be given a different Hamiltonian.
  - This leading to different results for the perturbation.