Homework 2: Quantum Harmonic Oscillator
DUE: Friday, October 28, 2016 (actually at 3am on 10/29)

Continuing on the idea of the harmonic oscillator of Homework 1:

(b) Calculate the first five *normalized* eigenfunctions (ϕ_n) and eigenvalues (ε_n) using a direct method. Be sure to use a forward- and backward-differencing for the boundary conditions (HINT: $3 + 2\Delta x\sqrt{KL^2 - \varepsilon_n} \approx 3$). For this calculation, use $x \in [-L, L]$ with $L = 4$ and choose $xspan = -L : 0.1 : L$. Save the absolute value of the eigenfunctions in a 5-column matrix (column 1 is ϕ_1, column 2 is ϕ_2 etc.) and the eigenvalues in a 1x5 vector. NOTE: This procedure solves for the *interior* points. So be sure at the end to include your first and last point.

ANSWERS: Should be written out as A3.dat (eigenfunctions) and A4.dat (eigenvalues)

(c) There has been suggestions that in some cases, nonlinearity plays a role such that

$$\frac{d^2\phi_n}{dx^2} - \left[\gamma|\phi_n|^2 + Kx^2 - \varepsilon_n\right]\phi_n = 0. \tag{1}$$

Depending upon the sign of γ, the probability density is focused or defocused. Find the first two *normalized* modes for $\gamma = \pm 0.05$ using shooting. For this calculation, use $x \in [-L, L]$ with $L = 2$ and choose $xspan = -L : 0.1 : L$. Save the absolute value of the eigenfunctions in a 2-column matrix (column 1 is ϕ_1 and column 2 is ϕ_2) and the eigenvalues in a 1x2 vector.

ANSWERS: For $\gamma = 0.05$, should be written out as A5.dat (eigenfunctions) and A6.dat (eigenvalues)
ANSWERS: For $\gamma = -0.05$, should be written out as A7.dat (eigenfunctions) and A8.dat (eigenvalues)

(d) For strongly nonlinear eigenfunctions, use the **bvp4c** to calculate the first three modes. Use the same output as in (c). Be sure to normalize.

ANSWERS: For $\gamma = 10$, should be written out as A9.dat (eigenfunctions) and A10.dat (eigenvalues)
ANSWERS: For $\gamma = -10$, should be written out as A11.dat (eigenfunctions) and A12.dat (eigenvalues)

(e) For a fixed value of the energy (specifically, take $\varepsilon_n = 1$, $\gamma = 0$ with $x \in [-L, L]$ and $L = 2$. For initial launch conditions, take $\phi = 1$ and $\phi_x = \sqrt{KL^2 - 1}$), perform a convergence study of the shooting method by controlling the error tolerance, TOL, in ODE45 and ODE23:

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TOL=1e-4;   OPTIONS = odeset('RelTol',TOL,'AbsTol',TOL);
[T,Y] = ODE45('F',TSPAN,Y0,OPTIONS);
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Show that indeed the schemes are fourth order and second order respectively by running the computation accross the computational domain and adjusting the tolerance. Use specifically the following values of $TOL = [1e-4\ 1e-5\ 1e-6\ 1e-7\ 1e-8\ 1e-9\ 1e-10]$. In particular, plot on a log-log scale the average step-size (x-axis) using the *diff* and *mean* command versus the tolerance (y-axis) for the above tolerance values. What are the slopes of these lines? Use the POLYFIT command to get the slopes. Note that the local error should be $O(\Delta t^5)$ and $O(\Delta t^3)$ respectively. What are the local errors for ODE113 and ODE15s? Save the slopes computed from the POLYFIT command with the log-log of the data as a 4x1 vector with the slopes of ODE45, ODE23, ODE113 and ODE15s respectively.

ANSWERS: Should be written out as A13.dat

(f) Compare your solutions in both (a) and (b) of **homework 1** with the exact Gauss-Hermite polynomial solutions for this problem (See wikipedia.com, for instance). Compute the error between your numerical solution and the exact solution for the values of the eigenfunctions and eigenvalues computed above. Specifically, calculate the following quantity for each eigenfunction $\| |\phi_n^{numerical}| - |\phi_n^{exact}| \|$ where $\|f(x)\| = \int_{-L}^{L} f(x)^2 dx$. For the eigenvalues, simply calculate the relative percent error $100 \times (|\varepsilon_n^{numerical} - \varepsilon_n^{exact}|/\varepsilon_n^{exact})$. The error vectors associated with the eigenfunctions and eigenvalues should be 5x1 vectors.

ANSWERS: For part (a), should be written out as A14.dat (eigenfunctions) and A15.dat (eigenvalues)
ANSWERS: For part (b), should be written out as A16.dat (eigenfunctions) and A17.dat (eigenvalues)

NOTE: For the tolerances in both the convergence (shooting method) of the ε_n in (a) and (c), and in the area for part (c), use a tolerance of 10^{-4}. As a final remark, my code takes 70 seconds.