

QUANTUM MECHANICS I

PHYS 516

Problem Set # 2

Distributed: Jan. 15, 2016

Due: January 22, 2016

1. Harmonic Oscillator 1: Plot the harmonic oscillator wavefunctions for the ground state $\psi_0(x)$ and the five lowest excited states $\psi_i(x)$, $i = 1 - 5$.

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!} \sqrt{\pi}} H_n(x) e^{-x^2/2}$$

where $H_n(x)$ are the classical Hermite polynomials with standard normalization: $H_n(x) = (2x)^n +$ terms of lower degree.

Solution: The harmonic oscillator wavefunctions were constructed by sweeping x from -5 to $+5$ in small steps ($dx = 0.01$), defining $\psi_0(x) = e^{-x^2/2} / \sqrt{\pi}$, and then using the recursion relation

$$\psi_{k+1}(x) = \sqrt{\frac{2}{k+1}} x \psi_k(x) - \sqrt{\frac{k}{k+1}} \psi_{k-1}(x)$$

and initializing with " $\psi_{-1}(x) = 0$ ". The recursion relation can be obtained from the differential and recursion relations for the Hermite polynomials (next problem set, Problem #4). The results are shown as the broad grey curves in Fig. 1.

2. Harmonic Oscillator 2: Solve the equation $-\frac{1}{2} \frac{d^2 \psi}{dx^2} + \frac{1}{2} x^2 \psi = E \psi$ (obtained by setting $m = k = \hbar = 1$ in the Schrödinger equation) numerically by discretizing along the line using a step size Δ and extending the part of the line that is discretized from $-a$ to $+a$. Play around with the parameters

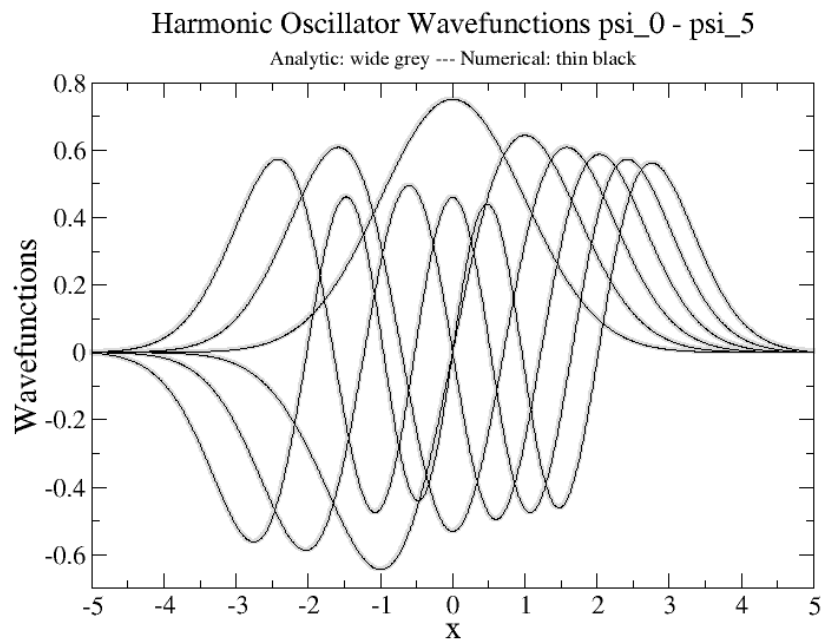


Figure 1: The ground state harmonic oscillator wavefunction $\psi_0(x)$ and first five excited states $\psi_i(x)$ are plotted. The analytically computed functions are shown by thick grey curves and the numerically computed wavefunctions are shown (superposed) by thin black curves.

Δ and a until you find reasonable values. Describe your frustration as you iterate to ‘reasonable values’. What values are you using? Then plot the ground state (no zero crossings) and the five lowest excited states and brag that you’ve done an analytically solvable problem numerically.

Solution: The interval $[-5, +5]$ was discretized with step size $dx = 0.01$, requiring $10/0.01 + 1 = 1001$ points. The x values and indices $i = 1 \cdots 1001$ are related $x = (i - 501)/100.0$. A tridiagonal matrix was created with $\frac{1}{2} \frac{2}{dx^2}$ along the diagonal and $-\frac{1}{2} \frac{1}{dx^2}$ along the sub/super diagonals. In addition, $\frac{1}{2}x^2$ was added along the diagonal. The diagonal was presented in a 1001 length column vector d and the off-diagonals presented in an array e (*Numerical Recipes* notation) and these arrays loaded into subroutines tqli and eigprt from same. The eigenvectors with the lowest six eigenvalues are plotted in Fig. 1 using the narrow black lines. Postprocessing of the numerical eigenvectors was done by multiplying by $\sigma(i)/\sqrt{dx}$, where $\sigma(i)$ is the sign of the 750th component of the i^{th} eigenvector (phase adjustment) and multiplying by a normalization coefficient (Problem 3). The lowest eigenvalues for this choice of parameters is: 0.499997, 1.499984, 2.499960, 3.499923, 4.499884.

3. Normalization Problem: If you look at the vertical scales on the plots of Problems 1 and 2, they are different. How do you reconcile this difference. Be quantitative.

Solution: The analytic and numerical eigenfunctions are scaled differently, so set $N\psi_{\text{num}}(x) = \psi(x)_{\text{anal}}$, where N is some normalization coefficient. Analytic and numerical integrations are done on the left and right:

$$\int_{-\infty}^{+\infty} |\psi_{\text{anal}}(x)|^2 = 1 \quad \sum_i |N\psi_{\text{num}}(i)|^2 \Delta = 1$$

Every sensible matrix eigenvalue routine outputs eigenvectors normalized to 1:

$$\sum_i |N\psi_{\text{num}}(i)|^2 \Delta = N^2 \Delta \sum_i |\psi_{\text{num}}(i)|^2 = N^2 \Delta = 1$$

As a result $N = 1/\sqrt{\Delta}$.

4. Plot $|\psi_{10}(x)|^2$ and compare with the plot by Dicke and Wittke in the handout.

Solution: The analytic computation of Problem 1 was extended to $\psi_{10}(x)$ and its square was plotted (Fig. 2).

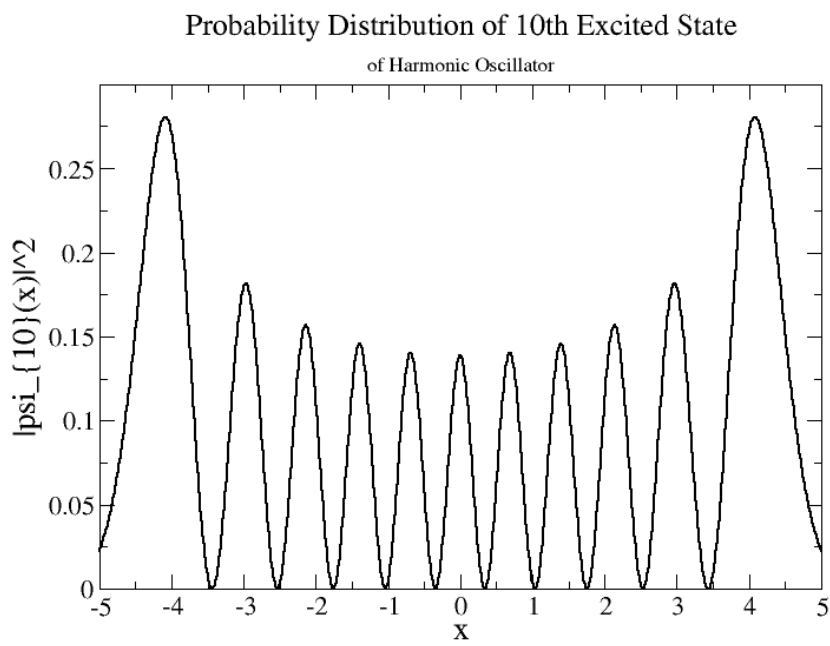


Figure 2: $|\psi_{10}(x)|^2$, where the wavefunction is constructed analytically.

5. Diatomic Molecules: Schrödinger derives an approximation to the spectrum of a diatomic molecule:

$$E_i \simeq \frac{l(l+1)\hbar^2}{2I_0} \left(1 - \frac{\epsilon}{1+3\epsilon}\right) + \left(n + \frac{1}{2}\right)\hbar\omega_0\sqrt{1+3\epsilon} \quad \epsilon = \frac{l(l+1)\hbar^2}{(I_0\omega_0)^2}$$

This occurs as Eq. (51) in his second paper. I have made the following modifications in his equations. (1) Interchanged $n \leftrightarrow l$, where n is now the harmonic oscillator quantum number and l is the orbital angular momentum quantum number, (2) $h \rightarrow \hbar$, $\nu_0 \rightarrow \omega_0$, (3) $\mu r_0^2 = A \rightarrow I_0$.

Carry out a Taylor series expansion of this energy expression in powers of ϵ (!! Please use Maple or other !!) and express the result in powers of $(n + \frac{1}{2})$ and $l(l+1)$:

$$E_i \simeq \sum_{p,q} D_{p,q} \left(n + \frac{1}{2}\right)^p [l(l+1)]^q$$

Solution: All the terms arising from the left hand term in the energy expression have $p = 1$ while those from the right hand term have $p = 1$. We carry out a Taylor series in ϵ on the left and right hand terms separately:

q	$p = 0$	$p = 1$
0		$(n + \frac{1}{2})\hbar\omega_0$
1	$\frac{1}{2}I_0\omega^2$	$\frac{3}{2}(n + \frac{1}{2})\hbar\omega_0$
2	$-\frac{1}{2}I_0\omega^2$	$-\frac{9}{8}(n + \frac{1}{2})\hbar\omega_0$
3	$3\frac{1}{2}I_0\omega^2$	$\frac{27}{16}(n + \frac{1}{2})\hbar\omega_0$
4	$-9\frac{1}{2}I_0\omega^2$	$-\frac{405}{128}(n + \frac{1}{2})\hbar\omega_0$
5	$27\frac{1}{2}I_0\omega^2$	$\frac{1701}{256}(n + \frac{1}{2})\hbar\omega_0$

Beware of Numerical Computations

Whenever you do a numerical computation you should turn yourself inside-out to feel comfortable that your results are believable. In the context of the current set of computations, this includes looking at the energies and eigenfunctions that are analytically available. The lower energies are just fine. A plot of energies up to $n = 50$ is given in Fig. 3. This shows there is a problem starting about $n = 10$. Another thing to do is look at the

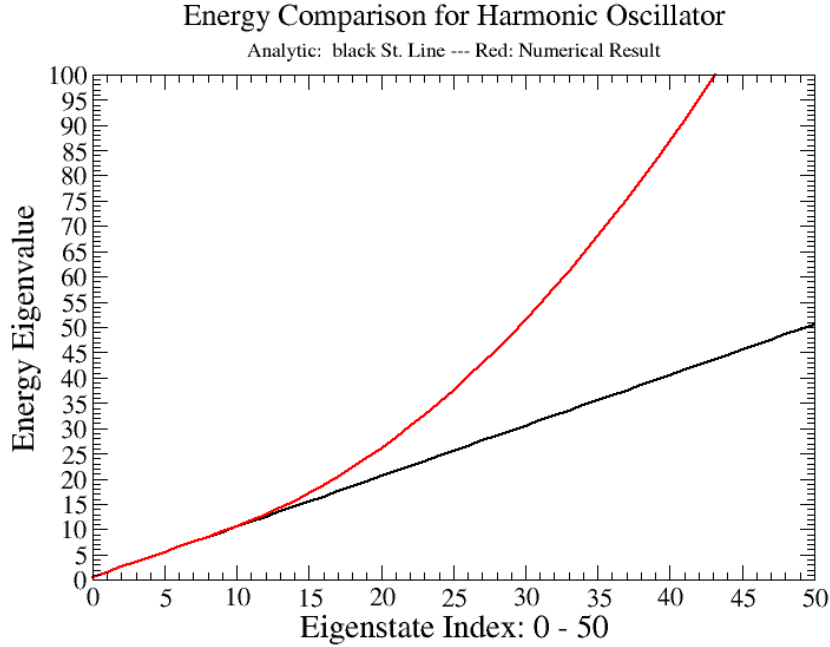


Figure 3: Energies of the lowest fifty eigenstates of the harmonic oscillator, computed analytically (red) and numerically (black).

wavefunctions to see if they vanish approaching the boundaries of the finite interval that was discretized. Starting at $n = 10$ you can see the beginnings of this problem: the values $\psi(\pm 5)$ start to pull away from zero.

A global picture of the disparity between the analytic and numerical values of the energy is shown in Fig. 4. Here there is a big disparity! Numerically, this is forced by the problem that the trace of the analytically constructed hamiltonian is $\sum(i + 1/2) \simeq 0.5 \times 10^6$ while the trace of the numerically constructed matrix $KE + PE$ is larger by about two orders of magnitude.

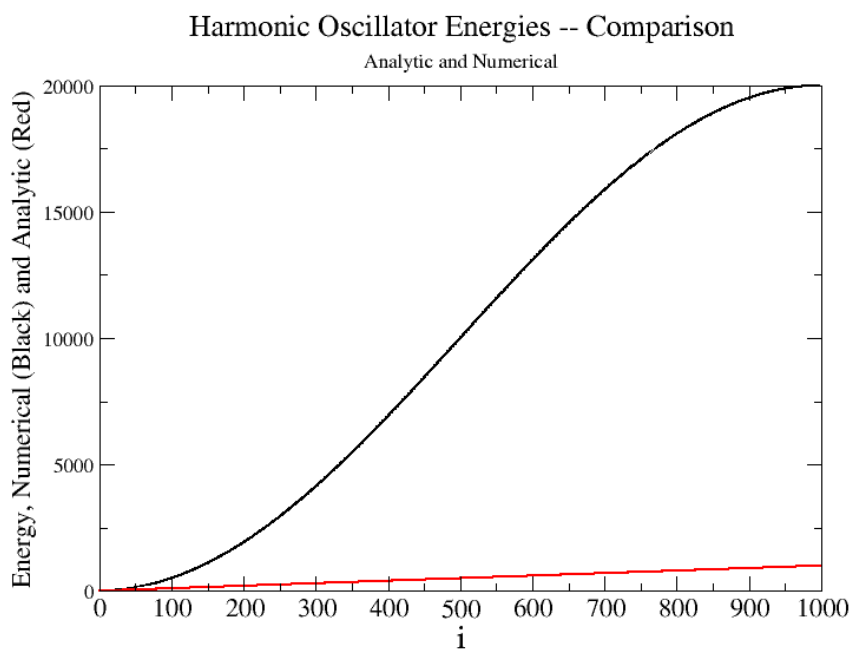


Figure 4: Energies of all the eigenstates of the harmonic oscillator, computed analytically (red) and numerically (black).