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Abstract

1 Problem 1

We solve the harmonic oscillator by writing down the classical Hamiltonian, replacing the momentum by $\frac{\hbar}{i}\frac{d}{dx}$, and solving. The classical Hamiltonian is:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \tag{1.1}$$

Replacing p with $\frac{\hbar}{i}\frac{d}{dx}$:

$$\{\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\}\Psi = E\Psi \tag{1.2}$$

$$\frac{d^2\Psi}{dx^2} - \frac{mkx^2}{\hbar^2}\Psi + \frac{2mE}{\hbar^2}\Psi = 0 \tag{1.3}$$

We now make a transformation $x = \gamma z$ into dimensionless coordinates.

$$\frac{1}{\gamma^2}\frac{d^2\Psi}{dz^2} - \frac{mk}{\hbar^2}\gamma^2 z^2\Psi + \frac{2mE}{\hbar^2}\Psi = 0 \tag{1.4}$$

$$\frac{d^2\Psi}{dz^2} - \frac{mk}{\hbar^2}\gamma^4 z^2\Psi + \frac{2mE}{\hbar^2}\gamma^2\Psi = 0 \tag{1.5}$$

$$\tag{1.6}$$

Table 22.6 of A&S has the solution for this general form, with the coefficient of the z term $2n+1-x^2$. The solutions are $e^{\frac{-x^2}{2}}H_n(x)$ with $H_n(x)$ the Hermite polynomials. Solving for the dimensionless parameter γ we find:

$$\frac{mk}{\hbar^2}\gamma^4 = 1 \tag{1.7}$$

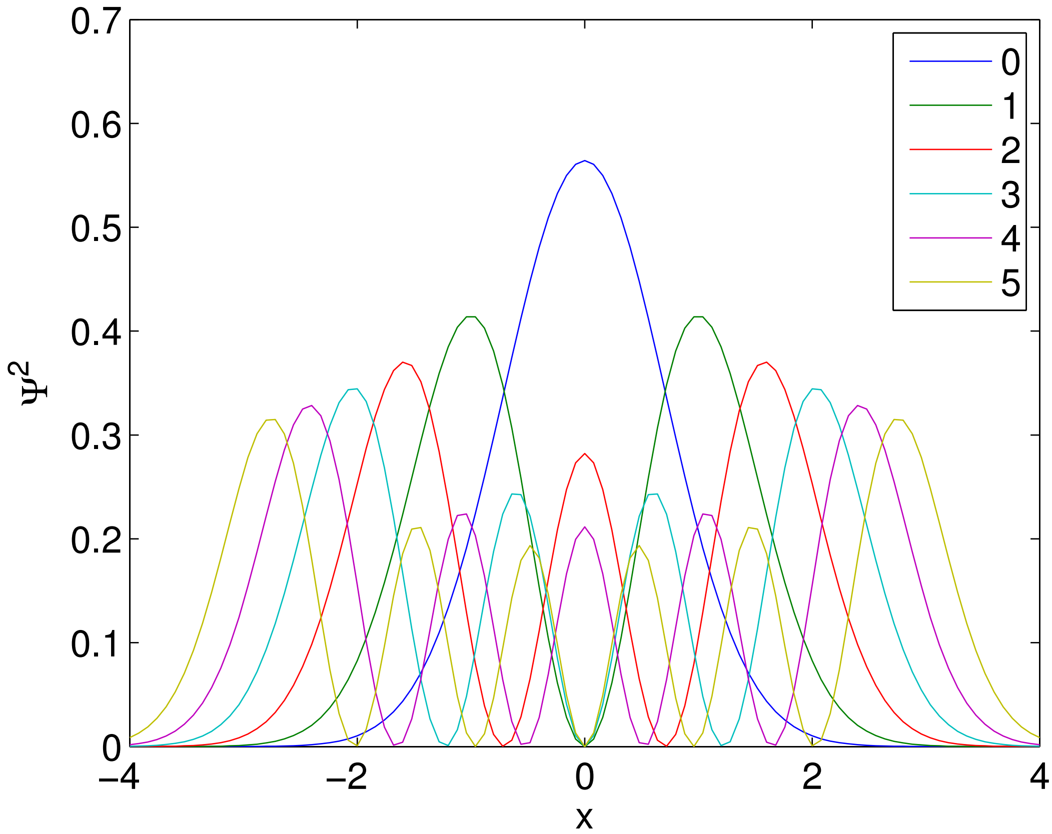
$$\gamma^2 = \frac{\hbar}{\sqrt{mk}} \tag{1.8}$$

$$\frac{2mE}{\hbar^2}\gamma^2 = 2n+1 \tag{1.9}$$

$$E = \frac{\hbar^2}{2m}\frac{\sqrt{mk}}{\hbar}(2n+1) = \hbar\sqrt{\frac{k}{m}}(n+\frac{1}{2}) \tag{1.10}$$

We incorporate the normalization constant (from A&S) to complete the expression for the wavefunctions, then plot the square of the first 6 wavefunctions.

$$\Psi(x)_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) \tag{1.11}$$



2 Problem 2

We now solve the quantum harmonic oscillator using a numerical method. We'll set $\hbar = k = m = 1$ to simplify the expressions. We approximate the second derivative as:

$$\frac{d^2}{dx^2} = \frac{x_{i+1} - 2x_i + x_{i-1}}{\Delta^2} \tag{2.1}$$

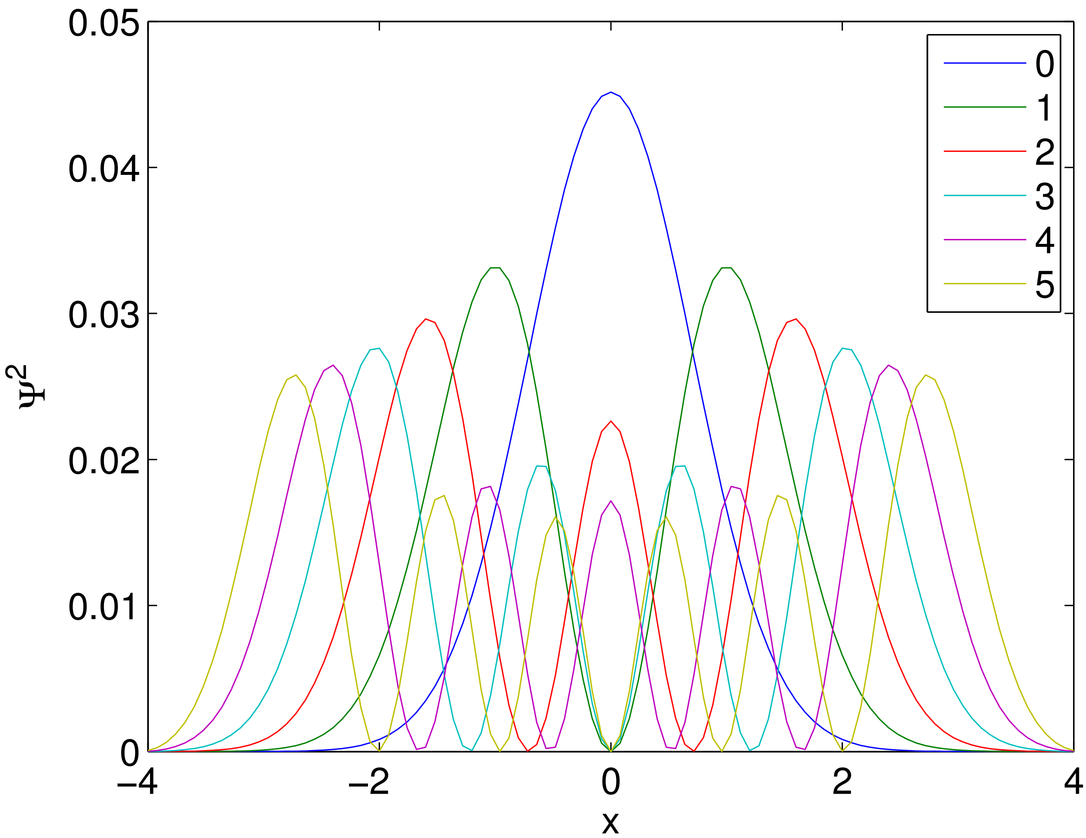
As a matrix operator this can be written:

$$\begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -2 \end{pmatrix} \tag{2.2}$$

The potential energy is simply the diagonal matrix with x_i^2's on the diagonal, multiplied by $\frac{1}{2}$. We can now write the Schrodinger equation in a matrix form:

$$(K_e + P_e)\Psi = E\Psi \tag{2.3}$$

With Ψ a column vector. This is clearly in the form of an eigenvalue problem, which we solve using MATLAB. The 6 lowest eigenvalues are (to within .01) 0.5, 1.5, 2.5, 3.5, 4.5 and 5.5 in close agreement with the analytical energy levels $n+\frac{1}{2}$ (ignoring the scaling factor). Increasing the number of lattice sites from 101 to 1001 improves the agreement to .001. We plot the eigenvectors corresponding to the 6 lowest eigenvalues.



3 Problem 3

We now solve the harmonic oscillator using a variational principle on the quadratic form of the Schrodinger equation. Again setting $\hbar = k = m = 1$, we have:

$$J = \int (\frac{d\Psi}{dx})^2 + \frac{1}{2}x^2\Psi^2 dx \tag{3.1}$$

We apply a normalization constraint to avoid the trivial solution $\Psi = 0$, and incorporate the constraint via Lagrange multipler.

$$\int \Psi^2 dx = 1 \tag{3.2}$$

$$J = \int (\frac{d\Psi}{dx})^2 + \frac{1}{2}x^2\Psi^2 dx = E \int \Psi^2 dx \tag{3.3}$$

We decompose Ψ into a sum of localized basis functions $\Psi_i = c_i e^{\frac{-(x-x_i)^2}{2\sigma^2}}$. We now need to calculate the integrals of $(\frac{d\Psi}{dx})^2$, $x^2\Psi^2$, and Ψ^2. We write Ψ^2 in this basis as:

$$\sum_i \sum_j c_i c_j e^{\frac{-(x-x_i)^2}{2\sigma^2}} e^{\frac{-(x-x_j)^2}{2\sigma^2}} \tag{3.4}$$

$$\sum_i \sum_j c_i c_j e^{\frac{-(x-x_i)^2-(x-x_j)^2}{\sigma^2}} \tag{3.5}$$

The integral of the exponential term from x=-4 to 4 is (according to Wolfram Alpha):

$$\frac{\sqrt{\pi}}{2}\sigma e^{\frac{-(i-j)^2}{4}}\{erf(\frac{x_i + x_j + 8}{2\sigma}) - erf(\frac{x_i + x_j - 8}{2\sigma})\} \tag{3.6}$$

Where we have set $\sigma = \Delta x$. For reasonably small values of σ the error function becomes a step function at 0, and the right hand term becomes 2 for all values of i and j. The exponential will suppress all terms where $|i - j|$ is not small. We cut off all terms with $|i - j| < 6$, so the next term is less then $\frac{1}{1000}$.

$$\int \sum_i \sum_j c_i c_j e^{\frac{-(x-x_i)^2-(x-x_j)^2}{\sigma^2}} = \sum_i \sum_{j=i-5}^{i+5} c_i c_j \sqrt{\pi}\sigma e^{\frac{-(i-j)^2}{4}} \tag{3.7}$$

For the potential term we need to caclulate the integral of $x^2\Psi^2$. This integral is not calculated by Wolfram Alpha, so we use the solution provided in class.

$$\int \sum_i \sum_j c_i c_j \frac{1}{2}x^2 e^{\frac{-(x-x_i)^2-(x-x_j)^2}{\sigma^2}} = \sum_i \sum_{j=i-5}^{i+5} c_i c_j \frac{\sqrt{\pi}}{2}\sigma e^{\frac{-(i-j)^2}{4}}\{(\frac{x_i + x_j}{2})^2 + \frac{1}{2}\sigma^2\} \tag{3.8}$$

We find the derivative of Ψ analytically, then calculate the integral of $(\nabla\Psi)^2$ using the previous integrals.

$$\nabla\Psi = \sum_i c_i \frac{d}{dx} e^{\frac{-(x-x_i)^2}{2\sigma^2}} \tag{3.9}$$

$$\nabla\Psi = \sum_i c_i \frac{-(x-x_i)}{\sigma^2} e^{\frac{-(x-x_i)^2}{2\sigma^2}} \tag{3.10}$$

$$\int(\nabla\Psi)^2 = \int \sum_i \sum_j c_i c_j \frac{x-x_i}{\sigma^2}\frac{x-x_j}{\sigma^2} e^{\frac{-(x-x_i)^2}{2\sigma^2}} e^{\frac{-(x-x_j)^2}{2\sigma^2}} \tag{3.11}$$

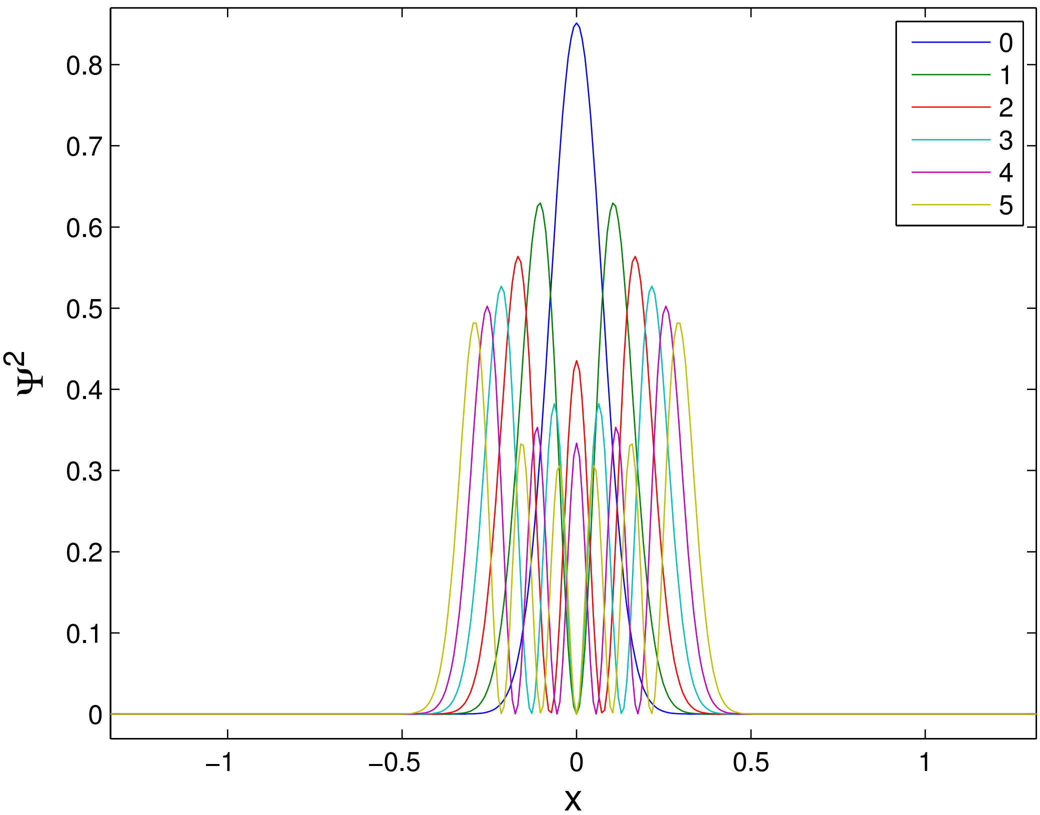
$$= \int \sum_i \sum_j c_i c_j \frac{1}{\sigma^2}(x^2 - xx_i - xx_j + x_i x_j) e^{\frac{-(x-x_i)^2}{2\sigma^2}} e^{\frac{-(x-x_j)^2}{2\sigma^2}} \tag{3.12}$$

$$= \sum_i \sum_j \frac{\sqrt{\pi}}{\sigma} e^{\frac{(i-j)^2}{4}} \{(\frac{x_i+x_j}{2})^2 + \frac{1}{2}\sigma^2 - (x_i+x_j)\frac{x_i+x_j}{2} + x_i x_j\} c_i c_j \tag{3.13}$$

$$= \sum_i \sum_j \frac{\sqrt{\pi}}{\sigma} e^{\frac{(i-j)^2}{4}} \{-\frac{(x_i+x_j)^2}{4} + \frac{1}{2}\sigma^2 + x_i x_j\} c_i c_j \tag{3.14}$$

$$= \sum_i \sum_{j=i-5}^{i+5} \frac{\sqrt{\pi}}{\sigma} e^{\frac{(i-j)^2}{4}} \{-\frac{(x_i+x_j)^2}{4} + \frac{1}{2}\sigma^2 + x_i x_j\} c_i c_j \tag{3.15}$$

Where we again only evaluate integrals for $|i-j| < 6$. We can now make a quadratic form from 3.7, 3.8 and 3.15 in the c's and set up the variational problem in matrix form. We plot the first 6 eigenvectors, using 1001 pts to help resolve the shapes.



These appear to have the right form, but scaled to the interval [-0.5:0.5].