The one-dimensional, time-independent Schrödinger's equation for the wave function $\psi(x)$ of a single particle of mass m in a potential $V(x)$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{1}$$

where E is the total energy. Depending on the shape of the potential, there may be bound states only, scattering states only, or both. In this assignment, we will investigate potentials for which there are bound states. When coupled with appropriate boundary conditions, Schrödinger's equation is an eigensystem in which bound states exist only at discrete eigenenergies. Computationally, we will represent the continuous wavefunction as a column vector of values at discrete points: $\psi(x_j) = \psi_j$, for $j = 0, 1, ..., N$. In practice, we specify boundary values for $\psi_0 = \psi_N = 0$, which implies that we are taking the potential at the boundaries to be infinite: $V_0 = V_N \to \infty$. In other words, we are embedding our potential inside an infinite square well. We do not explicitly include equations for the boundaries in our matrix problem. Linear differential operators that operate on the wavefunction become matrices. Using second-order central difference yields a tridiagonal matrix for the second derivative. Scalar multiplication by a known function yields a diagonal matrix with the values of the scalar at the discrete points down the diagonal. Thus:

$$\psi(x) \longrightarrow \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-2} \\ \psi_{N-1} \end{bmatrix}, \quad \frac{d^2}{dx^2} \longrightarrow \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & -2 \end{bmatrix}, \quad V(x) \longrightarrow \begin{bmatrix} V_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & V_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & V_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & V_{N-2} & 0 \\ 0 & 0 & 0 & \cdots & 0 & V_{N-1} \end{bmatrix}. \tag{2}$$

The Schrödinger's equation can then be written in matrix form:

$$\mathbf{H}\,|\psi\rangle = \lambda\,|\psi\rangle\,. \tag{3}$$

Exploration #1: Consider an infinite square well of width a. Let's choose a set of "natural" units for the problem and nondimensionalize Schrödinger's equation. Let's measure length in units of a and energy in units of $\hbar^2/(2ma^2)$. In these units, the eigenenergies should be $\tilde{E}_n = \pi^2 n^2$. Compute eigenvalues and eigenvectors. You should increase N until the $n = 8$ eigenenergy does not change at the 4th significant figure. Graph the first 8 eigenmodes. Also graph a few spurious modes. What do you notice about them that allows you to infer that they are probably not physical?

Exploration #2: Let's perturb the square well with a Gaussian perturbation: $\tilde{V}'(\tilde{x}) = \tilde{V}_0 \exp(-256\tilde{x}^2)$. First, choose $\tilde{V}_0$ to be 10% of the ground state energy. Compute the energy shifts for the first 8 modes. Next, choose the perturbation energy to be equal to the ground state energy. Again, compute the energy shifts for the first 8 modes. Graph the first 4 eigenfunctions for these perturbed potentials.

Recall from time-independent perturbation theory, the first order correction to the eigenenergies is given by:

$$E_n^{(1)} = \langle\psi_n^{(0)}|\,V'\,|\psi_n^{(0)}\rangle\,, \tag{4}$$

where V' is the perturbation potential. This is an integral, which you will need to compute numerically (say, with the trapezoidal rule). Compute the energy shifts using perturbation theory and see how they compare to the directly computed eigenenergies.

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Exploration #3: Consider the case of the quantum harmonic oscillator: $V(x) = m\omega_0^2 x^2/2$. We will embed this potential inside our infinite square well. In computational units, the potential is: $\tilde{V}(\tilde{x}) = (m^2\omega_0^2 a^4/\hbar^2)\tilde{x}^2$. You should verify that the coefficient in front of $\tilde{x}^2$ is dimensionless. We have to pick a natural frequency for our oscillator. We know that the classical turning points move outward as the energy increases. We do not want our eigenmodes to be affected by the infinite potential at the boundaries, so let's choose a sufficiently stiff oscillator such that, say, the classical turning points for the n^{th} eigenmode are located at $|x_C| = \alpha a$ (where $\alpha < 1$). Show that: $m^2\omega_0^2 a^4/\hbar^2 = (2n+1)^2/\alpha^4$. Let's choose $n = 12$ and $\alpha = 0.10$. Compute the first 8 eigenvalues and eigenvectors. Graph a few select eigenvectors and compare to exact eigenvectors (recall that the wave functions are Gaussian functions times Hermite polynomials; consult your favorite quantum mechanics textbook).

Exploration #4: Let's perturb the harmonic osciillator with a Gaussian perturbation: $\tilde{V}'(\tilde{x}) = \tilde{V}_0 \exp(-256\tilde{x}^2)$. First, choose $\tilde{V}_0$ to be 10% of the ground state energy. Compute the energy shifts for the first 8 modes. Next, choose the perturbation energy to be equal to the ground state energy. Again, compute the energy shifts for the first 8 modes. Graph the new ground state and first excited state eigenfunctions for these perturbations.

Recall from time-independent perturbation theory, the first order correction to the eigenenergies is given by:

$$E_n^{(1)} = \langle \psi_n^{(0)} | \, V' \, | \psi_n^{(0)} \rangle \,, \tag{5}$$

where V' is the perturbation potential. This is an integral, which you will need to compute numerically (say, with the trapezoidal rule). Compute the energy shifts using perturbation theory and see how they compare to the directly computed eigenenergies.