PHYS 581 Assignment 4

90 points total

Due Friday, March 14 (date flexible)

Instructions: All problems should be worked out in Mathematica, except for Question 1!

The one-dimensional time-dependent Schrödinger equation for a harmonic oscillator can be written as

$$-i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2}\right)\psi(x,t) \equiv \hat{H}\psi(x,t), \tag{1}$$

where m is the mass of the particle, ω is the natural frequency of the oscillator, $\hbar = h/2\pi$ is the modified Planck's constant, $\psi_n(x)$ are the associated wavefunctions (eigenstates), and $\hat{H}$ is the Hamiltonian (or Schrödinger operator). All of the eigenstates are subject to the boundary conditions $\psi(x) \to 0,\ \ x \to \pm\infty$. In the time-independent case, the Schrödinger equation reduces to

$$\hat{H}\psi_n(x) = E_n\psi_n(x). \tag{2}$$

1. (10 points) It isn't convenient to solve equations on a computer when there are units. To render Eqs. (1) and (2) dimensionless, it is convenient to introduce appropriate scaling factors d, τ, and ϵ to express units of length ($x = \tilde{x}d$), time ($t = \tilde{t}\tau$), and energy ($E_n = \tilde{E}_n\epsilon$), respectively, where the tilde-variables are dimensionless. Using these substitutions in Eq. (1) to render all terms dimensionless (including $\psi(x)$), obtain explicit expressions for d, τ, and ϵ in terms of the parameters $\hbar$, m, and ω.

2. (15 points) As discussed in the notes, a convenient basis for this equation are the Hermite polynomials $H_n(\tilde{x})$ (where $\tilde{x}$ is now explicitly dimensionless). As we saw in Assignment 3, the normalization factors get very large for $n \gg 1$, which is inconvenient. Instead, consider the modified Hermite polynomials $\tilde{H}(\tilde{x})$, defined by the recurrence relation
$$\tilde{x}\tilde{H}_n(\tilde{x}) = \sqrt{\frac{n+1}{2}}\tilde{H}_{n+1}(\tilde{x}) + \sqrt{\frac{n}{2}}\tilde{H}_{n-1}(\tilde{x}).$$
Use the Golub-Welsch (matrix) algorithm to obtain the Gaussian quadrature roots and weights of these modified Hermite polynomials for $N = 51$. What are the normalization factors h_n, $n = 0, \ldots, 50$, assuming the weight function is the same as for normal Hermite polynomials $w(\tilde{x}) = e^{-\tilde{x}^2}$?

3. (20 points) Work out the rule for the first derivative of the modified Hermite polynomials, i.e. an expression of the form
$$\frac{d}{d\tilde{x}}\tilde{H}_n(\tilde{x}) = f\left[\tilde{H}_{n-1}(\tilde{x}), \tilde{H}_n(\tilde{x})\right].$$
Using this and the recurrence relation in Question (2), obtain the simplest expression for
$$\frac{d^2}{d\tilde{x}^2}\left[\sqrt{w(\tilde{x})}\tilde{H}_n(\tilde{x})\right] = \frac{d^2}{d\tilde{x}^2}\left[e^{-\tilde{x}^2/2}\tilde{H}_n(\tilde{x})\right].$$

4. (20 points) Assume that the solutions are expressed as a superposition of modified Hermite polynomials as follows:
$$\psi_n(\tilde{x}) = \sqrt{w(\tilde{x})}\sum_m d_m^{(n)}\tilde{H}_m(\tilde{x}).$$
Obtain the $N \times N$ matrix $\hat{D}$ corresponding to the Hamiltonian / Schrödinger operator $\hat{H}$ for $N = 51$; see Eq. (1.62) in the notes. Calculate numerically the eigenvalues and eigenvectors by diagonalizing this matrix. List all the (dimensionless) eigenvalues $\tilde{E}_n$ and plot the eigenstates $\psi_n(\tilde{x})$ for the smallest few eigenvalues (in magnitude). Comment on the results.

5. (20 points) Now assume that the solutions are expressed as a superposition of DVR (Lagrange basis) functions as follows:
$$\psi_n(\tilde{x}) = \sum_j d_j^{(n)} \tilde{\ell}_j(\tilde{x}),$$
where
$$\tilde{\ell}_j(\tilde{x}) = \sqrt{w_j w(\tilde{x})} \sum_m \tilde{H}_m(\tilde{x}_j) \tilde{H}_m(\tilde{x});$$
see Eqs. (1.138) and (1.141) in the notes. Obtain the $N \times N$ matrix $\hat{D}$ corresponding to the Hamiltonian / Schrödinger operator $\hat{H}$ for $N = 51$; see Eq. (1.142) in the notes. Check that the term proportional to $\tilde{x}^2$ is diagonal. Calculate numerically the eigenvalues and eigenvectors by diagonalizing this matrix. List all eigenvalues $\tilde{E}_n$ in ascending order and plot the eigenstates $\psi_n(\tilde{x})$ for the lowest few eigenvalues. Comment on the results, and compare with the results obtained in Question (4) above.

6. (5 points) The results above are probably not that great for a good reason: the roots and weights have been calculated with too low a precision. If you ask Mathematica to increase the precision (by setting the WorkingPrecision parameter) do things improve?