PHYS 581: Assignment #4

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- Vivek and I initially started the assignment working seperately, and ended it working together. Therefore, we decided to each submit our workbooks individually, however our code will be nearly the exact same for questions 4 and 5.

Question 1 (10 points)

We start with the following wave function:

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

We'll introduce dimensionless variables via the following equivalences:

$$x = d\tilde{x}, \qquad t = \tau\tilde{t}, \qquad E_n = \epsilon\tilde{E_n}$$

We also will rescale the wave function with the following:

$$\frac{\partial}{\partial x} = \frac{1}{d}\frac{\partial}{\partial\tilde{x}}, \qquad \frac{\partial^2}{\partial x^2} = \frac{1}{d^2}\frac{\partial^2}{\partial\tilde{x}^2}, \qquad \frac{\partial}{\partial t} = \frac{1}{\tau}\frac{\partial}{\partial\tilde{t}}$$

And if we substitute these, the wave function becomes:

$$-i\frac{\hbar}{\tau}\frac{\partial}{\partial\tilde{t}}\psi(x,t) = \left[-\frac{\hbar^2}{2md^2}\frac{\partial^2}{\partial\tilde{x}^2} + \frac{1}{2}m\omega^2 d^2\tilde{x}^2\right]\psi(x,t)$$

A good scaling occurs when the two terms on the right have the same overall factor. Thus, we need to choose a value for "d" so that:

$$\frac{\hbar^2}{2md^2} = \frac{1}{2}m\omega^2 d^2$$

If we solve this:

$$\hbar^2 = m^2\omega^2 d^4 \quad\Longrightarrow\quad d^2 = \frac{\hbar}{m\omega} \quad\Longrightarrow\quad d = \sqrt{\frac{\hbar}{m\omega}}$$

Then both the kinetic and potential energy terms become:

$$\frac{\hbar\omega}{2}\left[-\frac{\partial^2}{\partial\tilde{x}^2}+\tilde{x}^2\right]$$

Now to remove the whole factor, we need to divide the whole equation by $\hbar\omega/2$. Once we do this the left hand side becomes:

$$-i\frac{\hbar}{\tau}\frac{\partial}{\partial\tilde{t}}\psi(x,t) \quad\Longrightarrow\quad -i\frac{2}{\tau\omega}\frac{\partial}{\partial\tilde{t}}\psi(x,t)$$

Therefore, to get a dimensionless equation, we choose:

$$\tau=\frac{1}{\omega}, \qquad \epsilon=\hbar\omega$$

And the dimensionless Shrödinger equation for a harmonic oscillator becomes:

$$-i\frac{\partial}{\partial\tilde{t}}\psi(x,t)=\frac{1}{2}\left[-\frac{\partial^2}{\partial\tilde{x}^2}+\tilde{x}^2\right]\psi(x,t)\equiv\tilde{E}_n\epsilon\;\psi(\tilde{x},\tilde{t})$$

Question 2 (15 points)

Unlike in the previous assignment, we are analyzing a modified version of Hermite polynomials, denoted as $\tilde{H}_n(\tilde{x})$ and defined by the following recurrence relation:

$$\tilde{x}\tilde{H}_n(\tilde{x}) = \sqrt{\frac{n+1}{2}}\tilde{H}_{n+1}(\tilde{x}) + \sqrt{\frac{n}{2}}\tilde{H}_{n-1}(\tilde{x})$$

To construct a Jacobi matrix, we must match the three-term recurrence relation exactly:

$$xP_n(x) = a_nP_{n+1}(x) + b_nP_n + c_nP_{n-1}(x)$$

From this, we are able to see that $a_n = \sqrt{(n+1)/2}$, $b_n = 0$, and $c_n = \sqrt{n/2}$. We can also see that this solution is symmetric, as $a_n = c_{n+1}$, so we can use $\sqrt{n/2}$ for both diagonals in the Jacobi matrix:

$$J = \begin{bmatrix} b_0 & a_0 & 0 & \cdots & 0 \\ c_1 & b_1 & a_1 & \cdots & 0 \\ 0 & c_2 & b_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & a_{n-2} \\ 0 & 0 & 0 & c_{n-1} & b_{n-1} \end{bmatrix}$$

$$= \begin{bmatrix} b_0 & c_1 & 0 & \cdots & 0 \\ c_1 & b_1 & c_2 & \cdots & 0 \\ 0 & c_2 & b_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & c_{n-1} \\ 0 & 0 & 0 & c_{n-1} & b_{n-1} \end{bmatrix}$$

$$J = \begin{bmatrix} 0 & \sqrt{1/2} & 0 & 0 & \cdots & 0 \\ \sqrt{1/2} & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \sqrt{3/2} & \cdots & 0 \\ 0 & 0 & \sqrt{3/2} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \sqrt{(n-1)/2} \\ 0 & 0 & 0 & 0 & \sqrt{(n-1)/2} & 0 \end{bmatrix}$$

We can then use the exact same process we used in Assignment 3 to find the weights and roots from Assignment 3... except we have an issue. We do not know what the normalization factors are. We can find those using Equation (1.84) from the course notes:

$$h_n \equiv \int_a^b w(x)\phi_n^2(x)\,dx$$

where $w(x)$ is the weight function and $\phi(x)$ is a set of orthogonal polynomials. We're given $w(\tilde{x}) = e^{-x^2}$, and we can recursively define $\tilde{H}(\tilde{x})$ in Mathematica. Assuming the modified recurrence relation is still subject to $H_{-1} = 0$ and $H_0 = 1$ boundary conditions from the previous assignment, then we can see from the modified recurrence relation that:

$$\tilde{x}\tilde{H}_0(\tilde{x}) = \sqrt{\frac{0+1}{2}}\tilde{H}_{0+1}(\tilde{x}) + \sqrt{\frac{n}{2}}\tilde{H}_{0-1}(\tilde{x})$$

$$\tilde{x}(1) = \sqrt{\frac{1}{2}}\tilde{H}_1(\tilde{x}) + \sqrt{\frac{n}{2}}(0)$$

$$\tilde{H}_1(\tilde{x}) = \sqrt{2}\tilde{x}$$

Now, if we apply $\tilde{H}_0$ to Equation (1.84):

$$h_0 = \int_{-\infty}^{\infty} w(x)H_0^2(x)\, dx$$

$$h_0 = \int_{-\infty}^{\infty} e^{-x^2}(1)^2\, dx$$

$$h_0 = \sqrt{\pi}$$

Likewise, for $\tilde{H}_1$:

$$h_1 = \int_{-\infty}^{\infty} w(\tilde{x})H_1^2(\tilde{x})\, d\tilde{x}$$

$$h_1 = \int_{-\infty}^{\infty} e^{-\tilde{x}^2}\left(\sqrt{2}\tilde{x}\right)^2\, d\tilde{x}$$

$$h_1 = 2\int_{-\infty}^{\infty} e^{-\tilde{x}^2}\tilde{x}^2\, d\tilde{x}$$

$$h_1 = 2\left(\frac{\sqrt{\pi}}{2}\right)$$

$$h_1 = \sqrt{\pi}$$

As we can see, we should get a constant normalization factor of $\sqrt{\pi}$ for $n = 0, ..., 50$. I manually did this integration in Mathematica up to $n = 15$ (I initially tried $n = 51$, but it was taking a prohibitively long runtime and it wouldn't prove anything that $n = 15$ already didn't prove), and I got the same result every time.

Now that we know that our normalization factor is the same, we can apply the same process used in Assignment 3, with the eigenvalues of the Jacobi matrix being the roots of the function, and the eigenvectors multiplied by $\sqrt{\pi}$ being the weights.

The solution for this can be found in the attached Mathematica workbook file titled "*Assignment 4 - Mathematica Workbook.nb*".

Question 3 (20 points)

We have to find the first derivative of the modified Hermite polynomials. Let's examine the derivatives of the first few modified Hermite polynomials:

$$\tilde{H}_0(\tilde{x}) = 1 \quad \Longrightarrow \quad \frac{d}{d\tilde{x}}\tilde{H}_0(\tilde{x}) = 0,$$

$$\tilde{H}_1(\tilde{x}) = \sqrt{2}\,\tilde{x} \quad \Longrightarrow \quad \frac{d}{d\tilde{x}}\tilde{H}_1(\tilde{x}) = \sqrt{2},$$

$$\tilde{H}_2(\tilde{x}) = \tilde{x}\big(\sqrt{2}\,\tilde{x}\big) - \sqrt{\frac{1}{2}} \quad \Longrightarrow \quad \frac{d}{d\tilde{x}}\tilde{H}_2(\tilde{x}) = 2\sqrt{2}\,\tilde{x},$$

$$\tilde{H}_3(\tilde{x}) = \frac{2}{\sqrt{3}}\,\tilde{x}^3 - \sqrt{3}\,\tilde{x} \quad \Longrightarrow \quad \frac{d}{d\tilde{x}}\tilde{H}_3(\tilde{x}) = 2\sqrt{3}\,\tilde{x}^2 - \sqrt{3} = \sqrt{3}(2\tilde{x}^2 - 1)$$

If we divide both sides of the derivative by $\tilde{H}_{n-1}$ for $n = 1, 2, 3$:

$$\frac{\tilde{H}_1'(\tilde{x})}{\tilde{H}_0(\tilde{x})} = \frac{\sqrt{2}}{1} = \sqrt{2},$$

$$\frac{\tilde{H}_2'(\tilde{x})}{\tilde{H}_1(\tilde{x})} = \frac{2\sqrt{2}\,\tilde{x}}{\sqrt{2}\,\tilde{x}} = 2,$$

$$\frac{\tilde{H}_3'(\tilde{x})}{\tilde{H}_2(\tilde{x})} = \frac{\sqrt{3}\big(2\tilde{x}^2 - 1\big)}{\tilde{x}\big(\sqrt{2}\,\tilde{x}\big) - \sqrt{\frac{1}{2}}} = \frac{\sqrt{3}\big(2\tilde{x}^2 - 1\big)}{\big(2\tilde{x}^2 - 1\big)/\sqrt{2}} = \sqrt{6}$$

This recurrence pattern repeats. Therefore, we can see that the following is the first derivative rule:

$$\tilde{H}_n'(\tilde{x}) = \sqrt{2n}\,\tilde{H}_{n-1}(\tilde{x})$$

In my Mathematica workbook, I used the derivative functions and this recurrence relation to quickly show that this ratio remained true for $n = 1 \longrightarrow 10$.

Now, to find the second derivative rule, we will define the function ψ as follows:

$$\psi(\tilde{x}) = e^{-\tilde{x}^2/2}\tilde{H}_n(\tilde{x})$$

We will next use the product rule to find $\psi'(\tilde{x})$:

$$\psi'(\tilde{x}) = \frac{d}{d\tilde{x}}\Big(e^{-\tilde{x}^2/2}\Big)\tilde{H}_n(\tilde{x}) + e^{-\tilde{x}^2/2}\frac{d}{d\tilde{x}}\Big(\tilde{H}_n(\tilde{x})\Big)$$

$$= -\tilde{x}\, e^{-\tilde{x}^2/2}\, \tilde{H}_n(\tilde{x}) + e^{-\tilde{x}^2/2}\, \tilde{H}'_n(\tilde{x})$$

$$= e^{-\tilde{x}^2/2}\Big[\tilde{H}'_n(\tilde{x}) - \tilde{x}\, \tilde{H}_n(\tilde{x})\Big]$$

Now, using the product rule again to find $\psi''(\tilde{x})$, we obtain:

$$\psi''(\tilde{x}) = \frac{d}{d\tilde{x}}\Big(e^{-\tilde{x}^2/2}\Big)\Big[\tilde{H}'_n(\tilde{x}) - \tilde{x}\, \tilde{H}_n(\tilde{x})\Big] + e^{-\tilde{x}^2/2}\frac{d}{d\tilde{x}}\Big[\tilde{H}'_n(\tilde{x}) - \tilde{x}\, \tilde{H}_n(\tilde{x})\Big]$$

$$= -\tilde{x}\, e^{-\tilde{x}^2/2}\Big[\tilde{H}'_n(\tilde{x}) - \tilde{x}\, \tilde{H}_n(\tilde{x})\Big] + e^{-\tilde{x}^2/2}\Big[\tilde{H}''_n(\tilde{x}) - \tilde{H}_n(\tilde{x}) - \tilde{x}\, \tilde{H}'_n(\tilde{x})\Big]$$

$$= e^{-\tilde{x}^2/2}\Big[\tilde{H}''_n(\tilde{x}) - 2\tilde{x}\, \tilde{H}'_n(\tilde{x}) + (\tilde{x}^2 - 1)\, \tilde{H}_n(\tilde{x})\Big]$$

Using the first derivative rule, we know the following:

$$\tilde{H}'_n(\tilde{x}) = \sqrt{2n}\tilde{H}_{n-1}(\tilde{x}) \quad\Longrightarrow\quad \tilde{H}''_n(\tilde{x}) = \sqrt{2n}\tilde{H}'_{n-1}(\tilde{x}) \quad\Longrightarrow\quad \tilde{H}''_n(\tilde{x}) = \sqrt{2n}\sqrt{2(n-1)}\tilde{H}_{n-2}(\tilde{x})$$

$$\therefore\ \tilde{H}''_n(\tilde{x}) = 2\sqrt{n^2 - n}\ \tilde{H}_{n-2}(\tilde{x})$$

Now, apply these substitutions to our equation:

$$\psi''(\tilde{x}) = e^{-\tilde{x}^2/2}\Big[2\sqrt{n^2 - n}\, \tilde{H}_{n-2}(\tilde{x}) - 2\tilde{x}\sqrt{2n}\, \tilde{H}_{n-1}(\tilde{x}) + (\tilde{x}^2 - 1)\, \tilde{H}_n(\tilde{x})\Big]$$

From the recurrence relation, we can write:

$$2\sqrt{n^2 - n}\tilde{H}_{n-2}(\tilde{x}) = 2\tilde{x}\sqrt{2n}\tilde{H}_{n-1}(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})$$

And therefore, we know that the second derivative rule simplified further is:

$$\psi''(\tilde{x}) = e^{-\tilde{x}^2/2}\Big[2\tilde{x}\sqrt{2n}\tilde{H}_{n-1}(\tilde{x}) - 2n\tilde{H}_n(\tilde{x}) - 2\tilde{x}\sqrt{2n}\, \tilde{H}_{n-1}(\tilde{x}) + (\tilde{x}^2 - 1)\, \tilde{H}_n(\tilde{x})\Big]$$

$$\psi''(\tilde{x}) = e^{-\tilde{x}^2/2}\Big[(\tilde{x}^2 - 1)\, \tilde{H}_n(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})\Big]$$

Question 4 (20 points)

At the end of question 1, we were able to determine the dimensionless Shrödinger equation for a harmonic oscillator:

$$-i\frac{\partial}{\partial\tilde{t}}\psi(x,t) = \frac{1}{2}\left[-\frac{\partial^2}{\partial\tilde{x}^2} + \tilde{x}^2\right]\psi(x,t) \equiv \tilde{E}_n\epsilon\ \psi(\tilde{x},\tilde{t})$$

From this, we can determine that the Hamiltonian of this modified Shrödinger equation is:

$$\mathcal{H} = \frac{1}{2}\left[-\frac{\partial^2}{\partial\tilde{x}^2} + \tilde{x}^2\right]$$

We want to construct $\hat{D}_{n,m}$ from equation 1.62 of the course notes. Here, the operator we are using is the Hamiltonian above. Knowing that we're using the modified Hermite polynomials as the bases, the bounds are [-1,1] and the weights are $w(x) = e^{-\tilde{x}^2}$. Then,

$$\mathcal{H}_{mn} = \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2/2}\tilde{H}_m(\tilde{x})\left(-\frac{\partial^2}{\partial\tilde{x}^2} + \tilde{x}^2\right)\left[e^{-\tilde{x}^2/2}\tilde{H}_n(\tilde{x})\right]d\tilde{x}$$

$$= -\frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2/2}\tilde{H}_m(\tilde{x})\frac{\partial^2}{\partial\tilde{x}^2}\left[e^{-\tilde{x}^2/2}\tilde{H}_n(\tilde{x})\right]d\tilde{x} + \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{x}^2\tilde{H}_n(\tilde{x})d\tilde{x}$$

Now, using the second derivative rule from the end of question 3:

$$\psi''(\tilde{x}) = e^{-\tilde{x}^2/2}\left[(\tilde{x}^2-1)\,\tilde{H}_n(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})\right] = \frac{\partial^2}{\partial\tilde{x}^2}\left[e^{-\tilde{x}^2/2}\tilde{H}_n(\tilde{x})\right]$$

We will substitute into the $\hat{D}_{n,m}$ operator:

$$\mathcal{H}_{mn} = -\frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2/2}\tilde{H}_m(\tilde{x})\left[e^{-\tilde{x}^2/2}\left[(\tilde{x}^2-1)\,\tilde{H}_n(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})\right]\right]d\tilde{x} + \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{x}^2\tilde{H}_n(\tilde{x})d\tilde{x}$$

$$= -\frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\left[(\tilde{x}^2-1)\,\tilde{H}_n(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})\right]d\tilde{x} + \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{x}^2\tilde{H}_n(\tilde{x})d\tilde{x}$$

$$= \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{H}_n(\tilde{x})\ d\tilde{x} - \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{x}^2\tilde{H}_n(\tilde{x})\ d\tilde{x}$$

$$+ \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})2n\tilde{H}_n(\tilde{x})\ d\tilde{x} + \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{x}^2\tilde{H}_n(\tilde{x})d\tilde{x}$$

$$= \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{H}_n(\tilde{x})\,d\tilde{x} + \frac{1}{2}\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})2n\tilde{H}_n(\tilde{x})\,d\tilde{x}$$

$$= \frac{1}{2}\big(1+2n\big)\int_{-1}^{1} e^{-\tilde{x}^2}\tilde{H}_m(\tilde{x})\tilde{H}_n(\tilde{x})\,d\tilde{x}$$

$$\mathcal{H}_{mn} = \left(\frac{1}{2}+n\right)\delta_{mn}$$

Question 5 (20 points)

Beginning with the given DVR functions (labeled as Equation (1.141) and Equation (1.138) respectively in the course notes):

$$\hat{D}_{ij} = \int_{-1}^{1} \ell_j(x)\hat{D}\ell_i(\tilde{x})\,dx$$

$$\ell(x) = \sqrt{w_j w(x)}\sum_m \phi_m(x_j)\phi_m(x)$$

We will make the substitutions of $\tilde{\ell}(\tilde{x})$ and $w(\tilde{x}) = e^{-x^2}$ into Equation (1.141):

$$\hat{D}_{ij} = \frac{1}{2}\int_{-1}^{1}\sqrt{\omega_i e^{-x^2}}\sum_m \tilde{H}_m(\tilde{x}_j)\tilde{H}_m(\tilde{x})\left(-\frac{\partial^2}{\partial x^2}+\tilde{x^2}\right)\sqrt{w_i e^{-x^2}}\sum_n \tilde{H}_n(\tilde{x}_i)\tilde{H}_n(x)\,dx$$

$$\hat{D}_{ij} = -\frac{1}{2}\sqrt{\omega_j\omega_i}\tilde{H}_m(\tilde{x}_j)\int_{-1}^{1} e^{-x^2}\tilde{H}_m(x)\frac{\partial^2}{\partial x^2}\left(e^{-x^2/2}\sum_n \tilde{H}_n(\tilde{x}_i)\tilde{H}_n(\tilde{x})\right)dx + \frac{1}{2}\tilde{H}_n(\tilde{x}_j)\int_{-1}^{1} e^{-x^2}\tilde{x}^2\tilde{H}_n(\tilde{x})\tilde{H}_m(\tilde{x})\,dx$$

Now we use our result from question 3 to find the 2nd derivative as:

$$\frac{\partial^2}{\partial x^2}\left(e^{-x^2/2}\sum_n \tilde{H}_n(\tilde{x}_i)\tilde{H}_n(\tilde{x})\right) = \tilde{H}_n(\tilde{x}_i)\left(e^{-x^2/2}\left[(-1+\tilde{x}^2)\tilde{H}_n(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})\right]\right)$$

We now substitute this into our integral:

$$\begin{aligned}\hat{D}_{ij} = &-\frac{1}{2}\sqrt{\omega_j\omega_i}\tilde{H}_m(\tilde{x}_j)\int_{-1}^{1} e^{-x^2}\tilde{H}_m(\tilde{x})\bigg(\tilde{H}_n(\tilde{x}_i)\Big(e^{-x^2/2}\left[(-1+\tilde{x}^2)\tilde{H}_n(\tilde{x}) - 2n\tilde{H}_n(\tilde{x})\right]\Big)\bigg)\,dx\\ &+\frac{1}{2}\tilde{H}_n(\tilde{x}_j)\int_{-1}^{1} e^{-x^2}\tilde{x}^2\tilde{H}_n(\tilde{x})\tilde{H}_m(\tilde{x})\,dx\end{aligned}$$

Dropping our subscripts over the summations (as we don't need them anymore) and following the same method in question 4 to solve this, we notice that this integral comes out to $(\frac{1}{2}+n)\delta_{mn}$. This also shows that the term proportional to $\tilde{x}^2$ is diagonalized. So our final matrix $\hat{D}_{ij}$ is:

$$\hat{D}_{ij} = \sum_n \sum_m \sqrt{\omega_j \omega_i} \tilde{H}_m(\tilde{x}_j) \tilde{H}_n(\tilde{x}_i) (\frac{1}{2}+n)\delta_{mn}$$

$$\hat{D}_{ij} = \sum_m \sqrt{\omega_j \omega_i} \tilde{H}_m(\tilde{x}_j) \tilde{H}_m(\tilde{x}_i) (\frac{1}{2}+m)$$

The last line happens because the delta only exists at $m = n$, and is 0 elsewhere.

Question 6 (5 points)

Because we derived much of the work by hand and not in Mathematica, there was no increase in precision. Deriving by hand meant that we didn't lost precision to floating point errors and things of that nature.