1. Harmonic Oscillator Matrix Elements. We have been considering the harmonic oscillator with Hamiltonian $H = p^2/2m + m\omega^2 x^2/2$. The energy eigenstates are $|\psi_n\rangle$ with energy eigenvalues $E_n = \hbar\omega(n + 1/2)$.

(a) Compute the matrices

$$\hat{x}_{nm} = \langle \psi_n \mid x \mid \psi_m \rangle \ , \quad \hat{p}_{nm} = \langle \psi_n \mid p \mid \psi_m \rangle \ , \quad \hat{E}_{nm} = \langle \psi_n \mid H \mid \psi_m \rangle \ .$$

These are the position, momentum, and energy operators in the *energy basis* or *energy representation*. The raising and lowering operators $a^\dagger$ and a will probably be useful.

Solution

Recall from lecture that

$$x_0 = \sqrt{\frac{\hbar}{m\omega}} \ , \quad x = \frac{x_0}{\sqrt{2}}\left(a + a^\dagger\right) \ , \quad p = \frac{\hbar}{i\sqrt{2}x_0}\left(a - a^\dagger\right) \ .$$

So

$$\begin{aligned}
\hat{x}_{nm} &= \frac{x_0}{\sqrt{2}}\left(\langle \psi_n \mid a \mid \psi_m \rangle + \left\langle \psi_n \mid a^\dagger \mid \psi_m \right\rangle\right) \\
&= \frac{x_0}{\sqrt{2}}\left(\left\langle a^\dagger \psi_n \mid \psi_m \right\rangle + \left\langle \psi_n \mid a^\dagger \psi_m \right\rangle\right) \\
&= \frac{x_0}{\sqrt{2}}\left(\left\langle \sqrt{n+1}\,\psi_{n+1} \mid \psi_m \right\rangle + \left\langle \psi_n \mid \sqrt{m+1}\,\psi_{m+1} \right\rangle\right) \\
&= \frac{x_0}{\sqrt{2}}\left(\sqrt{n+1}\,\delta_{n+1,m} + \sqrt{m+1}\,\delta_{n,m+1}\right) \ .
\end{aligned}$$

Or

$$\hat{x} = \frac{x_0}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \ .$$

Similarly

$$\begin{aligned}
\hat{p}_{nm} &= \frac{\hbar}{i\sqrt{2}x_0}\left(\langle \psi_n \mid a \mid \psi_m \rangle - \left\langle \psi_n \mid a^\dagger \mid \psi_m \right\rangle\right) \\
&= \frac{\hbar}{i\sqrt{2}x_0}\left(\left\langle a^\dagger \psi_n \mid \psi_m \right\rangle - \left\langle \psi_n \mid a^\dagger \psi_m \right\rangle\right) \\
&= \frac{\hbar}{i\sqrt{2}x_0}\left(\left\langle \sqrt{n+1}\,\psi_{n+1} \mid \psi_m \right\rangle - \left\langle \psi_n \mid \sqrt{m+1}\,\psi_{m+1} \right\rangle\right) \\
&= \frac{\hbar}{\sqrt{2}x_0}\left(-i\sqrt{n+1}\,\delta_{n+1,m} + i\sqrt{m+1}\,\delta_{n,m+1}\right) \ .
\end{aligned}$$

Or

$$\hat{p} = \frac{\hbar}{\sqrt{2}x_0}\begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & 0 & \dots \\ 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{4} & \dots \\ 0 & 0 & 0 & i\sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

It was shown in lecture that $H = \hbar\omega(aa^\dagger - 1/2)$. Using $a^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}$, we have $\hat{E}_{nm} = \hbar\omega(n+1/2)\,\delta_{nm}$ or

$$\hat{E} = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 3 & 0 & 0 & 0 & \dots \\ 0 & 0 & 5 & 0 & 0 & \dots \\ 0 & 0 & 0 & 7 & 0 & \dots \\ 0 & 0 & 0 & 0 & 9 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

End Solution

(b) Using ordinary matrix multiplication, show that $\hat{E} = \hat{p}^2/2m + m\omega^2\hat{x}^2/2$ and $\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar I$, where I is the identity matrix, $I_{nm} = \delta_{nm}$.

Solution

$$\frac{\hat{p}^2}{2m} = \frac{\hbar^2}{4mx_0^2}\begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & 0 & \dots \\ 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{4} & \dots \\ 0 & 0 & 0 & i\sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\times \begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & 0 & \dots \\ 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{4} & \dots \\ 0 & 0 & 0 & i\sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$= \frac{\hbar\omega}{4}\begin{pmatrix} 1 & 0 & -\sqrt{2} & 0 & 0 & \dots \\ 0 & 3 & 0 & -\sqrt{6} & 0 & \dots \\ -\sqrt{2} & 0 & 5 & 0 & -\sqrt{12} & \dots \\ 0 & -\sqrt{6} & 0 & 7 & 0 & \dots \\ 0 & 0 & -\sqrt{12} & 0 & 9 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

$$\frac{m\omega^2\hat{x}^2}{2} = \frac{m\omega^2 x_0^2}{4}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \dots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\times \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \dots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$= \frac{\hbar\omega}{4}\begin{pmatrix} 1 & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 3 & 0 & \sqrt{6} & 0 & \dots \\ \sqrt{2} & 0 & 5 & 0 & \sqrt{12} & \dots \\ 0 & \sqrt{6} & 0 & 7 & 0 & \dots \\ 0 & 0 & \sqrt{12} & 0 & 9 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Adding the matrices for $\hat{p}^2$ and $\hat{x}^2$, the off diagonal terms cancel and the result is

$$\frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 3 & 0 & 0 & 0 & \dots \\ 0 & 0 & 5 & 0 & 0 & \dots \\ 0 & 0 & 0 & 7 & 0 & \dots \\ 0 & 0 & 0 & 0 & 9 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \hat{E}\,.$$

$$\hat{x}\hat{p} = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \dots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\times \begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & 0 & \dots \\ 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{4} & \dots \\ 0 & 0 & 0 & i\sqrt{4} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$= \frac{\hbar}{2}\begin{pmatrix} i & 0 & -i\sqrt{2} & 0 & 0 & \dots \\ 0 & i & 0 & -i\sqrt{6} & 0 & \dots \\ i\sqrt{2} & 0 & i & 0 & -i\sqrt{12} & \dots \\ 0 & i\sqrt{6} & 0 & i & 0 & \dots \\ 0 & 0 & i\sqrt{12} & 0 & i & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

A similar calculation gives

$$\hat{p}\hat{x} = \frac{\hbar}{2}\begin{pmatrix} -i & 0 & -i\sqrt{2} & 0 & 0 & \dots \\ 0 & -i & 0 & -i\sqrt{6} & 0 & \dots \\ i\sqrt{2} & 0 & -i & 0 & -i\sqrt{12} & \dots \\ 0 & i\sqrt{6} & 0 & -i & 0 & \dots \\ 0 & 0 & i\sqrt{12} & 0 & -i & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

Or, we could notice that $\hat{p}$ and $\hat{x}$ must be Hermitian operators, so the Hermitian adjoint of $\hat{x}\hat{p}$ must be $\hat{p}^\dagger\hat{x}^\dagger = \hat{p}\hat{x}$. And we find the Hermitian adjoint of a matrix by transposing it and taking its complex conjugate. Subtracting the expressions for $\hat{x}\hat{p}$ and $\hat{p}\hat{x}$, we obtain the desired result.

Note that x and p involve the first power of the raising and lowering operators so they connect states separated by one quantum number. (The diagonals just above and just below the main diagonals of the matrices.) Their squares connect states to themselves and to states separated by two quantum numbers. This gives the main diagonal as well diagonals two above and two below the main diagonal.

——— End Solution ———

2. Harmonic Oscillator Coherent States. We've seen that the energy eigenstates of the quantum harmonic oscillator do not "oscillate" analogous to the classical motion. In lecture we considered a superposition of two states and showed we could get an oscillatory $\langle x \rangle$.

A more elaborate construction involves *coherent* states which are eigenfunctions of the annihilation operator:

$$a\varphi_\alpha = \alpha\varphi_\alpha \ ,$$

where α is a complex number.

(a) Show that $\varphi_\alpha(x, t = 0)$ can be expanded in the energy eigenstates (and normalized) as

$$\varphi_\alpha(x,0) = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\psi_n = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha a^\dagger)^n}{n!}\psi_0 \ .$$

Solution

The expansion coefficient is

$$\langle\psi_n \mid \varphi_\alpha\rangle = \frac{1}{\sqrt{n!}}\left\langle(a^\dagger)^n\psi_0 \mid \varphi_\alpha\right\rangle = \frac{1}{\sqrt{n!}}\left\langle\psi_0 \mid a^n\varphi_\alpha\right\rangle = \frac{\alpha^n}{\sqrt{n!}}\left\langle\psi_0 \mid \varphi_\alpha\right\rangle = \frac{\alpha^n}{\sqrt{n!}}\,C \ ,$$

where $\langle\psi_0 \mid \varphi_\alpha\rangle = C$ is just a number which we will determine by asking that φ_α be normalized.

$$1 = \langle\varphi_\alpha \mid \varphi_\alpha\rangle = |C|^2\sum_n\frac{\alpha^{*n}}{\sqrt{n!}}\sum_m\frac{\alpha^m}{\sqrt{m!}}\langle\psi_n \mid \psi_m\rangle = |C|^2\sum_n\frac{|\alpha|^{2n}}{n!} = |C|^2e^{|\alpha|^2} \ .$$

So, C is determined up to a phase, and we can take C to be real with

$$C = e^{-|\alpha|^2/2} \ .$$

End Solution

(b) Now that you have the expansion in energy eigenstates, the time dependence is fairly easy to determine. Show that

$$\varphi_\alpha(x,t) = \varphi_{\alpha(t)}(x,0)e^{-i\omega t/2} \ ,$$

where

$$\alpha(t) = \alpha(0)e^{-i\omega t} \ ,$$

and the shorthand $\varphi_{\alpha(t)}$ means: use the expression for φ_α with $\alpha(t)$ in place of α. In other words, the time dependence is found simply by multiplying the entire state by the phase factor $\exp(-i\omega t/2)$ and advancing the phase of α by $\exp(-i\omega t)$.

Solution

Using the expansion of $\varphi_\alpha(x,0)$ from part (a),

$$\varphi_\alpha(x,t) = e^{-|\alpha|^2/2}\sum_n\frac{\alpha^n}{\sqrt{n!}}\psi_n e^{-i(n+1/2)\omega t} = e^{-|\alpha|^2/2}\sum_n\frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}\psi_n e^{-i\omega t/2} \ .$$

which shows that we replace α by $\alpha \exp(-i\omega t)$ and multiply the whole thing by $\exp(-i\omega t)$.

End Solution

(c) Show that the $\langle x \rangle$ and $\langle p \rangle$ oscillate according to

$$\langle x \rangle = \sqrt{2}\, x_0\, |\alpha|\, \cos(\omega t - \delta)\,,$$
$$\langle p \rangle = -\sqrt{2}\, \frac{\hbar}{x_0}\, |\alpha|\, \sin(\omega t - \delta)\,,$$

where $x_0 = \sqrt{\hbar/m\omega}$ and δ is the phase of α, $\alpha = |\alpha| \exp(i\delta)$.

In other words, the motion of the expectation values is exactly the classical motion and α determines the amplitude and phase of the oscillator.

Solution

$$\begin{aligned}
\left\langle \varphi_{\alpha(t)} \mid x/x_0 \mid \varphi_{\alpha(t)} \right\rangle &= \frac{1}{\sqrt{2}} \left\langle \varphi_{\alpha(t)} \mid a + a^\dagger \mid \varphi_{\alpha(t)} \right\rangle \\
&= \frac{1}{\sqrt{2}} \left\langle \varphi_{\alpha(t)} \mid (a + a^\dagger)\, \varphi_{\alpha(t)} \right\rangle \\
&= \frac{1}{\sqrt{2}} \left(\alpha(t) + \alpha^*(t)\right) \\
&= \frac{1}{\sqrt{2}} \left(|\alpha| e^{-i\omega t + i\delta} + |\alpha| e^{i\omega t - i\delta} \right) \\
&= \sqrt{2}\, |\alpha|\, \cos(\omega t - \delta)\,. \\
\left\langle \varphi_{\alpha(t)} \mid p x_0/\hbar \mid \varphi_{\alpha(t)} \right\rangle &= \frac{1}{i\sqrt{2}} \left\langle \varphi_{\alpha(t)} \mid a - a^\dagger \mid \varphi_{\alpha(t)} \right\rangle \\
&= \frac{1}{i\sqrt{2}} \left\langle \varphi_{\alpha(t)} \mid (a - a^\dagger)\, \varphi_{\alpha(t)} \right\rangle \\
&= \frac{1}{i\sqrt{2}} \left(\alpha(t) - \alpha^*(t)\right) \\
&= \frac{1}{i\sqrt{2}} \left(|\alpha| e^{-i\omega t + i\delta} - |\alpha| e^{i\omega t - i\delta} \right) \\
&= -\sqrt{2}\, |\alpha|\, \sin(\omega t - \delta)\,.
\end{aligned}$$

End Solution

3. Uncertainty Relation for Coherent States. Calculate Δx^2 and Δp^2 for the coherent states introduced in the previous problem and determine the uncertainty product, $\Delta x\, \Delta p$.

Solution

We start by calculating $\left\langle (x/x_0)^2 \right\rangle$ and $\left\langle (px_0/\hbar)^2 \right\rangle$.

$$\begin{aligned}
\left\langle \begin{matrix} (x/x_0)^2 \\ (px_0/\hbar)^2 \end{matrix} \right\rangle &= \pm\frac{1}{2} \left\langle \varphi_{\alpha(t)} \mid (a \pm a^\dagger)^2 \mid \varphi_{\alpha(t)} \right\rangle \\
&= \pm\frac{1}{2} \left\langle \varphi_{\alpha(t)} \mid a^2 \pm aa^\dagger \pm a^\dagger a + a^{\dagger\,2} \mid \varphi_{\alpha(t)} \right\rangle \\
&= \pm\frac{1}{2} \left\langle \varphi_{\alpha(t)} \mid a^2 \pm 1 \pm 2a^\dagger a + a^{\dagger\,2} \mid \varphi_{\alpha(t)} \right\rangle \\
&= \pm\frac{1}{2} \left(\alpha^2 \pm 1 \pm 2\alpha^*\alpha + \alpha^{*\,2} \right) \\
&= \pm\frac{1}{2} \left(\alpha \pm \alpha^* \right)^2 + \frac{1}{2} \,.
\end{aligned}$$

In going from the second to the third line above, $[a, a^\dagger] = 1$ was used to ensure that a is on the right where it can operate to the right and produce α and $a^\dagger$ is on the left where it can operate to the left (becoming a) and produce α^* in the expectation value.

The first term in the last line (see previous problem) is $\langle x/x_0 \rangle^2$ (top) or $\langle px_0/\hbar \rangle^2$ (bottom)—just the things we need to subtract to get to the squared deviations. So

$$\Delta x^2 = \frac{x_0^2}{2} \,, \qquad \Delta p^2 = \frac{\hbar^2}{2x_0^2} \,,$$

and

$$\Delta x \, \Delta p = \frac{\hbar}{2} \,.$$

This is the minimum possible uncertainty product and the coherent states have a motion which is "as classical as it gets!" When $|\alpha|$ is large, the amplitudes of $\langle x \rangle$ and $\langle p \rangle$ are much larger than their uncertainties. This is an example of the Ehrenfest theorem. Coherent states have a Gaussian probability density. This and additional information about coherent states may be found in Schwabl, pp. 54–56 and Peebles, pp. 169–170.

End Solution

4. Harmonic Oscillator in 3D. Consider a 3-dimensional harmonic oscillator with Hamiltonian

$$H = \frac{\boldsymbol{p}^2}{2m} + \frac{m\omega^2 \boldsymbol{x}^2}{2} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{m\omega^2 x^2}{2} + \frac{m\omega^2 y^2}{2} + \frac{m\omega^2 z^2}{2} \,.$$

(a) Show that the energy eigenvalues are $E_n = \hbar\omega(n + 3/2)$.

Solution

Among the six variables, $\boldsymbol{x}$ and $\boldsymbol{p}$, the only non vanishing commutators are $[x, p_x]$, $[y, p_y]$, and $[z, p_z]$, so the Hamiltonian can be written (in an obvious way) as $H = H_x + H_y + H_z$ where the three terms on the RHS commute with each other. This means the eigenfunctions can be chosen to be eigenfunctions of H_x, H_y, and H_z simultaneously. Of course, these are just products of the 1D eigenfunctions.

$$\psi_{ijk}(x, y, z) = \psi_i(x)\,\psi_j(y)\,\psi_k(z)\;,$$

and

$$\begin{aligned}
H\psi_{ijk}(x, y, z) &= (H_x + H_y + H_z)\psi_i(x)\,\psi_j(y)\,\psi_k(z) \\
&= H_x\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) + H_y\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) + H_z\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) \\
&= \hbar\omega(i + 1/2)\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) + \hbar\omega(j + 1/2)\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) \\
&\qquad + \hbar\omega(k + 1/2)\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) \\
&= \hbar\omega(i + j + k + 3/2)\,\psi_i(x)\,\psi_j(y)\,\psi_k(z) \\
&= \hbar\omega(n + 3/2)\,\psi_{ijk}(x, y, z)\;,
\end{aligned}$$

where $n = i + j + k$ and n is any integer greater than 0 (since this is true of each of i, j, and k.

End Solution

(b) What is the degeneracy of level n? (That is, how many different states have energy $\hbar\omega(n + 3/2)$?)

Solution

We need to add up the number of ways for three non-negative integers to add up to n.

$$\begin{aligned}
m &= \sum_{i=0}^{n}\sum_{j=0}^{n-i} 1 \\
&= \sum_{i=0}^{n}(n - i + 1) \\
&= \sum_{i=0}^{n}(i + 1) \\
&= \frac{1}{2}(n + 1)(n + 2)\;.
\end{aligned}$$

As an interesting check, we might ask how many states are there with energy less than or equal to $\hbar\omega(n + 3/2)$. If we imagine a space with i, j, k axes and we go out to n on each axis and we pass a plane through these three points on the axes, then any lattice point in the positive octant between the origin and this plane (including the bounding planes and axes) corresponds to a state with energy less than or equal to $\hbar\omega(n+3/2)$. The lattice points in the positive octant (including the bounding planes and axes) correspond to all possible states. So, we just need to calculate the volume of the pyramid we've just constructed and (ignoring "edge effects") we'll have all the states with energy less than or equal to $\hbar\omega(n+3/2)$. Recall for a pyramid, the volume is 1/3 the base times the height, so $M \approx n^3/6$. This is certainly correct for large n. For small n, we know there is one state with energy $n = 0$, there are three with $n = 1$ (or four with $n \le 1$), and 6 with $n = 2$ (or 10 with $n \le 2$). A simple formula that satisfies this is

$$M = \frac{1}{6}(n+1)(n+2)(n+3)\,.$$

Note that

$$m = M(n) - M(n-1) = \frac{1}{6}\left((n+1)(n+2)(n+3) - n(n+1)(n+2)\right) = \frac{1}{2}(n+1)(n+2)\,.$$

——— End Solution ———

5. Scattering by a Square Potential. Consider a plane wave corresponding to a particle of mass m and energy E incident from the left on a potential barrier (or well) of width $2a$ and height V_0 (from $x = -a$ to $x = +a$ to be definite). Calculate the reflection and transmission coefficients. Be sure your results work for positive and negative V_0 and for any $E > 0$.

——— Solution ———

To the left and right of the potential barrier the plane wave solutions are $\exp(\pm ikx)$ where $k = \sqrt{2mE/\hbar^2}$. Within the barrier region, the plane wave solutions are $\exp(\pm iqx)$ where $q = \sqrt{2m(E-V_0)/\hbar^2}$. Note that we can handle the case of $E < V_0$ by allowing q to be imaginary which will give growing and decaying exponentials within the barrier region. Let I, II, III designate the region to the left of the barrier, within the barrier, and to the right of the barrier. Then the solution which has only an outgoing wave in region III and a unit amplitude incoming wave in region I is

$$\begin{aligned}
\psi_I &= e^{ikx} + Re^{-ikx}\,,\\
\psi_{II} &= Ae^{iqx} + Be^{-iqx}\,,\\
\psi_{III} &= Te^{ikx}\,.
\end{aligned}$$

To determine the four constants R, T, A, and B, we match the wave functions and derivatives at $x = -a$ and $x = +a$. However, it might be worth complicating things a bit by introducing C and D which we will set to 1 and 0 and writing

$$\begin{aligned}
\psi_I &= Ce^{ikx} + Re^{-ikx}\,,\\
\psi_{II} &= Ae^{iqx} + Be^{-iqx}\,,\\
\psi_{III} &= Te^{ikx} + De^{-ikx}\,.
\end{aligned}$$

We can write the matching conditions in matrix form

$$\begin{pmatrix} e^{-ika} & e^{+ika} \\ +ike^{-ika} & -ike^{+ika} \end{pmatrix} \begin{pmatrix} C \\ R \end{pmatrix} = \begin{pmatrix} e^{-iqa} & e^{+iqa} \\ +iqe^{-iqa} & -iqe^{+iqa} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} ,$$

and

$$\begin{pmatrix} e^{+iqa} & e^{-iqa} \\ +iqe^{+iqa} & -iqe^{-iqa} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{+ika} & e^{-ika} \\ +ike^{+ika} & -ike^{-ika} \end{pmatrix} \begin{pmatrix} T \\ D \end{pmatrix} .$$

Multiplying by the inverses of the matrices on the left,

$$\begin{aligned} \begin{pmatrix} C \\ R \end{pmatrix} &= \frac{-1}{2ik} \begin{pmatrix} -ike^{+ika} & -e^{+ika} \\ -ike^{-ika} & +e^{-ika} \end{pmatrix} \begin{pmatrix} e^{-iqa} & e^{+iqa} \\ +iqe^{-iqa} & -iqe^{+iqa} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\ &= \frac{-1}{2ik} \begin{pmatrix} (-ik-iq)e^{i(+k-q)a} & (-ik+iq)e^{i(+k+q)a} \\ (-ik+iq)e^{i(-k-q)a} & (-ik-iq)e^{i(-k+q)a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} , \end{aligned} \tag{1}$$

and

$$\begin{aligned} \begin{pmatrix} A \\ B \end{pmatrix} &= \frac{-1}{2iq} \begin{pmatrix} -iqe^{-iqa} & -e^{-iqa} \\ -iqe^{+iqa} & +e^{+iqa} \end{pmatrix} \begin{pmatrix} e^{+ika} & e^{-ika} \\ +ike^{+ika} & -ike^{-ika} \end{pmatrix} \begin{pmatrix} T \\ D \end{pmatrix} \\ &= \frac{-1}{2iq} \begin{pmatrix} (-ik-iq)e^{i(+k-q)a} & (+ik-iq)e^{i(-k-q)a} \\ (+ik-iq)e^{i(+k+q)a} & (-ik-iq)e^{i(-k+q)a} \end{pmatrix} \begin{pmatrix} T \\ D \end{pmatrix} . \end{aligned} \tag{2}$$

To get the overall relation between the wave in region I and the wave in region III we need to multiply the final matrix in equation (1) by the final matrix in equation (2). What we really want are the transmission and reflection coefficients. When we set $D = 0$ and $C = 1$, we find that $1 = M_{11}\,T$, where M_{11} is the 11 element of the matrix just described.

$$\begin{aligned} M_{11} &= \frac{-1}{4qk}\left(-(k+q)^2 e^{2i(k-q)a} + (k-q)^2 e^{2i(k+q)a}\right) \\ &= \frac{e^{2ika}}{4kq}\left(-(k^2+q^2)(e^{2iqa} - e^{-2iqa}) + 2kq(e^{2iqa} + e^{-2iqa})\right) \\ &= \frac{e^{2ika}}{2kq}\left(-i(k^2+q^2)\sin(2qa) + 2kq\cos(2qa)\right) \end{aligned}$$

Remember, $1 = M_{11}T$, so the transmission coefficient is $t = |T|^2 = 1/|M_{11}|^2$. Note that we don't need to go to the trouble of computing the probability current because, the wave number is the same in regions I and III. Also, since particles (probabilities) are conserved, the reflection coefficient $r = 1 - t$, so it will be enough to look at t. Let's assume for the moment that q is real ($E > V_0$). Then

$$t = \frac{4k^2q^2}{(k^2+q^2)^2\sin^2(2qa) + 4k^2q^2\cos^2(2qa)} .$$

Note that the transmission is unity whenever $2qa = n\pi$. Of course a way to think of this is that the waves reflected from the front and back of the barrier have a path difference which is an integral number of wavelengths (in the barrier region) and one of the reflected waves experiences an extra π phase shift due to reflection than the other. The interference effects all have to do with the extra path length inside the barrier region.

If $E < V_0$, then q is pure imaginary and it's probably easier to go back to the expression for M_{11} and substitute $q = i\kappa$, where κ is real.

$$M_{11} = \frac{e^{ika}}{2ik\kappa} \left(-i(k^2 - \kappa^2)(i\sinh(2\kappa a) + 2ik\kappa\cosh(2\kappa a)\right) .$$

Then

$$t = \frac{4k^2\kappa^2}{(k^2 - \kappa^2)^2 \sinh^2(2\kappa a) + 4k^2\kappa^2\cosh^2(2\kappa a)} .$$

Even though $E < V_0$ and a classical particle would bounce off the barrier (so the barrier region is forbidden classically), the quantum particle has a chance to tunnel through the barrier and come out the other side. Both hyperbolic functions become $\exp(2\kappa a)/2$ as $2\kappa a$ becomes large. In other words, the transmission coefficient is exponentially cut off as the barrier gets higher $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$ or wider. For $2\kappa a \ll 1$, the transmission coefficient approaches unity.

End Solution