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Problem 1: Solving the Harmonic Oscillator

Solving the differential equation form of the time-independent Schrödinger equation for the eigenstates of the harmonic oscillator Hamiltonian in 1D requires solving a second order differential equation. By using operator algebra, it is possible to simplify the solution to this problem.

The 1D harmonic oscillator is described by the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2. \tag{1}$$

Define the unitless variables

$$x = \frac{X}{\lambda}, \quad p = \frac{\lambda}{\hbar}P, \quad \lambda = \sqrt{\frac{\hbar}{m\omega}}. \tag{2}$$

such that the Hamiltonian has the form

$$H = \frac{\hbar\omega}{2}\left(p^2 + x^2\right). \tag{3}$$

Note that x and p are conjugate observables, $[x, p] = i$

(a) [2 pt] Using the harmonic oscillator operators

$$\hat{a} = \frac{1}{\sqrt{2}}(x + ip), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(x - ip), \quad \hat{n} = \hat{a}^\dagger\hat{a}, \tag{4}$$

and their commutation relations, show that the Hamiltonian can be written as

$$H = \hbar\omega(\hat{n} + \frac{1}{2}). \tag{5}$$

(b) [2 pts] Define the eigenstates of the operator $\hat{n}$:

$$\hat{n}|n\rangle = n|n\rangle, \tag{6}$$

with n some (unitless) numbers. Use the operator commutation relations to show that

$$\begin{aligned} \hat{a}|n\rangle &= c(n)|n-1\rangle \\ \hat{a}^\dagger|n\rangle &= d(n)|n+1\rangle. \end{aligned} \tag{7}$$

Derive expressions for $c(n)$ and $d(n)$. Show your work.

(c) [3 pts] The potential, $V(x) = \frac{\hbar\omega}{2}x^2 \geq 0$ for all x. Explain why this implies that:

1. The eigenenergies of the Harmonic Oscillator must be positive
2. The eigenvalues of $\hat{n}$ must be non-negative integers
3. There is a lowest eigenstate of $\hat{n}$, $|0\rangle$ defined by $\hat{a}|0\rangle = 0$.

(d) [2 pts] Show that results above define a first order differential equation in X that can be solved for the ground state harmonic oscillator wavefunction $\psi_0(X)$. Determine this equation and solve for this wavefunction.

(e) [1 pt] Use the result from (e) and the operators to determine the first excited state wavefunction for the harmonic oscillator, $\psi_1(X)$.

(a)

We know

$$H = \frac{\hbar\omega}{2}\left(p^2 + x^2\right),$$

so we want to write x and p in terms of $\hat{a}$ and $\hat{a}^+$. We have

$$\hat{a} = \frac{1}{\sqrt{2}}(x + ip)$$

$$\hat{a}^+ = \frac{1}{\sqrt{2}}(x - ip),$$

so

$$\sqrt{2}\,\hat{a} = x + ip, \quad \sqrt{2}\,\hat{a}^+ = x - ip$$

$$x = \sqrt{2}\,\hat{a}^+ + ip$$

$$\sqrt{2}\,\hat{a} = \left(\sqrt{2}\,\hat{a}^+ + ip\right) + ip$$

$$p = -\frac{i\left(\hat{a} - \hat{a}^+\right)}{\sqrt{2}}$$

and

$$\sqrt{2}\,\hat{a} = x + ip, \quad \sqrt{2}\,\hat{a}^+ = x - ip$$

$$ip = x - \sqrt{2}\,\hat{a}^+$$

$$\sqrt{2}\,\hat{a} = x + \left(x - \sqrt{2}\,\hat{a}^+\right)$$

$$x = \frac{\hat{a} + \hat{a}^+}{\sqrt{2}}.$$

Then

$$H = \frac{\hbar\omega}{2}\left[\left(\frac{-i(\hat{a} - \hat{a}^+)}{\sqrt{2}}\right)^2 + \left(\frac{\hat{a} + \hat{a}^+}{\sqrt{2}}\right)^2\right]$$

$$= \frac{\hbar\omega}{2}\left[-\frac{1}{2}\left(\cancel{\hat{a}\hat{a}} - \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} + \cancel{\hat{a}^+\hat{a}^+}\right) + \frac{1}{2}\left(\cancel{\hat{a}\hat{a}} + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + \cancel{\hat{a}^+\hat{a}^+}\right)\right]$$

$$= \frac{\hbar\omega}{2}\left[\frac{1}{2}\hat{a}\hat{a}^+ + \frac{1}{2}\hat{a}^+\hat{a} + \frac{1}{2}\hat{a}\hat{a}^+ + \frac{1}{2}\hat{a}^+\hat{a}\right]$$

$$= \frac{\hbar\omega}{2}\left[\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}\right]$$

(a), cont'd...

We know

$$[\hat{a}, \hat{a}^+] = 1,$$

so

$$\hat{a}\hat{a}^+ - \hat{a}^+\hat{a} = 1$$
$$\hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1$$

and

$$H = \frac{\hbar\omega}{2}\left[\left(\hat{a}^+\hat{a}+1\right) + \hat{a}^+\hat{a}\right]$$
$$= \frac{\hbar\omega}{2}\left[2\hat{a}^+\hat{a} + 1\right]$$
$$H = \hbar\omega\left(\hat{a}^+\hat{a} + \tfrac{1}{2}\right).$$

But

$$\hat{n} = \hat{a}^+\hat{a},$$

so

$$H = \hbar\omega\left(\hat{n} + \tfrac{1}{2}\right),$$

as expected.

(b)

We are given

$$\hat{n}|n\rangle = n|n\rangle.$$

We also have

$$\begin{aligned}[\hat{n}, \hat{a}^+] &= [\hat{a}^+\hat{a}, \hat{a}^+] \\ &= \hat{a}^+\hat{a}\hat{a}^+ - \hat{a}^+\hat{a}^+\hat{a} \\ &= \hat{a}^+(\hat{a}^+\hat{a}+1) - \hat{a}^+\hat{a}^+\hat{a} \\ &= \hat{a}^+\hat{a}^+\hat{a} + \hat{a}^+ - \hat{a}^+\hat{a}^+\hat{a} \\ &= \hat{a}^+.\end{aligned}$$

We want to show

$$\hat{a}^+|n\rangle = d(n)|n+1\rangle.$$

We have

$$\begin{aligned}\hat{n}\hat{a}^+|n\rangle &= \left([\hat{n},\hat{a}^+] + \hat{a}^+\hat{n}\right)|n\rangle \\ &= (\hat{a}^+ + \hat{a}^+\hat{n})|n\rangle \\ &= (n+1)\hat{a}^+|n\rangle\end{aligned}$$

This implies that $\hat{a}^+|n\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $(n+1)$. Since $\hat{n}$ applied to a state returns the number associated with the state, we know that we must have

$$\hat{a}^+|n\rangle = d(n)|n+1\rangle, \qquad (2)$$

where $d(n)$ is some constant that depends on n.

(b), cont'd...

Similarly, we have

$$
\begin{aligned}
[\hat{n}, \hat{a}] &= [\hat{a}^{+}\hat{a}, \hat{a}] \\
&= \hat{a}^{+}\hat{a}\hat{a} - \hat{a}\hat{a}^{+}\hat{a} \\
&= (\hat{a}\hat{a}^{+} - 1)\hat{a} - \hat{a}\hat{a}^{+}\hat{a} \\
&= \hat{a}\hat{a}^{+}\hat{a} - \hat{a} - \hat{a}\hat{a}^{+}\hat{a} \\
&= -\hat{a} \, .
\end{aligned}
$$

We want to show

$$\hat{a}|n\rangle = c(n)|n-1\rangle .$$

We have

$$
\begin{aligned}
\hat{n}\hat{a}|n\rangle &= \left([\hat{n},\hat{a}] + \hat{a}\hat{n}\right)|n\rangle \\
&= \left(-\hat{a} + \hat{a}\hat{n}\right)|n\rangle \\
&= (n-1)\hat{a}|n\rangle .
\end{aligned}
$$

This implies

$$\hat{a}|n\rangle = c(n)|n-1\rangle, \qquad (1)$$

where $c(n)$ is a constant that depends on n.

(b), cont'd...

Taking the complex conjugate of each side in ①, we get

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = |c(n)|^2 \langle n-1|n-1\rangle .$$

Since the eigenstates are orthonormal, we have

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = |c(n)|^2 .$$

But

$$\hat{n} = \hat{a}^{+}\hat{a}$$

and

$$\hat{n}|n\rangle = n|n\rangle ,$$

so

$$\langle n|\hat{n}|n\rangle = |c(n)|^2$$

$$\langle n|n|n\rangle = |c(n)|^2$$

$$n\langle n|n\rangle = |c(n)|^2$$

$$n = |c(n)|^2$$

and

$$c(n) = \sqrt{n} .$$

Then

$$\boxed{\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle} .$$

(b), cont'd...

Taking the complex conjugate of each side in (2), we get

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = |d(n)|^2 \langle n+1|n+1\rangle$$

$$\langle n|(\hat{a}^{+}\hat{a}+1)|n\rangle = |d(n)|^2$$

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle + \langle n|1|n\rangle = |d(n)|^2$$

$$\langle n|\hat{n}|n\rangle + \langle n|n\rangle = |d(n)|^2$$

$$\langle n|n|n\rangle + 1 = |d(n)|^2$$

$$n\langle n|n\rangle + 1 = |d(n)|^2$$

$$n+1 = |d(n)|^2$$

$$d(n) = \sqrt{n+1},$$

so

$$\boxed{\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle}$$

(c)

We know

$$V(x) = \frac{\hbar\omega}{2} x^2 \geq 0.$$

This implies that the eigenenergies must be positive because we know that the kinetic energy cannot be negative.

It also implies that the eigenvalues of $\hat{n}$ are positive because

$$V(x) = \frac{\hbar\omega}{2}\left(\frac{\hat{a}+\hat{a}^+}{2}\right)^2 \geq 0$$

$$= \frac{\hbar\omega}{4}\left(\hat{a}\hat{a} + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}^+\hat{a}^+\right) \geq 0$$

$$V(x)|n\rangle = \frac{\hbar\omega}{4}\left(\hat{a}\hat{a} + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}^+\hat{a}^+\right)|n\rangle$$

$$= \frac{\hbar\omega}{4}\left[\hat{a}\sqrt{n}\,|n-1\rangle + \hat{a}\sqrt{n+1}\,|n+1\rangle + \hat{a}^+\sqrt{n}\,|n-1\rangle + \hat{a}^+\sqrt{n+1}\,|n+1\rangle\right]$$

$$= \frac{\hbar\omega}{4}\left[\sqrt{n(n-1)}\,|n-2\rangle + (n+1)|n\rangle + (n)|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle\right]$$

$$= \frac{\hbar\omega}{4}\left[\sqrt{n(n-1)}\,|n-2\rangle + (2n+1)|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle\right]$$

In order for this to be ≥ 0, the eigenvalues of $\hat{n}$ must be positive. This also shows us that the lowest value of n is zero.
If we allowed $|-1\rangle$, we would have

$$a^+|-1\rangle = (-1+1)|0\rangle$$
$$= 0,$$

which makes no sense. So $|0\rangle$ must be our lowest eigenstate.

(d)

Let $|0\rangle = \psi_0$. Then

$$\hat{a}\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}(x + ip)\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}\left(\frac{X}{\lambda} + i\frac{\lambda}{\hbar}P\right)\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}X + \frac{i\lambda}{\hbar}\left(-i\hbar\frac{d}{dX}\right)\right)\psi_0 = 0$$

$$\left(\sqrt{\frac{m\omega}{\hbar}}X + \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dX}\right)\psi_0 = 0$$

$$\boxed{\frac{d\psi_0}{dX} = -\frac{m\omega}{\hbar}X\psi_0}$$

and

$$\int\frac{1}{\psi_0}d\psi_0 = \int -\frac{m\omega}{\hbar}X\,dX$$

$$\ln\psi_0 = -\frac{m\omega}{2\hbar}X^2 + C_1$$

$$\psi_0 = Ce^{-\frac{m\omega}{2\hbar}X^2}$$

where C is a constant. Normalizing...

$$\int|\psi_0|^2dx = 1$$

$$C^2\int e^{-\frac{m\omega}{\hbar}X^2}dx = 1$$

$$C^2\left(\sqrt{\frac{\pi\hbar}{m\omega}}\right) = 1$$

$$C = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

so

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}X^2}}.$$

(e)

We know $|1\rangle = \psi_1 = a^+\psi_0$. So

$$\psi_1 = a^+\psi_0$$
$$= \frac{1}{\sqrt{2}}(x - ip)\psi_0$$
$$= \frac{1}{\sqrt{2}}\left(\frac{X}{\lambda} - i\frac{\lambda}{\hbar}P\right)\psi_0$$
$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}X - \frac{i}{\sqrt{m\omega\hbar}}\left(-i\hbar\frac{d}{dX}\right)\right)\psi_0$$
$$= \sqrt{\frac{m\omega}{2\hbar}}X\psi_0 - \sqrt{\frac{\hbar}{2m\omega}}\frac{d\psi_0}{dX}$$
$$= \sqrt{\frac{m\omega}{2\hbar}}X\psi_0 - \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(-\frac{m\omega}{\hbar}X e^{-\frac{m\omega}{2\hbar}X^2}\right)$$
$$= \sqrt{\frac{m\omega}{2\hbar}}X\psi_0 + \sqrt{\frac{m\omega}{2\hbar}}X\psi_0$$

$$\boxed{\psi_1(x) = \sqrt{\frac{2m\omega}{\hbar}}X\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}X^2}}$$