

## 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

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

Define the unitless variables

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

such that the Hamiltonian has the form

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

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

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

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

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

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

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

$$\hat{n}|n\rangle = n|n\rangle, \quad (6)$$

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

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

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) Given:  $H = \frac{\hbar\omega}{2}(p^2 + x^2)$ ,  $[x, p] = i$

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

\* Rewrite  $H$  in terms  $a, a^\dagger$  then

$$\begin{aligned} \Rightarrow \sqrt{2}a &= (x + ip) & \Leftrightarrow & \quad x = \frac{1}{\sqrt{2}}(a + a^\dagger) \\ \sqrt{2}a^\dagger &= (x - ip) & & \quad p = \frac{i}{\sqrt{2}}(a - a^\dagger) \end{aligned}$$

$$\begin{aligned} \Rightarrow H &= \frac{\hbar\omega}{2} \left( \left[ \frac{-i}{\sqrt{2}}(a - a^\dagger) \right]^2 + \left[ \frac{1}{\sqrt{2}}(a + a^\dagger) \right]^2 \right) \\ &= \frac{\hbar\omega}{2} \left( \frac{-1}{2}(aa - a^\dagger a - aa^\dagger + a^\dagger a^\dagger) + \frac{1}{2}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger) \right) \\ &= \frac{\hbar\omega}{2} (aa^\dagger + a^\dagger a) \\ &= \frac{\hbar\omega}{2} (a^\dagger a + 1 + a^\dagger a) \quad (\text{from } [a, a^\dagger] = 1) \\ &= \hbar\omega(n + 1/2) \checkmark \end{aligned}$$

b) \* Remember that  $[n, a] = -a$ ,  $[n, a^\dagger] = a^\dagger$

$\Rightarrow$  Solve by using the above commutator relations

$$\begin{aligned} n(a|n\rangle) &= (an - a)|n\rangle \\ &= a(n-1)|n\rangle \\ &= (n-1)(a|n\rangle) \quad \Rightarrow a|n\rangle = c_n |n-1\rangle \end{aligned}$$

$$\begin{aligned} n(a^\dagger|n\rangle) &= (a^\dagger n + a^\dagger)|n\rangle \\ &= a^\dagger(n+1)|n\rangle \\ &= (n+1)(a^\dagger|n\rangle) \quad \Rightarrow a^\dagger|n\rangle = d_n |n+1\rangle \end{aligned}$$

$\Rightarrow$  Determine  $c_n$  and  $d_n$  through normalization

$$\langle n|a^\dagger a|n\rangle = |c_n|^2 \langle n-1|n-1\rangle$$

$$n \langle n|n\rangle = |c_n|^2$$

$$n = |c_n|^2 \Rightarrow \boxed{c_n = \sqrt{n}}$$

#1(cont.)

$$b) \quad \langle n | a a^\dagger | n \rangle = |d_n|^2 \langle n+1 | n+1 \rangle$$

$$\langle n | a^\dagger a + 1 | n \rangle = |d_n|^2$$

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

$$n+1 = |d_n|^2 \Rightarrow d_n = \sqrt{n+1}$$

- c) ① Given a potential  $V(x) = \frac{1}{2} \hbar \omega x^2 \geq 0$  for all  $x$  and combined with the fact that  $T \geq 0$  (since kinetic energy can never be negative), then  $(H = T + V) \geq 0$  at all times, thus its eigenenergies must also be positive

② We can rewrite our potential as:  $V = \frac{1}{2} \hbar \omega \left( \frac{a + a^\dagger}{\sqrt{2}} \right)^2$

$$\Rightarrow V = \frac{\hbar \omega}{4} (aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$$

$$V|n\rangle = \frac{\hbar \omega}{4} (aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)|n\rangle$$

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

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

\* For the above equation to be greater than or equal to 0,  $n$  must also be greater than or equal to 0

- ③ In order for the above to be true  $a|0\rangle = 0$  because  $n \geq 0$ . Following our work from part b

$$n(a|0\rangle) = (an - a)|0\rangle$$

$$= a(0-1)|0\rangle$$

$$= -a|0\rangle = c_n|-1\rangle$$

$$\langle 0 | -a^\dagger - a | 0 \rangle = |c_n|^2 \langle -1 | -1 \rangle$$

$$0 \langle 0 | 0 \rangle = |c_n|^2 \langle -1 | -1 \rangle$$

$$0 = |c_n|^2 \langle -1 | -1 \rangle$$

$$\hookrightarrow \langle -1 | -1 \rangle = 0$$

#1 (cont.)

d) If we let  $\psi_0 = \psi_0$

$$a \psi_0 = 0$$

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

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

$$\frac{1}{\sqrt{2}} \left( \frac{1}{\lambda} x + i \frac{\lambda}{\hbar} \left( -i \hbar \frac{\partial}{\partial x} \right) \right) \psi_0 = 0$$

$$\frac{1}{\sqrt{2}} \left( \frac{1}{\lambda} x + \lambda \frac{\partial}{\partial x} \right) \psi_0 = 0$$

$$\frac{1}{\lambda} x \psi_0 = -\lambda \frac{\partial \psi_0}{\partial x}$$

$$\int x \partial x = \int -\lambda^2 \frac{\partial \psi_0}{\psi_0}$$

$$\frac{1}{2\lambda^2} x^2 + C = \ln(\psi_0)$$

$$\exp \left[ \frac{-x^2}{2\lambda^2} + C \right] = \psi_0$$

$$\hookrightarrow \psi_0 = C \exp \left[ \frac{m\omega x^2}{2\hbar} \right]$$

\* Normalizing our wavefunction

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

$$1 = C^2 \int \left| \exp \left[ \frac{m\omega}{2\hbar} x^2 \right] \right|^2 dx$$

$$1 = C^2 \int \exp \left[ \frac{m\omega}{\hbar} x^2 \right] dx$$

$$1 = C^2 \sqrt{\frac{\pi \hbar}{m\omega}}$$

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

$$\Rightarrow \psi_0 = \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \exp \left[ \frac{m\omega}{2\hbar} x^2 \right]$$

#1 (cont.)

e) \* Following a similar progression to part d

$$|1\rangle = \psi_1 = a^\dagger |0\rangle$$

$$\psi_1 = \frac{1}{\sqrt{2}} (x - c p) \psi_0$$

$$= \frac{1}{\sqrt{2}} \left( \frac{x}{\lambda} - i \frac{\lambda}{\hbar} (-i \hbar \frac{\partial}{\partial x}) \right) \psi_0$$

$$= \frac{1}{\sqrt{2}} \left( \frac{x}{\lambda} - \lambda \frac{\partial}{\partial x} \right) \psi_0$$

$$= \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}} x - \sqrt{\frac{\hbar}{m\omega}} \frac{\partial}{\partial x} \right) \left[ \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \exp \left[ -\frac{m\omega}{2\hbar} x^2 \right] \right]$$

$$= \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}} x \psi_0 - \sqrt{\frac{\hbar}{m\omega}} \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \left( -x \frac{m\omega}{\hbar} \right) \exp \left[ -\frac{m\omega}{2\hbar} x^2 \right] \right)$$

$$= \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}} x \psi_0 + \sqrt{\frac{m\omega}{\hbar}} x \psi_0 \right)$$

$$= \sqrt{\frac{2m\omega}{\hbar}} x \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \exp \left[ -\frac{m\omega}{2\hbar} x^2 \right]$$