Week 4

Observables and Hermitian Operators

4.1 Harmonic Oscillator: Raising and Lowering Operators

1/22: • **Raising operator**: The operator defined as follows. *Denoted by* $\hat{\boldsymbol{a}}_+$, $\boldsymbol{a}_+$. *Given by*

$$\hat{a}_+ = \frac{1}{\sqrt{2\hbar m\omega}}[-i\hat{\vec{p}} + m\omega\hat{\vec{x}}]$$

• **Lowering operator**: The operator defined as follows. *Denoted by* $\hat{\boldsymbol{a}}_-$, $\boldsymbol{a}_-$. *Given by*

$$\hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}}[i\hat{\vec{p}} + m\omega\hat{\vec{x}}]$$

• **Number operator**: The operator defined as follows. *Denoted by* $\boldsymbol{a}_+\boldsymbol{a}_-$. *Given by*

$$a_+a_- = \hat{a}_+ \circ \hat{a}_- = \frac{1}{2\hbar m\omega}\left[\hat{\vec{p}}^2 + m^2\omega^2x^2 - im\omega[\hat{\vec{p}}, \hat{\vec{x}}]\right]$$

• Properties of these operators.

  – We can express $\hat{\vec{p}}, \hat{\vec{x}}$ in terms of a_+, a_- via

$$\hat{\vec{p}} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-) \qquad \hat{\vec{x}} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-)$$

    ■ It follows that

$$[\hat{\vec{p}}, \hat{\vec{x}}] = \frac{i\hbar}{2}[a_+ - a_-, a_+ + a_-] = \frac{i\hbar}{2}([a_+, a_-] - [a_-, a_+]) = i\hbar[a_+, a_-]$$

    ■ Consequently, since $[\hat{\vec{p}}, \hat{\vec{x}}] = -i\hbar$, we have that

$$[a_+, a_-] = -1$$

    ■ We also have that

$$[a_-, a_+] = 1$$

  – Since $[\hat{\vec{p}}, \hat{x}] = -i\hbar$ and $\omega^2 = k/m$, we have that

$$\begin{aligned}
a_+a_- &= \frac{1}{2\hbar m\omega}\left[\hat{\vec{p}}^2 + m^2\omega^2x^2 - m\hbar\omega\right] \\
&= \frac{1}{\hbar\omega}\left[\underbrace{\frac{\hat{\vec{p}}^2}{2m} + \frac{kx^2}{2}}_{\hat{H}} - \frac{\hbar\omega}{2}\right] \\
\hat{H} &= \hbar\omega\left(a_+a_- + \frac{1}{2}\right)
\end{aligned}$$

- Because of the properties of $[a_+, a_-]$ proven above, we similarly have that

$$\hat{H} = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)$$

- We can also derive this equation in a manner exactly analogous to the first one.

- How does the number operator act on the eigenstate $|\psi_n\rangle$ of the harmonic oscillator?
  - Since $E_n = \hbar\omega(n + 1/2)$, we have that

$$\begin{aligned}
\hbar\omega\left(a_+ a_- + \frac{1}{2}\right)|\psi_n\rangle &= \hat{H}\,|\psi_n\rangle \\
\hbar\omega\left(a_+ a_- + \frac{1}{2}\right)|\psi_n\rangle &= \hbar\omega\left(n + \frac{1}{2}\right)|\psi_n\rangle \\
a_+ a_-\,|\psi_n\rangle &= n\,|\psi_n\rangle
\end{aligned}$$

- How do the raising and lowering operators act on the eigenstate $|\psi_n\rangle$ of the harmonic oscillator?
  - Using a number of the above substitutions, we have that

$$\begin{aligned}
\hat{H}(a_+\,|\psi_n\rangle) &= \left[\hbar\omega\left(a_+ a_- + \frac{1}{2}\right)\right](a_+\,|\psi_n\rangle) \\
&= \hbar\omega\left(a_+ a_- a_+ + \frac{1}{2}a_+\right)|\psi_n\rangle \\
&= \hbar\omega a_+\left(a_- a_+ + \frac{1}{2}\right)|\psi_n\rangle \\
&= \hbar\omega a_+\left(a_+ a_- + 1 + \frac{1}{2}\right)|\psi_n\rangle \\
&= \hbar\omega a_+\left(n + 1 + \frac{1}{2}\right)|\psi_n\rangle \\
&= E_{n+1}(a_+\,|\psi_n\rangle)
\end{aligned}$$

  - This means that $\hat{H}$ acts on $a_+\,|\psi_n\rangle$ the same way it acts on $|\psi_{n+1}\rangle$. In other words, it must be that

$$a_+\,|\psi_n\rangle \propto |\psi_{n+1}\rangle$$

  - Similarly,

$$\hat{H}(a_-\,|\psi_n\rangle) = E_{n-1}(a_-\,|\psi_n\rangle)$$

    so

$$a_-\,|\psi_n\rangle \propto |\psi_{n-1}\rangle$$

  - These actions are why a_+, a_- are called the *raising* and *lowering* operators!
  - We now seek to determine the constants of proportionality.
  - First off, note that a_+ and a_- are adjoints, i.e.,

$$a_+^\dagger = a_-$$

    - This identity is evident from the original $\hat{a}_+, \hat{a}_-$ definitions, where the only difference between the two definitions is the conjugacy of the imaginary momentum term!
    - Is this correct, or do I have to appeal to the formal $\langle\psi_i|\hat{a}_+\psi_j\rangle = \langle\hat{a}_+^\dagger\psi_i|\psi_j\rangle$ definition??

- Then for a_+, we know that if

$$a_+ |\psi_n\rangle = c_+ |\psi_n\rangle$$

then

$$\begin{aligned} c_+^2 &= c_+^2 \langle\psi_{n+1}|\psi_{n+1}\rangle \\ &= \langle c_+\psi_{n+1}|c_+\psi_{n+1}\rangle \\ &= \langle a_+\psi_n|a_+\psi_n\rangle \\ &= \langle\psi_n|a_+^\dagger a_+|\psi_n\rangle \\ &= \langle\psi_n|a_-a_+|\psi_n\rangle \\ &= \langle\psi_n|a_+a_- + 1|\psi_n\rangle \\ &= (n+1)\langle\psi_n|\psi_n\rangle \\ &= n+1 \end{aligned}$$

so that, taking square roots,

$$c_+ = \sqrt{n+1}$$

- By the same method — namely

$$c_-^2 = \langle a_-\psi_n|a_-\psi_n\rangle = \langle\psi_n|a_+a_-|\psi_n\rangle = n$$

we can also learn that

$$c_- = \sqrt{n}$$

- Therefore,

$$a_+ |\psi_n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle \qquad\qquad a_- |\psi_n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle$$

- Note that what we have done here to derive this fact is far more slick than working directly with the unintuitive and complicated formal definitions of a_+, a_-.

- Now is a good time to mention a bit more about Dirac notation.
  - A "ket" represents a vector in a Hilbert space, so $|\psi_n\rangle$ demonstrates that we are talking about the wave function as a vector in the abstract linear algebra sense, not as a function $\psi_n : \mathbb{R}^4 \to \mathbb{C}$.
  - A "bra" represents a linear functional on a Hilbert space. In quantum mechanics, the linear functional $\langle\eta|$ is given by

$$\langle\eta| := \int \mathrm{d}^3\vec{r}\;\eta^*$$

  - Observe that this "functional" does indeed map any $|\psi_n\rangle$ given to it as an argument to a number $\langle\eta|\psi_n\rangle$!

- $|\psi_n\rangle$ can be defined in terms of a_+, $|\psi_0\rangle$, and constants.
  - Observe that since $a_+ |\psi_0\rangle = |\psi_1\rangle$ and $a_+ |\psi_1\rangle = \sqrt{2}\,|\psi_2\rangle$, we have that

$$|\psi_2\rangle = \frac{a_+}{\sqrt{2}}|\psi_1\rangle = \frac{a_+^2}{\sqrt{2}}|\psi_0\rangle$$

  - Similarly,

$$|\psi_3\rangle = \frac{a_+}{\sqrt{3}}|\psi_2\rangle = \frac{a_+^3}{\sqrt{3\cdot 2}}|\psi_0\rangle$$

  - Generalizing, we have that

$$|\psi_n\rangle = \frac{a_+^n}{\sqrt{n!}}|\psi_0\rangle$$

- Thus, we have that
$$\psi_n(x) = \left(\frac{1}{\sqrt{2\hbar m\omega}}\right)^n \frac{1}{\sqrt{n!}} \left(-\hbar\frac{\mathrm{d}}{\mathrm{d}x} + xm\omega\right)^n \psi_0(x)$$
where we may recall that
$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \mathrm{e}^{-m\omega x^2/2\hbar}$$
- Final observations about the raising and lowering operators.
  - Since $a_- |\psi_0\rangle = 0$ (as we may readily verify by direct computation), we have that
$$\hbar\frac{\mathrm{d}\psi_0}{\mathrm{d}x} + m\omega x\psi_0 = 0$$
  - We also know that
$$\mathrm{d}(\ln(\psi_0)) = -\frac{m\omega}{\hbar}\frac{\mathrm{d}x^2}{2}$$
so
$$\psi_0 \propto \mathrm{e}^{-m\omega x^2/2\hbar}$$
    - What is the point of this line?? What new information does it give us?
- Raising and lowering operators allow us to compute the kinetic and potential energy of the harmonic oscillator.
  - Kinetic energy.
$$\begin{aligned}
\left\langle \psi_n \middle| \frac{\hat{p}^2}{2m} \middle| \psi_n \right\rangle &= -\frac{\hbar\omega}{4} \langle \psi_n|(a_+ - a_-)^2|\psi_n\rangle \\
&= -\frac{\hbar\omega}{4} \langle \psi_n|a_+^2 + a_-^2 - a_+a_- - a_-a_+|\psi_n\rangle \\
&= -\frac{\hbar\omega}{4} \Big[\underbrace{\langle \psi_n|a_+^2|\psi_n\rangle}_{\propto \langle\psi_n|\psi_{n+2}\rangle} + \underbrace{\langle \psi_n|a_-^2|\psi_n\rangle}_{\propto \langle\psi_n|\psi_{n-2}\rangle} - \underbrace{2\langle \psi_n|a_+a_-|\psi_n\rangle}_{2n\langle\psi_n|\psi_n\rangle} - \underbrace{\langle \psi_n|1|\psi_n\rangle}_{\langle\psi_n|\psi_n\rangle} \Big] \\
&= \frac{\hbar\omega}{4}(2n+1) \\
&= \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right) \\
&= \frac{E_n}{2}
\end{aligned}$$
  - Potential energy.
$$\begin{aligned}
\langle \psi_n|\hat{H}|\psi_n\rangle &= E_n \\
\left\langle \psi_n \middle| \frac{\hat{p}^2}{2m} \middle| \psi_n \right\rangle + \left\langle \psi_n \middle| k\frac{\hat{x}^2}{2} \middle| \psi_n \right\rangle &= \frac{E_n}{2} + \frac{E_n}{2} \\
\left\langle \psi_n \middle| k\frac{\hat{x}^2}{2} \middle| \psi_n \right\rangle &= \frac{E_n}{2}
\end{aligned}$$
  - Implication: In an energy eigenstate, the harmonic oscillator has equal values of kinetic and potential energies!

- Computing more observables.
  - We can show that

$$\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle = \langle\psi_n|\hat{\vec{p}}|\psi_n\rangle = 0 \qquad \langle\psi_n|\hat{\vec{x}}^2|\psi_n\rangle = \frac{\hbar\omega}{k}\left(n+\frac{1}{2}\right) \qquad \langle\psi_n|\hat{\vec{p}}^2|\psi_n\rangle = \hbar\omega m\left(n+\frac{1}{2}\right)$$

- It follows from the above computations and the facts that

$$\Delta x^2 = \langle\psi_n|\hat{\vec{x}}^2|\psi_n\rangle - (\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle)^2 \qquad \Delta p^2 = \langle\psi_n|\hat{\vec{p}}^2|\psi_n\rangle - (\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle)^2$$

that

$$\Delta x^2 \cdot \Delta p^2 = \hbar^2\left(n+\frac{1}{2}\right)^2$$
$$\Delta x \cdot \Delta p = \frac{\hbar}{2}(2n+1)$$

  - Implication: The ground state $\psi_0(x)$ is represented by a Gaussian since in this case, $\Delta x \cdot \Delta p = \hbar/2$.
- Review from last class.
  - Mostly stuff I already wrote down.
  - One new equation formalizing the even/odd solutions:

$$f_n(x) = (-1)^n f_n(-x)$$

  - The first four Hermite polynomials:

$$H_0(\xi) = 1 \qquad H_1(\xi) = 2\xi \qquad H_2(\xi) = 4\xi^2 - 2 \qquad H_3 = 8\xi^3 - 12\xi$$

  - Summary of the characteristics of E_n: The energy is quantized and grows linearly with n in quanta of $\hbar\omega$, and has a minimum value $\hbar\omega/2$.
  - As with other time-independent potentials, the general solution to the Schrödinger equation will be

$$\psi(x,t) = \sum_n c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar}$$

where

$$\langle\psi|\hat{H}|\psi\rangle = \sum_n |c_n|^2 E_n$$