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

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

    - 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 $a_- \left|\psi_0\right\rangle = 0$ (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.

$$\begin{aligned}
\left\langle \psi_n \middle| \frac{\hat{p}^2}{2m} \middle| \psi_n \right\rangle &= -\frac{\hbar\omega}{4} \left\langle \psi_n \middle| (a_+ - a_-)^2 \middle| \psi_n \right\rangle \\
&= -\frac{\hbar\omega}{4} \left\langle \psi_n \middle| a_+^2 + a_-^2 - a_+a_- - a_-a_+ \middle| \psi_n \right\rangle \\
&= -\frac{\hbar\omega}{4} \Big[\underbrace{\left\langle \psi_n \middle| a_+^2 \middle| \psi_n \right\rangle}_{\propto \langle\psi_n|\psi_{n+2}\rangle} + \underbrace{\left\langle \psi_n \middle| a_-^2 \middle| \psi_n \right\rangle}_{\propto \langle\psi_n|\psi_{n-2}\rangle} - \underbrace{2\left\langle \psi_n \middle| a_+a_- \middle| \psi_n \right\rangle}_{2n\langle\psi_n|\psi_n\rangle} - \underbrace{\left\langle \psi_n \middle| 1 \middle| \psi_n \right\rangle}_{\langle\psi_n|\psi_n\rangle} \Big] \\
&= \frac{\hbar\omega}{4}(2n+1) \\
&= \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right) \\
&= \frac{E_n}{2}
\end{aligned}$$

  - Potential energy.

$$\begin{aligned}
\left\langle \psi_n \middle| \hat{H} \middle| \psi_n \right\rangle &= E_n \\
\left\langle \psi_n \middle| \frac{\hat{p}^2}{2m} \middle| \psi_n \right\rangle + \left\langle \psi_n \middle| k\frac{\hat{x}^2}{2} \middle| \psi_n \right\rangle &= \frac{E_n}{2} + \frac{E_n}{2} \\
\left\langle \psi_n \middle| k\frac{\hat{x}^2}{2} \middle| \psi_n \right\rangle &= \frac{E_n}{2}
\end{aligned}$$

  - 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

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

4.2 Time Dependence and Coherent States

1/24: - Review of the harmonic oscillator.
  - Our Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{kx^2}{2} = \frac{\hat{\vec{p}}^{\,2}}{2m} + \frac{k\hat{\vec{x}}^{\,2}}{2}$$

    - We have an analogy with the classical $\omega^2 = k/m$.
  - Under this Hamiltonian, $\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle$ implies that

$$E_n = \hbar\omega\left(\frac{1}{2}+n\right)$$

  - The raising and lowering operators are given by

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

    - Together, these imply that

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

    - We also have that

$$\begin{aligned} a_+a_-\left|\psi_n\right\rangle &= n\left|\psi_n\right\rangle & \qquad a_+\left|\psi_n\right\rangle &= \sqrt{n+1}\left|\psi_{n+1}\right\rangle \\ [a_-,a_+] &= 1 & a_-\left|\psi_n\right\rangle &= \sqrt{n}\left|\psi_{n-1}\right\rangle \end{aligned}$$

    - We call a_+a_- the number operator.
    - We should go home and learn these formulas.
  - The full eigenstate is

$$\psi(x,t) = \sum_{n=0}^{\infty} \underbrace{c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar}}_{\psi_n(x,t)}$$

  - Two properties of this eigenstate.
    1. We have that

$$\left|\psi\right\rangle = \sum_{n=0}^{\infty} c_n\mathrm{e}^{-iE_nt/\hbar}\left|\psi_n\right\rangle$$

       which implies that

$$\sum_{n=0}^{\infty} |c_n|^2 = 1$$

       since $\langle\psi|\psi\rangle = 1$ and $\langle\psi_n|\psi_m\rangle = \delta_{nm}$.
    2. We have that

$$\langle\psi|\hat{H}|\psi\rangle = \sum_{n=0}^{\infty} |c_n|^2 E_n$$

  - We have that

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

    - Note that this makes sense because the sum $E_n/2 + E_n/2$ of potential and kinetic should be E_n, and it will be!
  - Additionally, recall that we have

$$\hat{\vec{p}}^2 \propto (a_+ - a_-)^2 \qquad \hat{\vec{x}}^2 \propto (a_+ + a_-)^2$$

    - Thus, we have that

$$\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle = \langle\psi_n|(a_+ - a_-)|\psi_n\rangle = 0 \qquad \langle\psi_n|\hat{\vec{x}}|\psi_n\rangle = \langle\psi_n|(a_+ + a_-)|\psi_n\rangle = 0$$

  - The harmonic oscillator is a very important problem in physics, and we should know it by heart! (In order to pass the class.)
- Recall as well that there is a correspondence between the Dirac notation and the functional notation, given by

$$\psi_n(x) \mapsto \left|\psi_n\right\rangle$$

  - As an additional example,

$$\frac{1}{\sqrt{2\hbar m\omega}}\left[-\hbar\frac{\mathrm{d}}{\mathrm{d}x} + m\omega x\right]\psi_n(x) = \sqrt{n+1}\psi_{n+1}(x) \quad\mapsto\quad a_+\left|\psi_n\right\rangle = \sqrt{n+1}\left|\psi_{n+1}\right\rangle$$

- One more example:

$$\hbar\frac{\mathrm{d}\psi_0}{\mathrm{d}x}+m\omega x\psi_0(x)=0 \quad\mapsto\quad a_-\left|\psi_0\right\rangle=0$$

  - Note that solving this ODE yields the solution

$$\psi_0=C\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

  - It appears that this is how we intuitively derive the ansatz we used last Friday!

- Now we start on some new content.
- Observe that

$$\begin{aligned}\frac{2m\omega\hat{\vec{x}}}{\sqrt{2\hbar m\omega}}&=a_++a_-\\ \hat{\vec{x}}&=\sqrt{\frac{\hbar}{2m\omega}}(a_++a_-)\end{aligned}$$

- In classical mechanics, the solution to the harmonic oscillator is

$$x(t)=A\sin\omega t+B\cos\omega t$$

- We now investigate the observables of $|\psi\rangle$.
- To start with, we show how $\langle\psi|\hat{\vec{x}}|\psi\rangle$ varies with time. This will lead into a discussion of something called coherent states. Let's begin.
  - We start with

$$\langle\psi|\hat{\vec{x}}|\psi\rangle=\sum_{m,n=0}^{\infty}c_m^*c_n\mathrm{e}^{i(E_m-E_n)t/\hbar}\left\langle\psi_n|\hat{\vec{x}}|\psi_n\right\rangle$$

  - We can algebraically manipulate the above to

$$\begin{aligned}\langle\psi|\hat{\vec{x}}|\psi\rangle&=\sum_{m,n=0}^{\infty}c_m^*c_n\mathrm{e}^{i(\hbar\omega(m-n))t/\hbar}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta_{m,n+1}+\sqrt{n}\delta_{m,n-1}\right)\\ &=\sum_{n=0}^{\infty}c_{n+1}^*c_n\mathrm{e}^{i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}+\sum_{n=1}^{\infty}c_{n-1}^*c_n\mathrm{e}^{-i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n}\\ &=\sum_{n=0}^{\infty}c_{n+1}^*c_n\mathrm{e}^{i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}+\sum_{n=0}^{\infty}c_n^*c_{n+1}\mathrm{e}^{-i\omega t}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}\\ &=\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t)\left[\sum_{n=0}^{\infty}\left(c_{n+1}^*c_n+c_n^*c_{n+1}\right)\sqrt{n+1}\right]\\ &\quad+\sqrt{\frac{\hbar}{2m\omega}}\sin(\omega t)\left[\sum_{n=0}^{\infty}\left(c_{n+1}^*c_n-c_n^*c_{n+1}\right)\sqrt{n+1}\right]\end{aligned}$$

  - Thus,

$$\langle\psi|\hat{\vec{x}}|\psi\rangle=A\cos\omega t+B\sin\omega t$$

    where

$$\begin{aligned}A&=2\operatorname{Re}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{\hbar}{2m\omega}} & B&=2\operatorname{Im}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{\hbar}{2m\omega}}\\ &=\operatorname{Re}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{2\hbar}{m\omega}} & &=\operatorname{Im}\left[\sum_{n=0}^{\infty}c_{n+1}^*c_n\sqrt{n+1}\right]\sqrt{\frac{2\hbar}{m\omega}}\end{aligned}$$

- Now for large values of n,

$$\sqrt{n+1}\sqrt{\frac{2\hbar}{m\omega}} = \sqrt{\frac{2\hbar\omega(n+1)}{m\omega^2}} \approx \sqrt{\frac{2E_n}{m\omega^2}}$$

  where

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \qquad x = A\sin\omega t \qquad E = \frac{m\omega^2 A^2}{2} \qquad A = \sqrt{\frac{2E}{m\omega^2}}$$

  - How can we just ignore the real and imaginary sum terms??
- Now take the harmonic oscillator. Notice that $\sum_n$ is dominated by large values of $n \approx \bar{n}$, close to $\bar{n}$, where $\bar{n} \gg 1$. Thus,

$$\langle\psi|\hat{\vec{x}}|\psi\rangle = \sqrt{\frac{2E\bar{n}}{m\omega^2}}\sum_{n=0}^{\infty}\mathrm{Re}\left[\sum c_{n+1}^* c_n\right]\sin\omega t$$

  and

$$\langle\psi|\hat{\vec{x}}^{\,2}|\psi\rangle - (\,\langle\psi|\hat{\vec{x}}|\psi\rangle)^2 \neq 0$$

- This is *not* classical motion.
- The states that come closest to realizing classical motion are called **coherent states**.

- **Coherent state**: A state in which the uncertainty in $\hat{\vec{x}}$ is minimized.
- Example:
  - We have that

$$a_-\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle \qquad a_-\left|\psi_0\right\rangle = 0\left|\psi_0\right\rangle$$

  - Then

$$\frac{\hbar}{2m\omega}\left[\,\langle\alpha|(a_+ + a_-)^2|\alpha\rangle - (\,\langle\alpha|(a_+ + a_-)|\alpha\rangle)^2\right] = \frac{\hbar}{2}$$
$$\frac{\hbar}{2m\omega}\left[\,\langle\alpha|a_+^2 + a_+a_- + a_-a_+ + a_-^2|\alpha\rangle - (\,\langle\alpha|(a_+ + a_-)|\alpha\rangle)^2\right] = \dots$$

  - We'll finish this up next time.