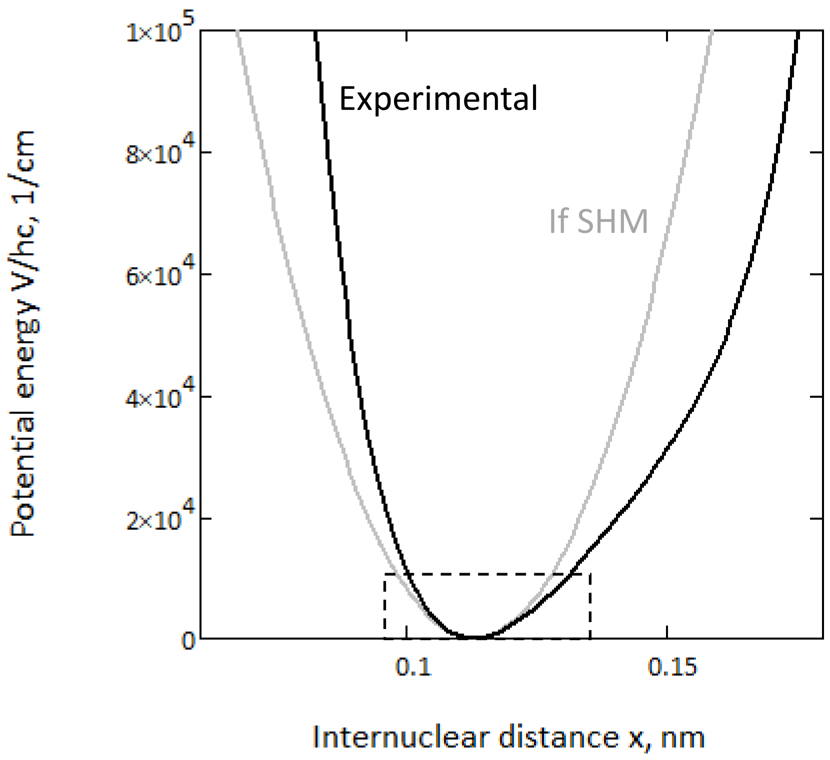
Today in Physics 237: quantum harmonic oscillator, the easy way

- Its Schrödinger equation, and the relation of the ideal 1-D quantum simple harmonic oscillator to vibrational states of diatomic molecules.
- Commutators, and the canonical commutator of x and $\hat{p}$
- Raising and lowering operators
- Operator-algebra solution to the time-independent Schrödinger equation for the quantum simple harmonic oscillator.
- Ground state, and nonzero zero-point energy

$^{12}C^{16}O$



The 1-D quantum harmonic oscillator

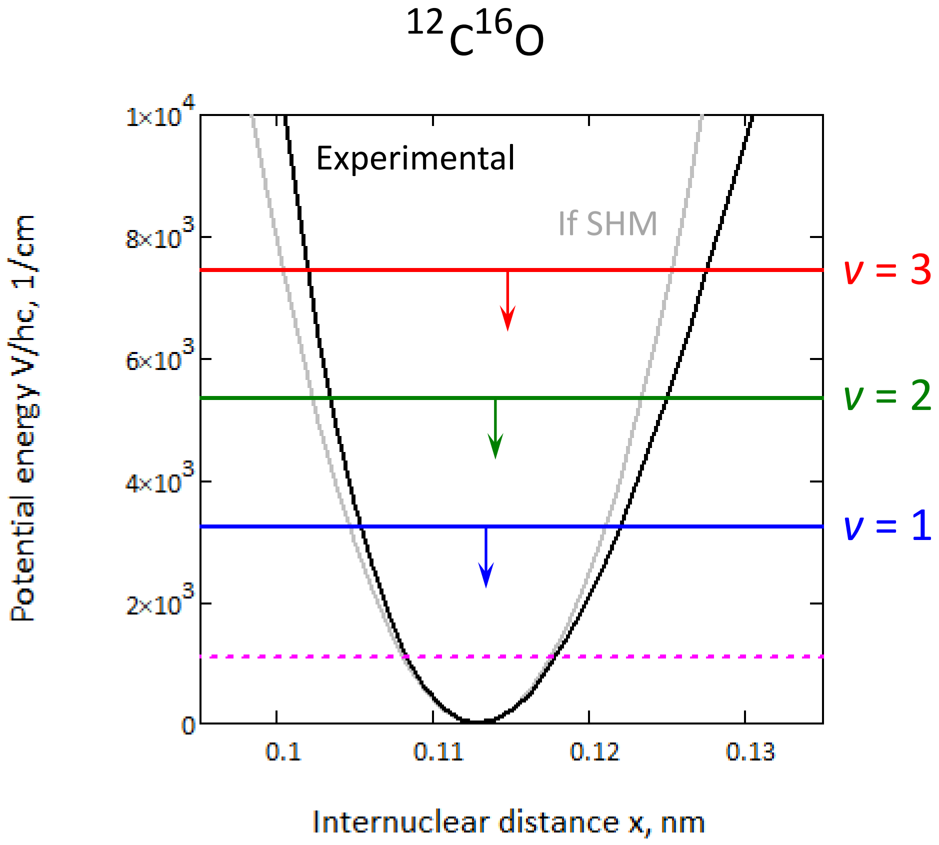
- Start with the potential energy of a classical 1-D simple harmonic oscillator,

$$V(x)=\frac{1}{2}kx^2=\frac{1}{2}m\omega^2x^2 \quad ,$$

where x is the displacement from the oscillator's equilibrium position.

- m could be a single quantum subject to a spring-like restoring force, or the **reduced mass** m' of two quanta which are bound together by a spring-like force but otherwise free, like an isolated **diatomic molecule**.
  - For example, CO: $m'\cong\frac{m_C m_O}{m_C+m_O}u=\frac{12\times16}{12+16}u=6.86u \quad ,$

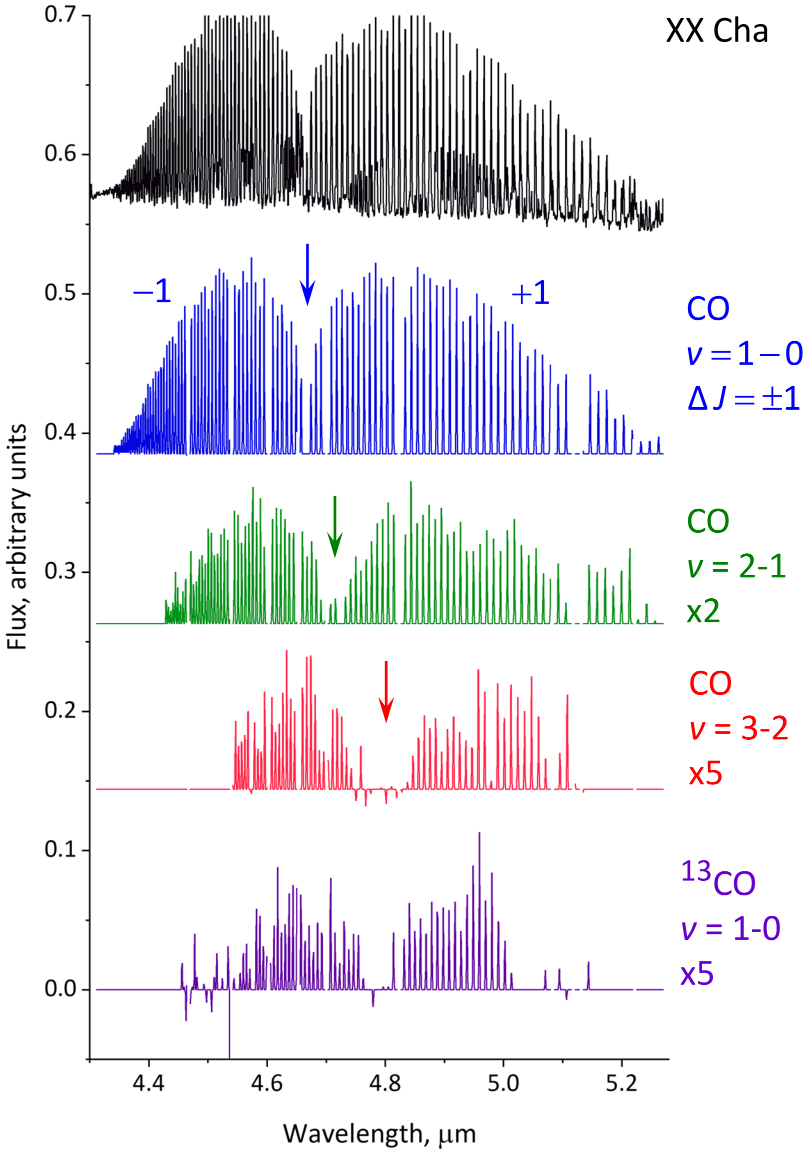
    where u is the atomic mass unit.
- Then solve $\hat{H}\psi=\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi=E\psi \quad .$



The 1-D quantum harmonic oscillator (continued)

- Most diatomic molecules, particularly the heavier ones, are described well by the simple harmonic oscillator potential, meaning that the vibrational states are approximately uniformly spaced.

- The effect of **anharmonicity** is usually that the energy spacing decreases with increasing energy, as marked with the arrows at right for the emission spectrum of cosmically-very-abundant $^{12}\mathrm{C}^{16}\mathrm{O}$.
  - CO is not particularly heavy. By the third excited state, the energy spacing has decreased by about as much as that of the first excited state in the next-more-massive diatomic molecule $^{13}\mathrm{C}^{16}\mathrm{O} \quad \left(^{13}\mathrm{CO}\right)$.
  - The forest of emission lines on either side of the wavelength of the vibrational transitions at right are the **rotation-vibration transitions** of the molecule, which we will discuss in due time.
  - The quantum anharmonic oscillator is not hard to solve. However, the uniformly-spaced energies of the quantum simple harmonic oscillator allow us easy access to a diabolically useful technique.



Data from JWST/NIRSpec; Henning et al. 2024

Solution by operator algebra

We will solve the quantum simple harmonic oscillator in two ways: by an algebraic shortcut now, and by brute-force solution starting next class. The short way:

- Again, the time independent S.E.: $\hat{H}\psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right)\psi = \frac{1}{2m}\left(\hat{p}^2 + m^2\omega^2 x^2\right)\psi = E\psi$.

  It would easy to solve if we could factor the term in brackets to have the form $\hat{Q}_1\hat{Q}_2$.

- Let's consider two operators which come *close* to providing this factoring:

$$\left.\begin{aligned} \hat{a}_+ &= \frac{1}{\sqrt{2m\hbar\omega}}(-i\hat{p} + m\omega x) \\ \hat{a}_- &= \frac{1}{\sqrt{2m\hbar\omega}}(+i\hat{p} + m\omega x) \end{aligned}\right\} \quad \text{or, more compactly,} \quad \hat{a}_\pm = \frac{1}{\sqrt{2m\hbar\omega}}(\mp i\hat{p} + m\omega x) \quad .$$

- Multiply them with ψ, to remind us that there are operators here; we must keep x and d/dx in their original order:

Solution by operator algebra (continued)

$$\hat{a}_-\hat{a}_+\psi = \frac{1}{2m\hbar\omega}(i\hat{p}+m\omega x)(-i\hat{p}+m\omega x)\psi = \frac{1}{2m\hbar\omega}\left(\hat{p}^2 + m^2\omega^2x^2 - m\omega xi\hat{p} + ipm\omega x\right)\psi$$

$$= \frac{1}{2m\hbar\omega}\left[\hat{p}^2 + m^2\omega^2x^2 - im\omega\left(x\hat{p}-\hat{p}x\right)\right]\psi \quad .$$

This is almost the Hamiltonian operating on ψ, apart from the cross term we are trying to simplify away.

- Now define the **commutator** of two operators as $\left[\hat{P},\hat{Q}\right] = \hat{P}\hat{Q} - \hat{Q}\hat{P}$; then we see that the cross term contains the commutator of x and $\hat{p}$:

$$\hat{a}_-\hat{a}_+\psi = \frac{1}{2m\hbar\omega}\left(\hat{p}^2 + m^2\omega^2x^2\right)\psi - \frac{i}{2\hbar}[x,\hat{p}]\psi \quad .$$

- And, magically, that last term has a simple and memorable form, though it doesn't vanish:

$$[x,\hat{p}]\psi = -i\hbar\left(x\frac{d\psi}{dx} - \frac{d}{dx}x\psi\right) = -i\hbar\left(\cancel{x\frac{d\psi}{dx}} - \psi\frac{dx}{dx} - \cancel{x\frac{d\psi}{dx}}\right) = i\hbar\psi \quad \Rightarrow \quad \boxed{[x,\hat{p}] = i\hbar}$$

Canonical commutator

Solution by operator algebra (continued)

- And we are left with

$$\hat{a}_-\hat{a}_+\psi = \frac{1}{2m\hbar\omega}\left(\hat{p}^2 + m^2\omega^2x^2\right)\psi - \frac{i}{2\hbar}(i\hbar)\psi \quad \Rightarrow \quad \hat{H} = \frac{1}{2m}\left(\hat{p}^2 + m^2\omega^2x^2\right) = \boxed{\hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)} \ .$$

- Also, $\hat{a}_-$ and $\hat{a}_+$ **do not commute**, i.e. their commutator is not zero. To see this quickly, repeat the last page but start with these two operators in the reverse order:

$$\hat{a}_+\hat{a}_-\psi = \frac{1}{2m\hbar\omega}\left(-i\hat{p} + m\omega x\right)\left(i\hat{p} + m\omega x\right)\psi = \frac{1}{2m\hbar\omega}\left(\hat{p}^2 + m^2\omega^2x^2 + m\omega x i\hat{p} - ipm\omega x\right)\psi$$

$$= \frac{1}{2m\hbar\omega}\left[\hat{p}^2 + m^2\omega^2x^2 + im\omega\left(x\hat{p} - \hat{p}x\right)\right]\psi = \frac{1}{\hbar\omega}\left[\hat{H} + \frac{i}{2}(-i\hbar)\right]\psi$$

$$\Rightarrow \quad \hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right) = \boxed{\hbar\omega\left(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2}\right)} \Rightarrow \boxed{\left[\hat{a}_-, \hat{a}_+\right] = 1} \ .$$

subtract upper line from lower

Solution by operator algebra (continued)

- In terms of our new operators $\hat{a}_\pm$, the time-independent Schrödinger equation becomes $\hat{H}\psi = \hbar\omega\left(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2}\right)\psi = E\psi$.
- To see what these operators actually are, we next consider the states $\hat{a}_\pm\psi$, and the eigenvalues of the Hamiltonian operating on these states. Remember throughout that ψ stays on the right; and that operators $\hat{H}, \hat{a}_+, \hat{a}_-$ **do not** commute with one another but **do** commute with constants $E, \hbar\omega, 1/2$. And use $\left[\hat{a}_-, \hat{a}_+\right] = 1$. Here goes:

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

Use $\hat{a}_-\hat{a}_+ = \hat{a}_+\hat{a}_- + 1$

$$= \hat{a}_+\hbar\omega\left(\hat{a}_+\hat{a}_- + 1 + \frac{1}{2}\right)\psi = \hat{a}_+\left(\hat{H} + \hbar\omega\right)\psi = \hat{a}_+\left(E + \hbar\omega\right)\psi = \left(E + \hbar\omega\right)\hat{a}_+\psi \quad ;$$

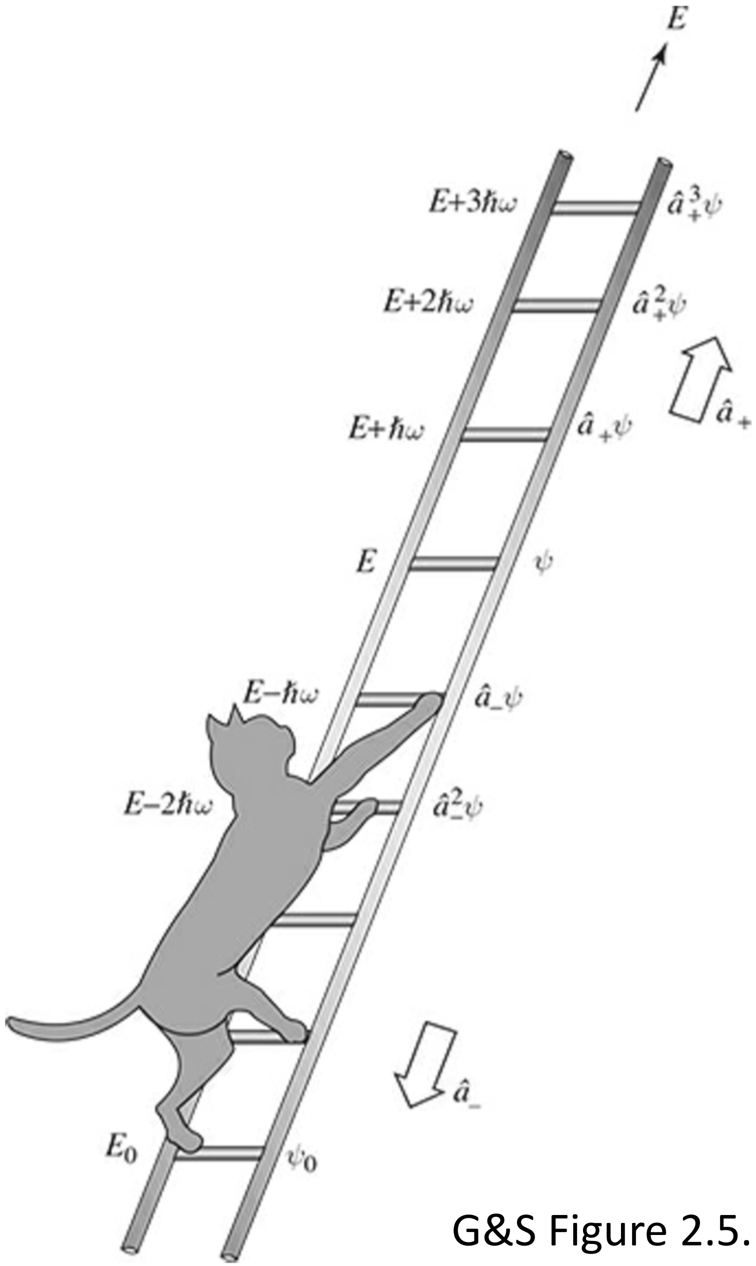
$$\hat{H}\left(\hat{a}_-\psi\right) = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)\left(\hat{a}_-\psi\right) = \hbar\omega\left(\hat{a}_-\hat{a}_+\hat{a}_- - \frac{1}{2}\hat{a}_-\right)\psi = \hbar\omega\hat{a}_-\left(\hat{a}_+\hat{a}_- - \frac{1}{2}\right)\psi$$

Use $\hat{a}_+\hat{a}_- = \hat{a}_-\hat{a}_+ - 1$

$$= \hat{a}_-\hbar\omega\left(\hat{a}_-\hat{a}_+ - 1 - \frac{1}{2}\right)\psi = \hat{a}_-\left(\hat{H} - \hbar\omega\right)\psi = \hat{a}_-\left(E - \hbar\omega\right)\psi = \left(E - \hbar\omega\right)\hat{a}_-\psi \quad .$$

Solution by operator algebra (continued)

- Summary: $\boxed{\hat{H}\left(\hat{a}_{\pm}\psi\right)=\left(E\pm\hbar\omega\right)\left(\hat{a}_{\pm}\psi\right)\quad .}$
- In English: when $\hat{a}_{+}$ or $\hat{a}_{-}$ operate on a state ψ which is a solution to the S.E. with energy eigenvalue *E*, the result is another state which is a different solution to the S.E., that has energy eigenvalue $E+\hbar\omega$ or $E-\hbar\omega$, respectively.
- In other words: $\hat{a}_{+}$ and $\hat{a}_{-}$ **raise and lower**, respectively, the energy of the system by the amount $\hbar\omega$. They are therefore called **raising** or **lowering operators**, respectively, or **ladder operators**, collectively.
  - Originally called **creation** or **annihilation operators**, respectively. Lots of particle physicists still call them that.
  - Invented by Paul Dirac in the 1940s; first treated extensively in the third edition of his quantum-mechanics textbook.



G&S Figure 2.5.

The ground state

- According to Problems 2.2 and 2.3 on last week's assignment, there cannot be a solution to the Schrödinger equation with an energy eigenvalue less than the minimum of V.

- So if one starts with a solution ψ and repeatedly applies to it the lowering operator $\hat{a}_-$, one will eventually get zero, or a non-normalizable solution.

- Suppose the result is **zero**. That can be used to determine the last state ψ_0 just before zero:

$$\hat{a}_-\psi_0 = \frac{1}{\sqrt{2m\hbar\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0 \quad \Rightarrow \quad \frac{d}{dx}\psi_0 = -\frac{m\omega}{\hbar}x\psi_0$$

Separate and integrate

$$\int\frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}\int x dx \quad \Rightarrow \quad \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + A' \quad \Rightarrow \quad \psi_0 = Ae^{-m\omega x^2/2\hbar}$$

Gaussian; use Lecture 2 green pages to integrate and normalize

$$1 = \int\psi_0^*\psi_0 dx = |A|^2\int_{-\infty}^{\infty}e^{-m\omega x^2/\hbar}dx = |A|^2\sqrt{\frac{\pi\hbar}{m\omega}} \quad \Rightarrow \quad \boxed{\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-m\omega x^2/2\hbar}}\,.$$

Ground state

The ground state (continued)

- The energy of the ground state:

$$\hat{H}\psi_0 = \hbar\omega\left(\hat{a}_+\cancelto{0}{\hat{a}_-\psi_0} + \frac{1}{2}\psi_0\right) = \frac{\hbar\omega}{2}\psi_0$$

$$\Rightarrow \boxed{E_0 = \frac{\hbar\omega}{2}}\ .$$

Zero-point energy

- And all the excited states and their energies:

$$\boxed{\begin{aligned} &\psi_v(x) = A_v\left(\hat{a}_+\right)^v\psi_0(x) \\ &E_v = \left(v+\frac{1}{2}\right)\hbar\omega \quad , \quad v = 0,1,2,\ldots \end{aligned}}$$

We'll find the normalization constants next time.