# 9/9/2024

- Review by example
  - General Uncertainty Principle
  - Harmonic Oscillator
- Infrared Spectroscopy
- Google Drive Folder Link Setup
- Exercise 1: Introduction to Google Colab

- This lecture and exercise is designed to help you achieve the following learning objectives
  - Use the general uncertainty principle to evaluate limits on the simultaneous specification of a pair of quantities
  - Describe how analytical models help interpret various experimental spectra
  - Use Google Colab to run python computer code and to annotate results

# Review by Example

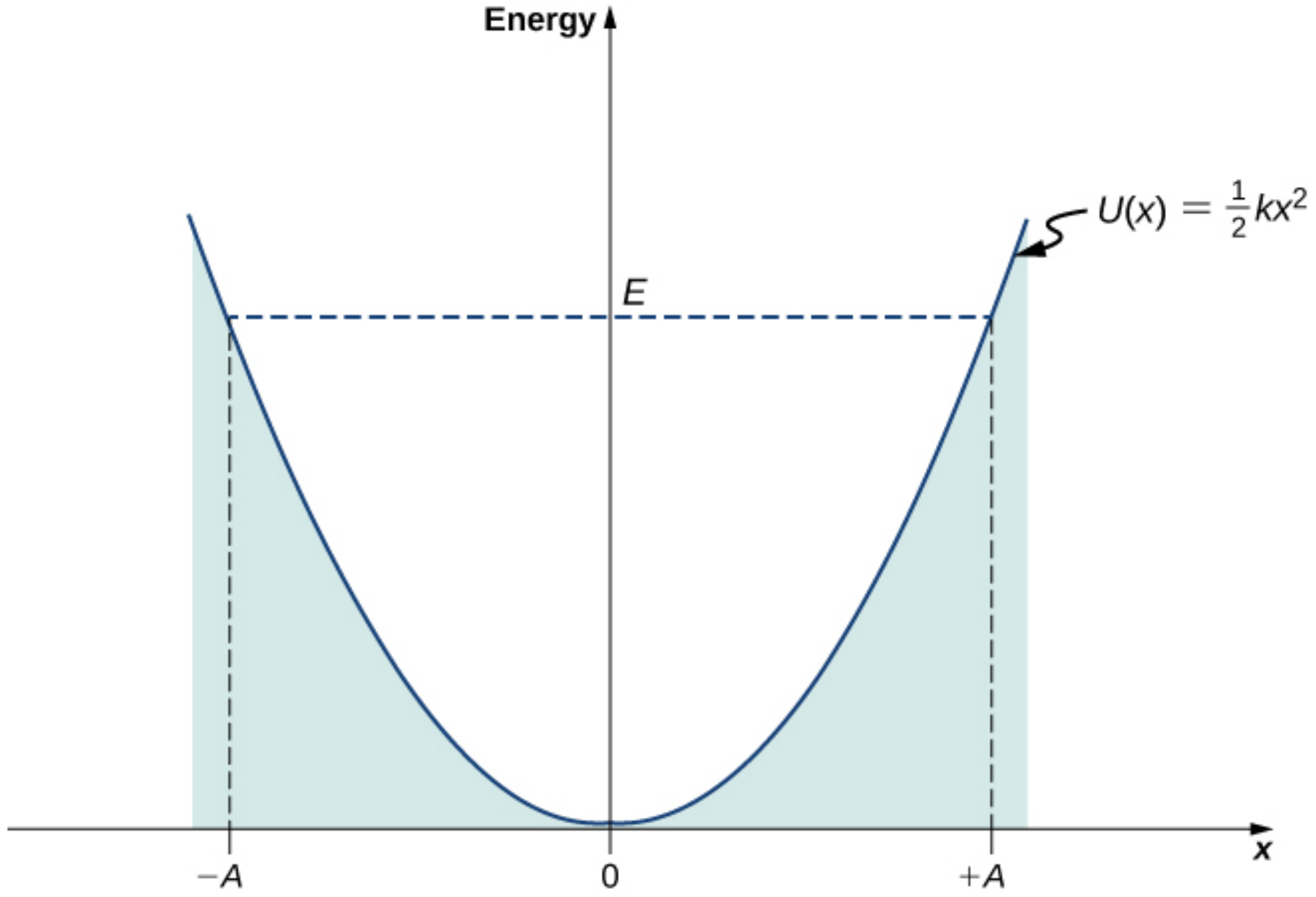
# GUT example

- Using the general uncertainty principle $\Delta A \Delta B \geq \frac{1}{2}\left|\left\langle[\hat{\mathbf{A}}, \hat{\mathbf{B}}]\right\rangle\right|$, evaluate the limitation on the simultaneous specification of kinetic energy and potential energy

- $\left[\hat{\mathbf{T}}, \hat{\mathbf{V}}\right] f = \hat{\mathbf{T}}\hat{\mathbf{V}} f - \hat{\mathbf{V}}\hat{\mathbf{T}} f = -\frac{\hbar^2}{2m}\frac{d^2 Vf}{dx} + V\frac{\hbar^2}{2m}\frac{df}{dx}$
- $\frac{d^2 Vf}{dx^2} = \frac{d}{dx}\left[f\frac{dV}{dx} + V\frac{df}{dx}\right] = f\frac{d^2 V}{dx^2} + 2\frac{df}{dx}\frac{dV}{dx} + V\frac{d^2 f}{dx^2}$
- $\left[\hat{\mathbf{T}}, \hat{\mathbf{V}}\right] f = -\frac{\hbar^2}{2m}\left[f\frac{d^2 V}{dx^2} + 2\frac{df}{dx}\frac{dV}{dx}\right] = i\hat{\mathbf{C}} f$
- Therefore, $\Delta T \Delta V \geq \frac{\hbar^2}{4m}\left|\left\langle \frac{d^2 V}{dx^2} + 2\frac{dV}{dx}\frac{d}{dx}\right\rangle\right|$

# Harmonic Oscillator

- $V(x) = \frac{1}{2}kx^2$
- The Hamiltonian is $\hat{\mathbf{H}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}k_f x^2$
- The energies are $E_\nu = \left(\nu + \frac{1}{2}\right)\hbar\omega$, where $\nu = 0,1,2,...$
  - $\omega = \sqrt{\frac{k_f}{m}}$
  - $\nu$ starts at 0, not 1
  - Spacings between energy levels are constant




https://phys.libretexts.org/Bookshelves/University_Physics/University_Physics_(OpenStax)/University_Physics_III_-_Optics_and_Modern_Physics_(OpenStax)/07%3A_Quantum_Mechanics/7.06%3A_The_Quantum_Harmonic_Oscillator

# HO Example

- The oscillation of the atoms around their equilibrium positions in the molecule HI can be modeled as a harmonic oscillator of mass $m \approx m_H$ (the iodine atom is almost stationary) and force constant $k_f = 313.8\ N\ m^{-1}$. Evaluate the separation of energy levels and predict the wavelength of light needed to induce a transition between neighboring levels.

- $m = 1.008 \times 10^{-3}\ \text{kg mol}^{-1} / 6.022 \times 10^{23}\ \text{particles/mol} = 1.674 \times 10^{-27}\ \text{kg}$
- $\omega = \sqrt{\dfrac{k_f}{m}} = \sqrt{\dfrac{313.8\ \text{N m}^{-1}}{1.674 \times 10^{-27}\ \text{kg}}} = 4.33 \times 10^{14}\ \text{s}^{-1}$
- $\lambda = \dfrac{hc}{\Delta E} = \dfrac{hc}{\hbar\omega} = \dfrac{2\pi c}{\omega} = 4.35\ \mu m$

# Infrared Spectroscopy

# Dipoles

- Molecules with permanent dipole moments will generate oscillating dipoles when they vibrate.

- Which of the following diatomic molecules will exhibit an infrared spectrum?

    A. HBr

    B. $H_2$

    C. CO

    D. $I_2$

- HBr and CO

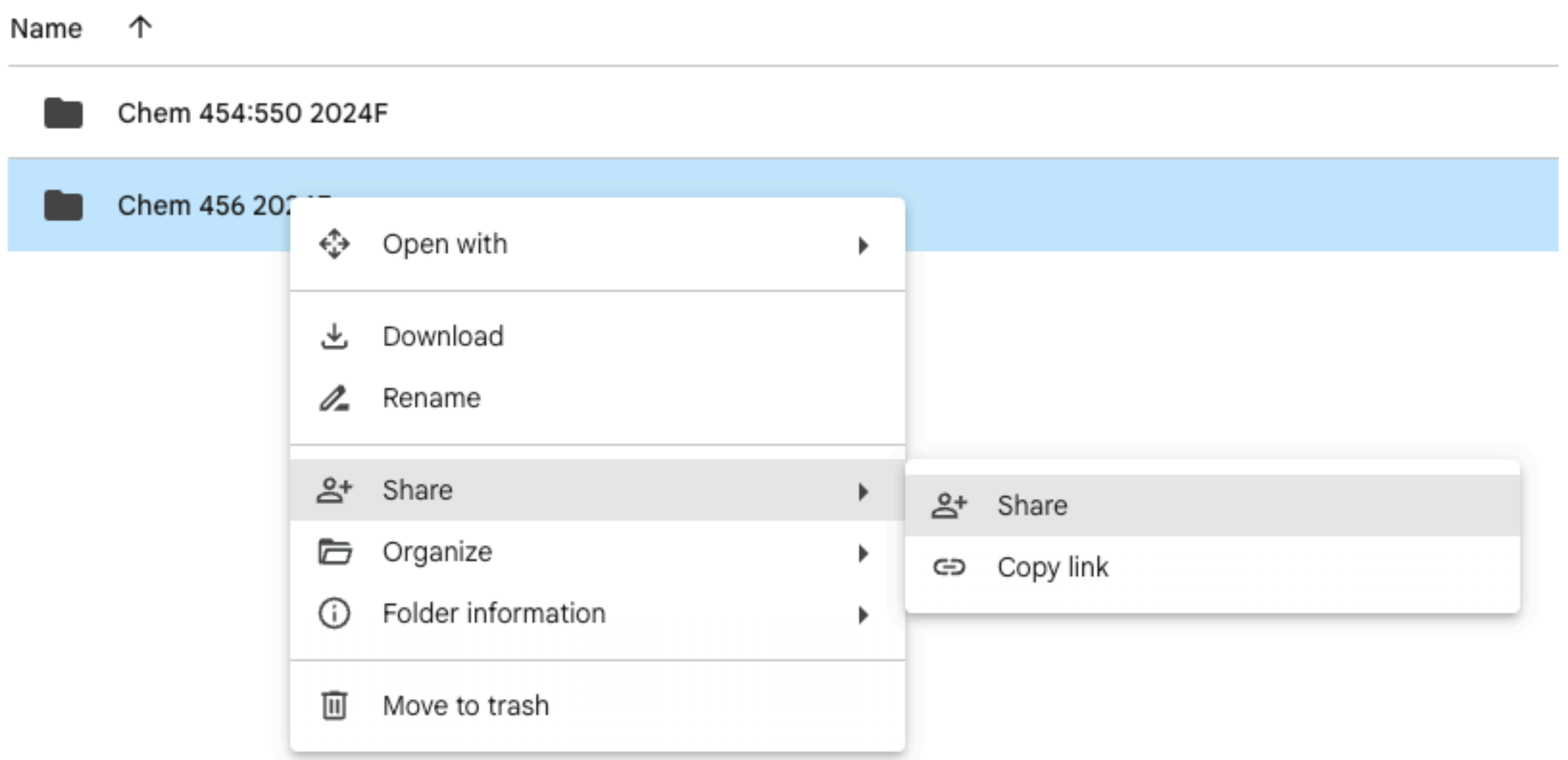
# Identification by IR

- In the HO model, $\Delta E = \hbar\nu_{obs}$ or $\Delta E = h\nu_m$
- $\nu_{obs} = \sqrt{\dfrac{k}{\mu}}$ or $\nu_m = \dfrac{1}{2\pi}\sqrt{\dfrac{k}{\mu}}$ and $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$
- An unknown diatomic oxide has a vibrational frequency of ω = 1904 cm$^{-1}$ and a force constant of 1607 N m$^{-1}$. Identify the molecule. (a) CO (b) BrO (c) NO (d) $^{13}$CO
- $\nu_m = \omega c = (1904\ \text{cm}^{-1})(2.99 \times 10^{10}\ \text{cm s}^{-1}) = 5.706 \times 10^{13}\ \text{s}^{-1}$
- $\mu = \dfrac{(2\pi)^2 k}{\nu_m^2} = \dfrac{(2\pi)^2(1607\ \text{N m}^{-1})}{(5.706 \times 10^{13}\ \text{s}^{-1})^2} = 1.250 \times 10^{-26}$ kg for a single molecule
- $\mu = (1.250 \times 10^{-23}\ \text{g})(6.022 \times 10^{23}\text{mol}^{-1}) = 7.528\ \text{g mol}^{-1}$ for a mol of particles
- For NO, $\dfrac{m_1 m_2}{m_1 + m_2} = \dfrac{14 \times 16}{14 + 16}\ \text{g mol}^{-1} = 7.5\ \text{g mol}^{-1}$

# Review

- What is necessary for a transition between vibrational states to be observed in infrared spectroscopy?
- What is the difference between mass and reduced mass?

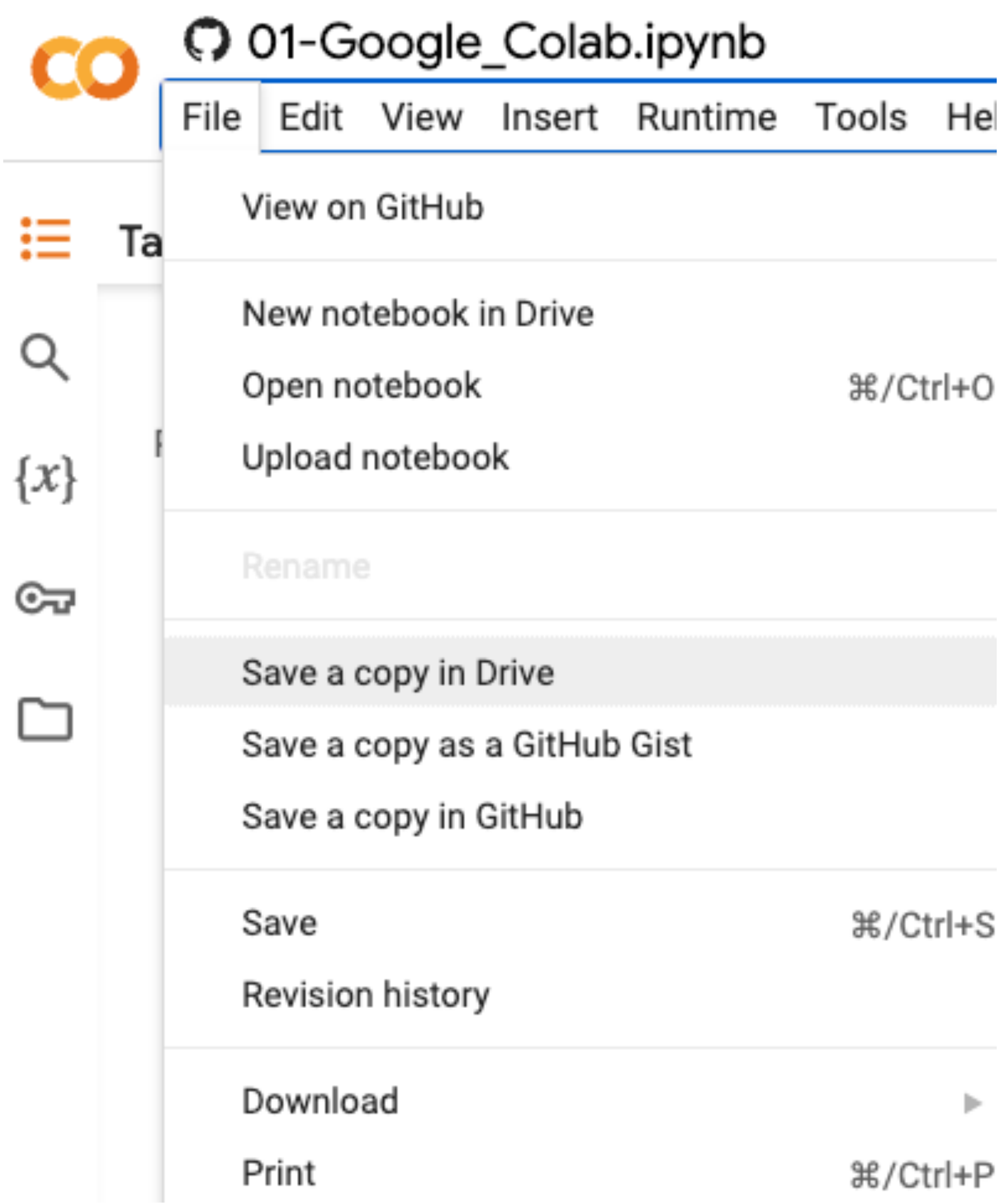
# Google Drive Folder Setup




- Log in to Google Drive. This can be a school account or a personal account.
- Create a folder for this class called “Chem550-2024F”
- Create the subfolder “exercises”. This should be exactly correct, <u>including lowercase</u>.
- Right click on the folder.
- Select “Share”
- Share the folder with me, <u>dminh@iit.edu</u>, and the TA, <u>tnguyen48@hawk.iit.edu</u>.

# Exercise 1: Introduction to Google Colab

https://colab.research.google.com/github/daveminh/Chem550-2024F/blob/main/exercises/01-Google_Colab.ipynb




- After following this link, you should
  - save a copy of the notebook to Google Drive
  - rename it to 01-Google_Colab.ipynb
  - move it to your class folder under the “exercises” folder
  - work on and save the notebook