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

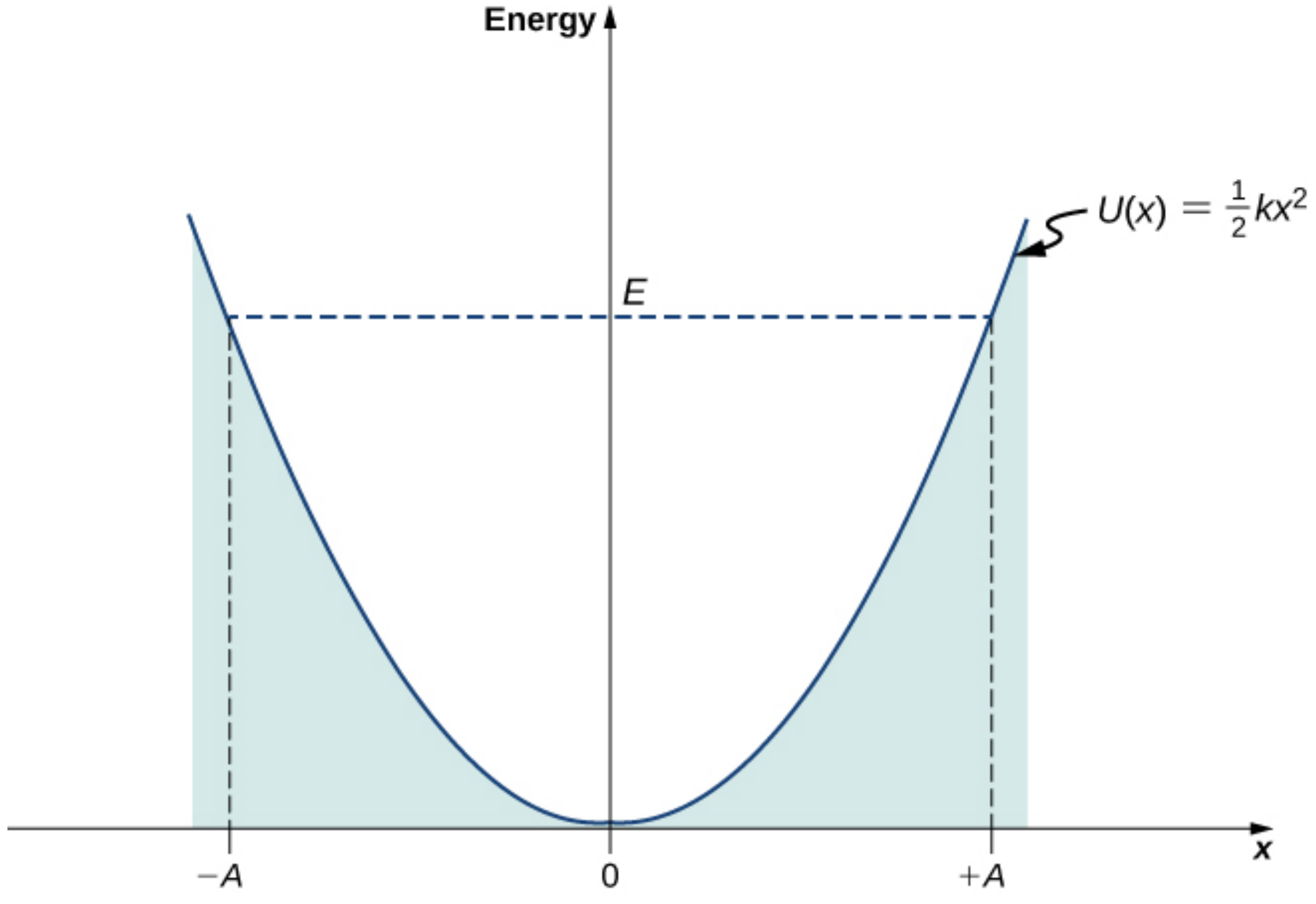
Review by Example

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

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 $\nu = 0,1,2,...$
  - $\omega = \sqrt{\frac{k_f}{m}}$
  - ν 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.

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

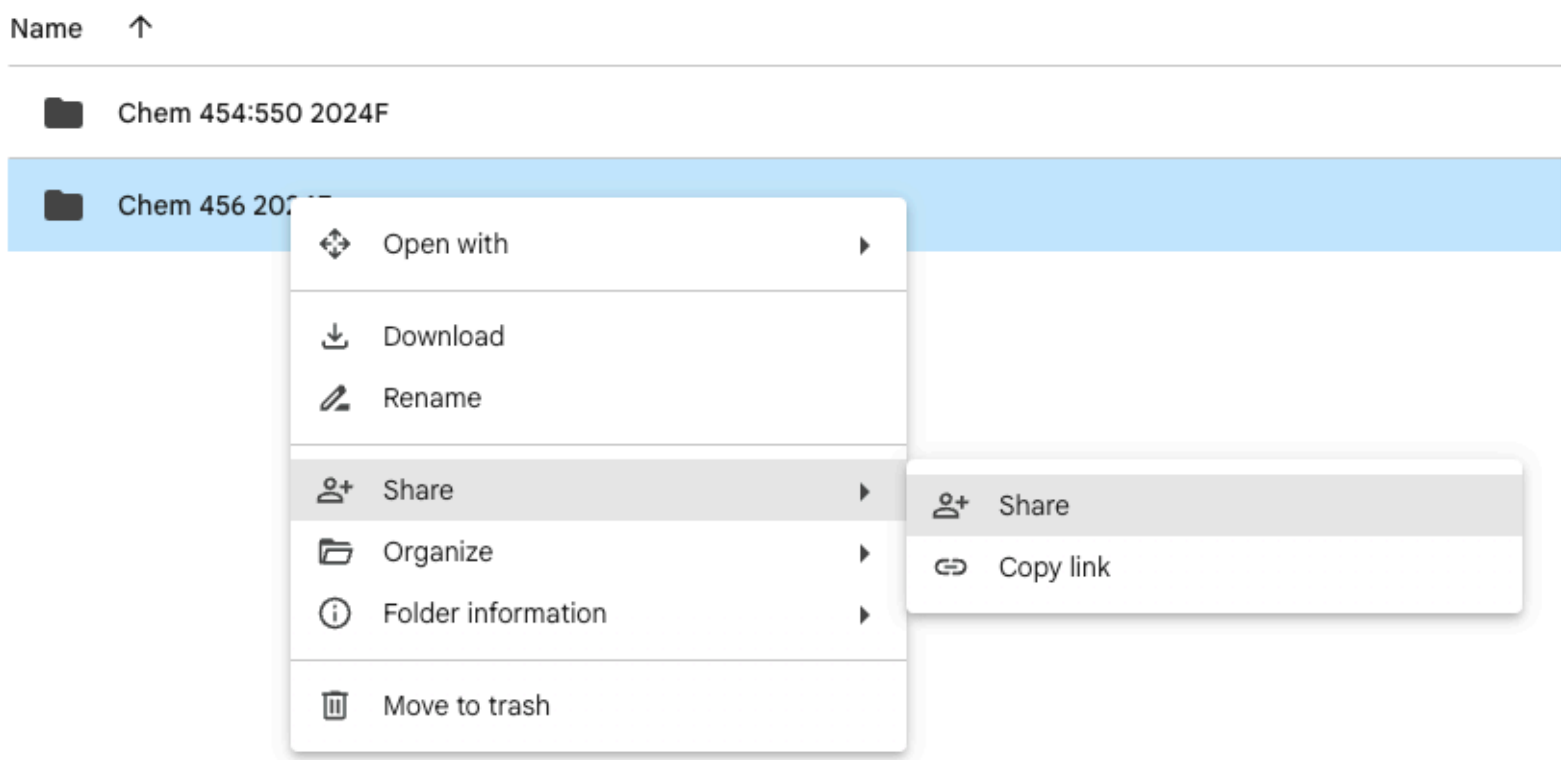
Identification by IR

- In the HO model, $\Delta E = \hbar\nu_{obs}$ *or* $\Delta E = h\nu_m$
- $\nu_{obs} = \sqrt{\frac{k}{\mu}}$ or $\nu_m = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$ and $\mu = \frac{m_1 m_2}{m_1 + m_2}$
- 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

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?

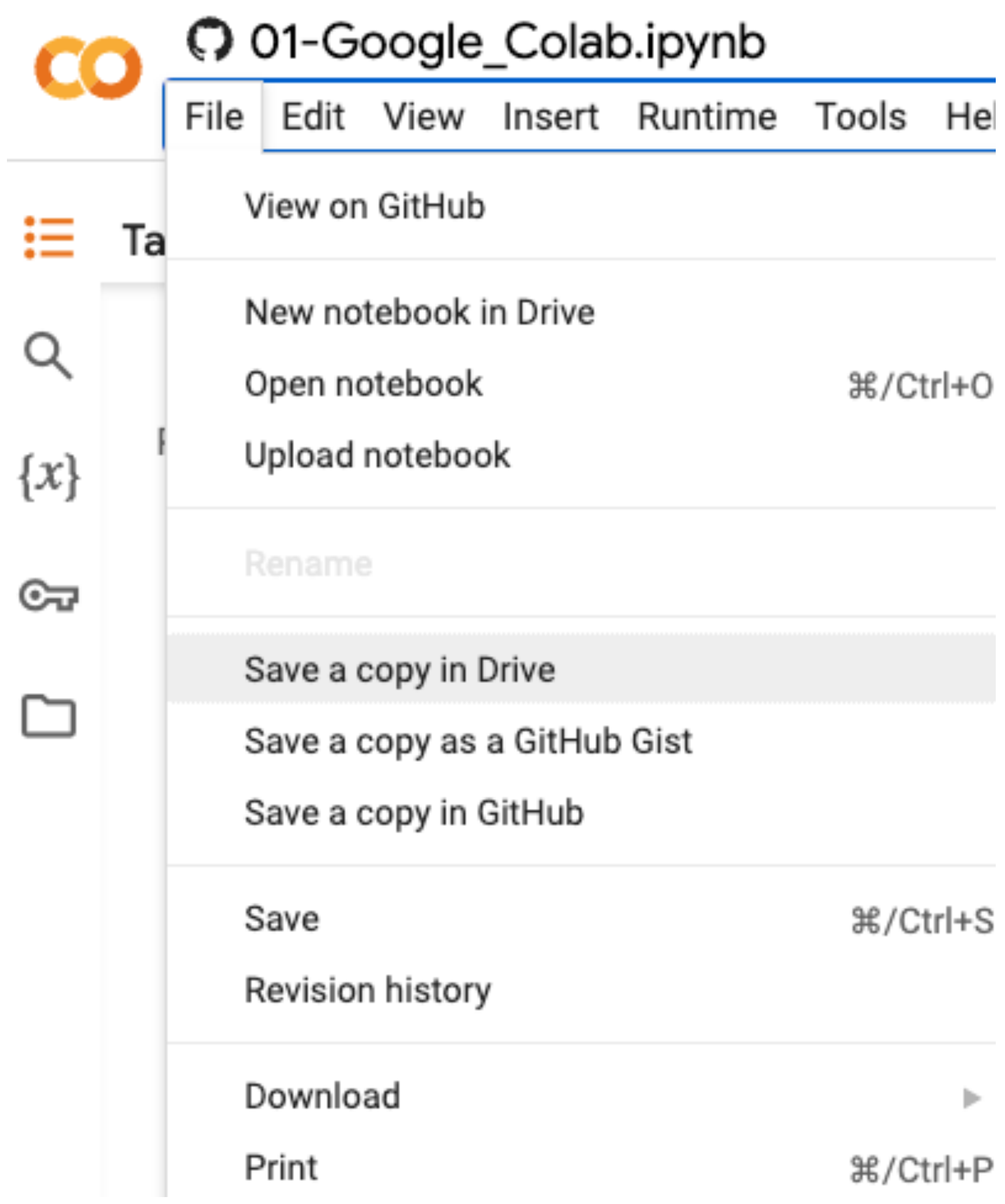
Google Drive Folder Setup



- 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