

CHEM352: PHYSICAL CHEMISTRY II
NOTES AFTER OFFICE HOURS - 04/03

1. Matrix determinants and visualization of the linear transformations: the **3Brown1Blue** youtube channel: "Cramer's rule, explained geometrically — Essence of linear algebra, chapter 12" explains visually the cramers rule for solving linear equations. You would probably need watch several earlier videos in the series to understand the visualization of the linear transformation and determinants first. The series finishes with a visualization of eigenfunctions and eigenvalues of some matrices, it might be useful for people needing more visuals.
2. James questioned me about different review topics and took some notes. Here's a list:
 - Gas phase spectroscopy – large biomolecules, peptides, proteins, biopolymers, etc. 2nd and tertiary of gas phase, solvation shells, transfer molecule into gas phase, IR – vibrational. Little in rotational, some specific techniques (mass spec and tandem mass spec (fragmented mass spec)) ion Mobility spectroscopy
 - QM/MM – look up lecture Noble prize lecture. Molecule as a spring. Introduce quantum mechanics. Application
 - Force field – how to do simulations in practices - force field construction, parameterization and MD algorithms.
 - Density functional theory – reformulation of wavefunction mechanics. What is density functional theory. Electron density is the main element instead of wavefunction. How does using electron density work. Introduces different functionals. How different energies are defined.
 - Hartree-Fock and Electron Correlation – represent wave function as single slate determinants. Carries approximation the neglects electron correlation. Develop theory to more details. Introduce few methods which reintroduces electron correlation. Hartree-Fock 1 chapter of textbook and 2-3 papers on electron correlation
3. From chapter 13 we will cover Rot-Vib spectroscopy and Anharmonic vibrations.