

Light matter interaction part I and II

Part I

- Fundamentals of light-matter interaction (DC limit: field-dipole; AC field-transition dipole): scattering, absorption, emission
- Energy levels: from NMR to x-rays; it's all the same thing
- Boltzmann: thermal occupation of levels
- Some differences between different types of spectroscopies (at different photon energies):
 - Microwave (NMR: spin relaxation; pulse field gradient techniques, MRI)
 - IR (vibrational: Raman, IR, what determines x-section?)
 - Optical (electronic: singlet/triplets states; Jablonski Diagram, Franck Condon principle, FRET)
 - X-rays (XAS; XPS; core levels)

Part II

- Bloch equations that describe time-evolution of 2-level system
- Linear spectroscopy ($E \rightarrow P \rightarrow E'$; E and E' out-of-phase for resonant absorption)
- Line shape theory: homogeneous & inhomogeneous broadening, Kubo model, Time-domain-Frequency-domain equivalence (free induction decay), Motional narrowing
- Non-linear spectroscopy as a means to determine line shape contributions: ladder climbing, chirped pulses, higher-order Bloch equations

Fundamentals: light/wave

- Electric-magnetic fields
- Lorentz transformations
- Maxwell's equations
- Wave equation in free space
- Wave equation in a medium, linear and non-linear polarization terms

Light-matter interactions part I and II

Part I

- Complex optical constants
 - Complex Refractive Index (Permittivity, Susceptibility, Conductivity), Kramers-Kronig Relations, Dielectric Spectroscopy
 - Characteristic penetration depth
 - Reflectivity and Hagen-Rubens Relation
- Atomistic Theory of the Optical Properties
 - Free electrons without Dumping
 - Free electrons with Dumping or Classical Free Electron Theory of Metals: Drude Model
 - Bound electrons or Classical Electron Theory of Dielectric Materials: Lorentz Model
 - Contribution of Free Electrons and Harmonic Oscillators to the Optical Constants
- Interband and Intraband Transitions and Dispersion

Part II

- Reflection/Transmission (Refraction), Fresnel Factors, Layered Media, AR coatings, Ellipsometry, Brewster Angle Microscopy
- Scattering from particles
- Extinction, Absorption, Beer's Law

Lasers and Pulse propagation

Lasers

- Gain vs absorption. Beer's law. 2, 3, and 4 - level systems
- Laser basics: gain, loss and the cavity. Laser threshold condition
- Laser modes: pulse formation by modelocking, passive and active modelocking
- Amplification, direct and regenerative

Ultrashort pulse propagation

- Chromatic dispersion and optical phase
- Group and phase refractive index
- Chirp coefficients (GVD, TOD, ...)
- Effect of GVD and TOD on short optical pulses
- Pulse compression in prisms and gratings
- Basics of pulseshaping and arbitrary waveform generation

Nonlinear optics

- Basics with harmonic potential well, anharmonic symmetric and antisymmetric potential well
- Introduce SHG, SFG, DFG
- Phase matching, doubling with nonlinear crystals, autocorrelation
- Optical parametric amplification, principle topas, vacuum fluctuations, saturation used to get stable output, old (superfluorescence) vs. new (white light) topas
- DFG signal, idler
- SHG and SFG spectroscopy

Group theory and selection rules

- Selection rules IR and Raman for diatomics
- Point group, symmetry operations
- Character tables, what is written in them, how to use them
- Selection rules IR and Raman for larger molecules based on group theory combine to get selection rules for SFG. Maybe expansion to non-vanishing χ^2 elements

Quantum mechanics

Time-independent Schrodinger equation

- Wavefunction and energy level/ eigenfunction and eigenvalue
- Ground State vs. Excited State
- Superposition of the eigenfunctions; quantum-classical correspondence
- Experimental observables

Time-dependent Schrodinger equation

- First-order perturbation: Collision-induced excitation
- Second-order perturbation
- External Field; Schrodinger picture, vs. Heisenberg picture, vs. Interaction picture
- Transition probability
- Fermi Golden rule

Ray optics

- Fermat's principle of least time
- Reflection
- Refraction – Snell Law
- Mirrors, lenses and prisms
- Fiber optics - total internal reflection
- Microscope and telescope
- Optical aberrations

Fourier optics

- Fourier transform pairs and basic concepts of the transform
- Lens (or circular aperture) as a Fourier transform
- Superposition of fields (waves)
- Interferometry: basic examples (Mach Zender / Michelson), heterodyne detection in spectroscopy, Frequency domain fringes
- Laser pulses and Fourier considerations
- Diffraction: single slit, Young's double slit, many slits, gratings
- Fraunhofer criterion and Fresnel diffraction (only an overview)

Near-field spectroscopy

- From bulk to surface to Mie plasmons
- The evanescent field
- Light-plasmon coupling, dispersion relation, Otto/Kretschmann configurations for FTIR/ATR
- Near-field spectroscopy examples: SPR, SERS/SEIRAS, nearfield SHG scattering

Light polarization

- Polarization of light (linear, circular, unpolarized)
- Jones formalism to describe polarizing optics
- Linear polarizers & Malus law
- Modifying polarization: Scattering, Reflection
- Modifying polarization: birefringence, $\lambda/4$, $\lambda/2$, $\lambda/8$
- Jones formalism to describe polarizing optics
- Optical activity and circular dichroism
- Experiments using polarization: Brewster angle, anisotropy decays (Kerr effect, fluorescence, infrared pump-probe, IR pump-SFG probe)

Data analysis

- Expected value, variance, co-variance
- discrete data and their distribution (chi², likelihood, student-t....)
- Filters and windows, Fourier transform, frequency response
- Fourier transform, convolution, deconvolution (e.g. instrument response functions)
- Correlation analysis, regression analysis (linear fit)
- Fitting: Linear regression for orthogonal parameters, non-linear regression for interdependent parameters
- Minimization methods: Levenberg-Marquardt, Simplex
- Errors: statistical, systematic, errors in fit parameters