

Fundamentals of Spectroscopy for Optical Remote Sensing

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Spectroscopy is a science branch studying the interactions between radiation and matter. Three major aspects of spectroscopy, in the modern view, include:

- (1) Fundamental study of matter structures and internal interactions (e.g., atomic and molecular structures along with various orbital, spin and nuclear interactions).
- (2) Applied study of environmental properties (e.g., remote sensing of atmospheric parameters, chemical analysis, etc.). The main contents are identification of chemical composition and measurement of their quantity using spectroscopy, and measurement of environmental conditions like wind and temperature through spectroscopy analysis.
- (3) Fundamental study of dynamical processes on a molecular level. Development of time-resolved spectroscopy and femtosecond lasers play an essential role in the study of fast dynamical processes, allowing better analysis of spectral information and its transformation into models of structures and processes.

There are many reasons why spectroscopy is important and so a “must learn” knowledge. Spectroscopy is the fundamental for many modern sciences and technologies, and it has found very wide applications. Spectroscopy is a very important approach to study the fundamental matter (fundamental particles, atoms, and molecules, etc.) structures and internal interactions, and to study the dynamical processes. Spectroscopy is often used in physics, analytical chemistry, biology, medicine, and material sciences for the identification of substances through the spectrum emitted from them or absorbed in them, and for study of fast dynamical processes through time-resolved spectroscopy. Spectroscopy is heavily used in astronomy and remote sensing. They are used either to measure the chemical composition and physical properties of objects or to measure related environmental properties like velocities and temperatures from Doppler shift and broadening of spectral lines. Spectroscopy is the fundamental for all remote sensing technologies. We hope to help students to develop the abilities and fundamental knowledge so that students can learn new things for innovation and revolution in the future.

As described in our textbook “Laser Spectroscopy” by W. Demtröder, there are many fascinating applications of spectroscopy, such as LIDAR, single-molecule detection, laser femtosecond chemistry and biology, etc. However, to achieve such fascinating applications, we must know the fundamentals of laser spectroscopy, like the numerous novel approaches to achieve high sensitivity, high resolution (spectral, spatial, and temporal), high precision, and ultra-fast spectroscopy. Such laser spectroscopy is based on the understanding of why and how spectral lineshape, linewidth, and line intensity are formed, and why some transitions are allowed but some are not. Such understanding comes from the understanding of theories of atomic and molecular structures and spectra, and from the understanding of theories of radiation (or quantum) transitions. Of course, all of such spectroscopy starts with the basics of quantum physics, quantum mechanics, electromagnetism, lasers, optics, etc.

The thoughts outlined above help form the teaching philosophy and course structure for the spectroscopy class. For this graduate entry-level class of spectroscopy, we will start with “Part I. Introduction to Quantum Physics and Spectroscopy” that consists of the first three chapters. Chapter 1 provides a review of several experimental facts that led to the quantum

concepts. These experiments were chosen not only for their intriguing features of how to analyze experimental results to test existing theories and discovery new things, but also for their usefulness in optical remote sensing applications. Wave-particle duality is discussed in Chapter 2, as it is a very important concept to understanding many experimental phenomena, including optical remote sensing. The duality concept is also essential in quantum mechanics understanding. Basics of quantum mechanics will be introduced in Chapter 3 to provide a systematic and mathematic approach to treat modern spectroscopy problems. These three chapters form the first part of this class and serve as a preparation for Part II to Part IV that are the main body of the spectroscopy class.

“Part II. Fundamentals of Atomic Spectroscopy” consists of four chapters. After Chapter 4 of an introduction to atomic spectroscopy, we use a large Chapter 5 to study atomic structures and energy levels along with their relationships to the interactions within and outside atoms. Using hydrogen atom as an example, it is shown how we can solve Schrodinger equation to derive energy levels and atomic structures. Then such method is applied to alkali atoms that have single valence electron. External field influences, such as Zeeman and Stark effects, are discussed after calculating the hyperfine structures. Multiple-electron atoms are treated at the end of this chapter. Chapter 6 is devoted to radiation transitions, and it provides a few models to show how quantum transitions are understood and calculated. Selection rules are introduced for different types of transitions, such as electric dipole transition, magnetic dipole transition, and electric quadrupole transition, etc. Armed with the energy level and transition probability information of individual atoms, we discuss in Chapter 7 how atomic spectral lines are formed and how to calculate spectral line strength, width, and shape, etc. This is mainly achieved through considering statistical information of an atom assembly.

“Part III. Fundamentals of Molecular Spectroscopy” consists of six chapters. After Chapter 8 of an introduction, Chapters 9–12 study the rotational, vibrational, Raman and electronic spectroscopy of molecules, respectively. Many concepts are introduced here, but they are relatively easier than the fundamental concepts in atomic spectroscopy.

“Part IV. Fundamentals of Laser Spectroscopy” consists of six chapters. Chapter 13 describes the basics of laser spectroscopy. Following this, Chapter 14 studies how to achieve the highest detection sensitivity in Doppler-limited laser spectroscopy, while Chapter 15 figures out how to achieve very high spectral resolution in laser spectroscopy, i.e., Doppler-free laser spectroscopy. Chapter 16 is devoted to ultra-fast or time-resolved spectroscopy for studying fast dynamical processes. Chapter 17 will introduce the new development in spectroscopy field, and Chapter 18 will discuss several fascinating applications of laser spectroscopy.

We define this spectroscopy class as an entry-level graduate class, because we emphasize the fundamental concepts and devote our efforts to help students to build a very solid foundation in the spectroscopy field. High-level quantum mechanics calculations used in this class are few, but the basic quantum mechanics and spectroscopy calculations are covered. Students will gain such capabilities from this class that they can go on to read advanced spectroscopy and advanced quantum mechanics books and papers to figure out the in-depth calculations or take more advanced spectroscopy or quantum mechanics classes for such calculations.