7. PATTERNS AND MODELS

We now want to discuss the role of pattern analysis in its application to physics. We spend some time on the meaning of the terms *model* and *alternative model*. Acoustics provides some interesting, visualizable analogs for the models we will use in atomic physics. We then introduce some popular models [box, well, coulomb rigid rotor] for the most important atomic/molecular systems, and we see how they serve to explain the line spectra, continuous spectra, and other observable properties.

7.1 PATTERN RECOGNITION & DEVELOPMENT OF MODELS

Pattern Recognition by Humans

Human beings react to order and pattern in remarkable ways. Our sensory systems are adapted to recognize familiar signals even when they are present only marginally in a welter of other signals and noise, for example the ability of two persons to converse in a typical party where other conversations and loud music are present. Another example is our ability to the intelligibility of garbled ($e \rightarrow j$ $i \rightarrow b$ $a \rightarrow x$ $o \rightarrow k$) text:

THIS SJNTJNCJ HAS A SINGLJ LJTTJR MISTYPJD
ANOTHJR SJNTJNCJ HAS TWO JRRONJOUS SYMBOLS BNSJRTJD
WJ DO THJ SXMJ THBNG WBTH THRJJ CHXRXCTJRS RJPLXCJD.
WJ CKULD CKNTBNUJ WBTH FKUR SUBSTBTUTBKNS

We are adept in filling in missing pieces when the pattern seems familiar, so tht ths sntnc cn b ndrstd vn whn th vwls r rmvd frm th wrds. Jig saw puzzles and detective novels, public address messages in airport terminals, interpretation of clinical X-rays, ... there are countless examples where a trained observer can make useful interpretations from scant data, or from data almost totally buried in noise. .

Indeed an individual's survival in the everyday world involves thousands of actions done in response to fragmentary clues interpreted (often reflexively) on the basis of a conceptual model of that world that the individual has gradually built on earlier experience. A single clue is usually not enough; we respond best to a correlated sequence of clues as received in the form of spatial or temporal patterns in our sensory apparatus.

> We use the same sort of pattern recognition in the sciences: Once we get a few pieces of data that seem correlated with a particular conceptual model, we then use the model to guide our search for more data, and we acquire more belief in the model as additional, confirming data is found. This model helps us to organize our observations and thus make sense of the world; alas it is also the seed of preconceptions that lead us to disregard data that seems somehow discordant. If the first part of the message is very familiar it prepares us:
>
> (a) to look for certain items in the future and
> (b) to ignore input that does not seem to be part of that pattern.

Patterns Tell About Their Sources : Acoustic Examples

Spectral patterns help assign a geometry to the system that produces the spectrum.

We have seen (Cf. Sec. 6) that much can be learned from examination of a single spectral line, and we now work to interpret the overall pattern formed by the entire set of lines emitted (or absorbed) by the atom. By "pattern" we mean a systematic, quantitative relationship between the frequencies (and amplitudes) of the different lines in the atom's spectrum. To be considered useful, such a pattern should not only give us an economical representation for the data already obtained but should also guide us toward future experiments. As already discussed in Sec. 2, the discovery of patterns is an important precursor to the development of models and theories [Cf. also H. F. Judson's book *Patterns*]

> Music provides us with many familiar examples of the remarkable response of humans to a spectral patterns.

For instance, if one first hears a tune played in C-major there is no difficulty recognizing the same melody if it is played in D-major since it is the *ratio* of frequencies which dominates the listener's perception of harmony and of melodic line. Similarly, with only a bit of musical experience and again on the basis of distinctive frequency ratios, one can recognize when a tune is being played in a minor key. And one can tell when a melody written in a major key is played, by accident or design, in a minor key,

Spectral Patterns and Physical Structures

Moving somewhat closer to our study of the relation of spectra to structure, there is the ability of many persons to recognize the instruments of the orchestra. Most listeners can recognize the sound from a cello, a viola, or a violin as having been produced from a bowed string instrument; they can distinguish it from the sound produced by the plucked string instruments such as a guitar, banjo, or mandolin. These two classes of instrument differ in the way that oscillations are driven and in the rate that vibrational energy is converted to acoustic radiation. However the two classes have the same stretched-string geometry in their oscillating elements and this gives them a recognizably similar harmonic pattern of a fundamental plus integer overtones. The woodwinds and the brasses are closely related because they too produce distinct musical notes with harmonic overtones... a characteristic that we associate with a structure in which something long and narrow (string, or column of air in a tube) is vibrating. This long, thin geometry leads to a vibrational spectrum in which the mode frequencies are an integer multiples of a fundamental frequency; in fact the octave and other important intervals of Western music are characterized by the same set of simple integer relationships between frequencies.

> (Other physical geometries (e.g.. the circular disk, drumhead, bell) have a quite different, pattern of overtones; indeed the output of such instruments is so anharmonic that one often cannot assign a musical pitch to the sound they generate. Bells, drums, and cymbals are musically quite distinct from harmonically resonant structures, and there is no difficulty in distinguishing them from the strings, woodwinds, and brasses.)

If two sources produce spectral patterns that show some similarities but differ in details, then by experimentally modifying one of the sources we may better understand how they are similar and just why they differ as they do. For example in order to understand the physical differences between a guitar and a mandolin, one should make at least one set of measurements in which a guitar is compared to a mandolin which has had one string removed from each of its pairs. Similarly, comparisons between Lithium and Beryllium are easier to make if one also studies Beryllium with one electron removed (Be^+) because it then has the same number of electrons as Lithium.

The association of spectral pattern with system geometry is one that carries over easily from acoustics to atomic physics and quantum mechanics. If two sources produce spectral patterns with a common ratio of corresponding frequencies, experience suggests that the sources are very likely to be of the same class and share a common geometry. and we can then use the absolute value of the frequencies to identify the particular species (for example, violoncello, viola, and violin in the viol family, or potassium, sodium, and lithium in the family of alkali atoms).

This can be carried further. If you remove one of the two electrons from the normal helium atom (thus producing a positive helium ion), the ion produces an optical spectrum with a pattern essentially identical to (but at frequencies much higher than) the one produced by the normal hydrogen atom. The forces have increased (compared to ordinary hydrogen) because of the increased charge of the nucleus: The spectral pattern of the helium ion shifts to higher frequencies, much as happens as one increases the tension on the strings of a guitar.

> These extrapolations have their limits, of course. The one-electron ions He^+, Li^{++}, Be^{+++}, B^{+4}, C^{+5}, ... do produce spectra that are proportional to but higher than that produced by atomic hydrogen. However, the spectra from the heavier one electron ions (e.g. Ar^{+19} … U^{+91} deviate more and more from exact proportionality to hydrogen as the nuclear charge Z increases because the effects of relativity, quantum electrodynamics, and finite nuclear size become proportionally more important.

Comment on Scaling: The frequencies in the spectrum of a given system depend on the mass of the system components (heavy objects oscillate slowly) and on the strength of the forces that hold the system together (strong forces lead to fast oscillations). The frequencies associated with the solar system are quite low (10^{-6} Hz) because the masses are so large and the gravitational force is so weak. Macroscopic objects such as violin strings oscillate mechanically at frequencies up to 10^{+4} Hz or so, and ultrasound can be generated by the 10^{+5} Hz radiation from vibrating quartz plates. Atoms and molecules have the motion of small masses governed by the electric (r^{-2}) force, and so they have spectra with frequencies that can exceed 10^{+14} Hz.

Can Spectra Mislead? Models and "Reality"

A word of caution is in order here because spectra can be misleading:

Through experience we come to associate the waveform of radiation emitted (or absorbed) by a system as a definite indicator of its structure: For example a stretched string, when plucked, bowed, or hammered, yields a spectrum that is some superposition of a lowest (fundamental) frequency and overtones that come at integer multiples of the fundamental. So when we hear a spectrum with this pattern, we may tend to identify the source as *actually being* a vibrating, stretched string.

> The phrase *actually being* is critical to our study of quantum mechanics because from a limited set of observables we are creating an apparent reality in our mind's eye.

For example, if your technician brings in the graph of an acoustic spectrum that shows a fundamental plus overtones, and if there is a closed violin case visible in the corner of the lab, you might conclude immediately that a vibrating string was the source of the spectrum. But the actual source of the spectrum might also have been an organ pipe!

Of course the assignment of an actual structure from the observed spectrum is still subject to ambiguity.... the source that sounds like a violin might actually be a Moog synthesizer with no structural resemblance whatever to the mechanical system that it mimics so effectively. In fact modern synthesizers are so good that the listener who relies entirely on the perceived spectrum to deduce the structure of the source is often hard put to distinguish between the synthetic and the real spectrum. In making a mental model of the situation, then, the listener has the freedom to conceptualize the source either as a synthesizer or as a more traditional instrument. The observer has a choice of model to represent the system being observed.

When working to understand a particular source of sound, the observer can distinguish between alternative models by measuring properties of the source other than the emitted acoustic spectrum.... for example the tension on the strings and the nut-bridge distance in a violin. But such a new look at the source is not always feasible... in many cases (particularly in astrophysics) the spectrum is all we have.

Models and Reality

The hydrogen atom has a spectrum with frequencies that decrease dramatically as its total internal energy increases. With the hypothesis that the atom has a heavy nucleus [supported by Rutherford's scattering experiments] and a light electron [supported by the studies of J.J. Thomson and R.A. Millikan], Bohr was able to create a planetary model of the atom that had remarkable similarities to the solar system. The success of that representation of hydrogen was dramatic; indeed its success made it difficult for many to accept the alternative, and ultimately more successful, quantum mechanical representation.

Pictures and words are necessary to describe physical models, but if the model enjoys some success then the tacit acceptance of its visual construct and its terminology can severely impede the discussion of other alternatives. This is particularly true when applying the concept of a trajectory to quantum mechanical situations, as we have seen in our analysis of interference phenomena (Sec. 3). We should rely less on preconceptions and more on observations. Although we often find it easier to work with a representation that is known not to match all the observations (e.g. we can do quite a bit of physics with non-relativistic classical mechanics), we must continue to remind ourselves (particularly when the "wave-particle duality" comes up for discussion!) that representations are just models and not a statement of actual being in the philosophical sense.

7.2 MODELS FOR ATOMIC AND MOLECULAR STRUCTURE

Experiments yield wealth of data, and the long efforts to sort the visual and numerical patterns are analogous to taxonomy in the biological sciences. Organization of the observed patterns is assisted by conceptual models devised according to the intuition and experience of researchers in the field. In this effort certain conceptual models emerge as basic in that they are not only amenable to calculation but also have broad applicability for analysis of experiments done with atoms, molecules, and nuclei.

> One should actually say "electrons, photons, ..atoms, ions, molecules, nuclei, solids, ..." but this is awkward, so we rely on the reader to recognize the word "atom" as a generic representation of all of the above when appropriate.

Important, Basic Models in Quantum Mechanics

Models are chosen for various reasons, including:

(a) the apparent relationship between the model and the data,
(b) the ease of solution of associated equations of motion.
(c) the degree of agreement between predictions and observation
(d) the conceptual elegance and aesthetic appeal of the theory

Models in quantum mechanics are used to describe the phenomena of atomic, molecular and particle physics. Models usually begin with a specific visualization and then, as anthropomorphic preconceptions are removed, the models acquire more emphasis on relationships between observables. As a consequence, the theories also become more abstract, and we will encounter this particularly in our study of the harmonic oscillator.

Among the most important models in quantum mechanics are:

a) Particle in a box

The model of a single particle in a piecewise constant potential (deep square well, finite well, multiple wells) which applies to situations in nuclear and molecular physics, and which is also useful for the quantum theory of solids.

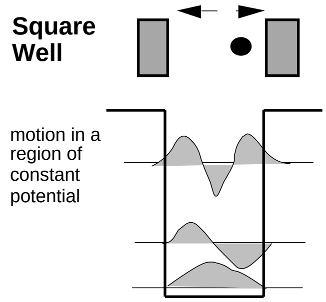


Fig 7.1 Deep Well and Eigenfunctions

b) Harmonic Oscillator

The model of a mass bound with a linear restoring force (harmonic oscillator) which applies *inter alia* to molecules and to crystal lattices; after a significant generalization this model also underlies the highly successful quantum theory of the electromagnetic field.

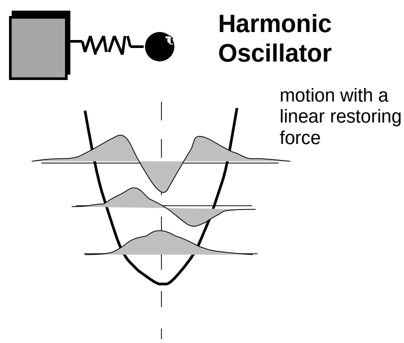


Fig 7.2 Harmonic Oscillator and Eigenfunctions

c) Rigid Rotor

The model of masses bound to one another at a nearly fixed distance (rigid rotor) which is used for molecular theory, and which provides the semi-classical approach to the quantum theory of angular momentum.

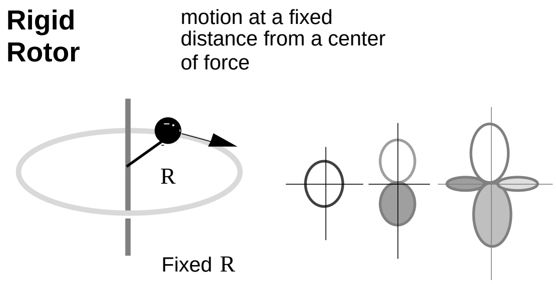
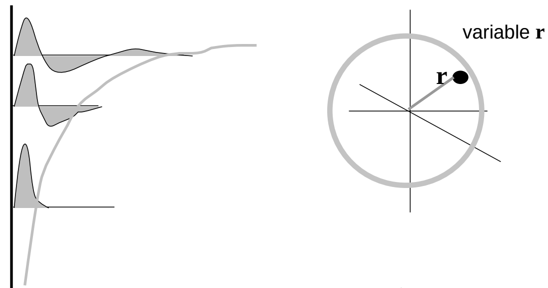


Fig 7.3 Rigid Rotor and Eigenfunctions

d) Hydrogen atom

The model of a single particle in a Coulomb potential which is used for one-electron atoms (hydrogen, muonium, positronium) and ions (He , Li , ..), and which is extended to more complicated atoms and to charges in solids (e.g. F-centers, excitons).



Radial Motion in a $\frac{1}{r^2}$ potential

Fig 7.4 Coulomb Potential and Eigenfunctions

e) Spin in a Field

The model of a spin - particle in a magnetic field which explains the Zeeman effect in optical and radiofrequency spectra, and which leads us to the general quantum theory of angular momentum.

When Models Don't Fit

Many physical systems do not fit neatly into the categories defined by these simple models. Often the atom or molecule of interest is significantly more complicated than the idealized model. In that case the analysis of data often proceeds with a modification of the most appropriate simple model, as when one uses a one-electron model to describe the optical spectrum of an alkali atom. Or it may be that the analysis proceeds by combining simple models, as when one uses a rotor model and harmonic oscillator model together for a description of the microwave spectrum of a diatomic molecule.

There are only a few physical models that have tractable solutions, so physicists cling to them, as drowning sailors to a raft, as they strive to understand their world. And in this they have attained an astonishing degree of success. One can only marvel that the principles underlying a planetary model used to describe the solar system (diameter 10^{+13} m) also apply to a model used to describe the atom (diameter of 10^{-10} m). And one can only admire the physicists who, not being satisfied with 1% agreement between theory and experiment, examine the small discrepancies and thereby uncover the marvels of relativity and quantum electrodynamics.

7.3 FROM LINE SPECTRA TO A THERMAL SPECTRUM

An interesting situation arises when individual atoms are in such close proximity to other atoms that interatomic forces become comparable to the internal forces that bind the atom. In this context it is interesting to consider the spectrum emitted from a gas of hot atoms in the limits of low and high gas densities. The radiation from a gas is almost entirely attributable to the motion of valence electrons (since the massive positive ions move slowly), so the spectrum is a measure of the potential that governs the motion of those electrons.

In the limit of low densities where the interatomic spacing is much larger than the electron orbits, each electron tends to maintain an association with its parent atomic ion. The electron motions in this limit are quite orderly and the radiation from the dilute sample of gas consists of well-defined spectral lines in a pattern characteristic of the atomic species present in the gas.

As the density of the sample gas increases, the typical interatomic spacing becomes comparable to the electron orbit size and the perturbations from near neighbors broaden and shift the spectral lines from the atoms. The dominant atomic species in the gas still reveal themselves in the spectrum, but the fine details of individual atom structure blur as interatomic and molecular processes become more important.

In the limit of high densities the interatomic spacing is smaller than the valence electron orbits. Each electron is now strongly influenced by the presence of several nearby ions as well as by other electrons; the motions of the electrons are disorderly and not particularly characteristic of the atoms that comprise the sample.

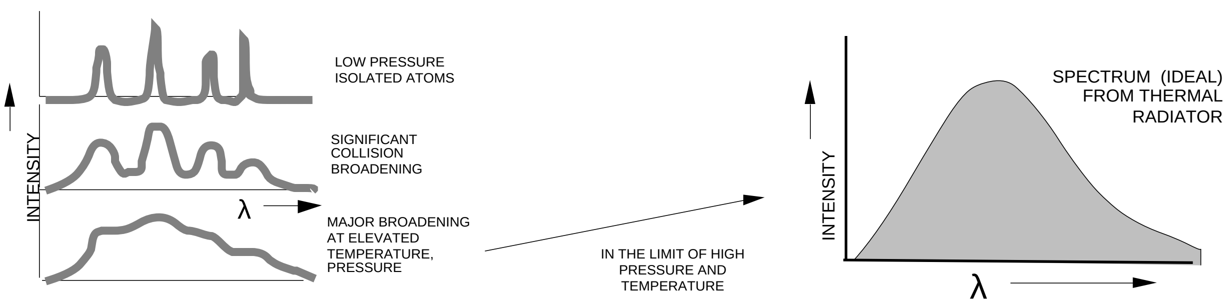


Fig 7.4 Evolution of Line Spectrum to Black Body Continuum

The Black Body Spectrum: If the high-density sample is in thermodynamic equilibrium, then the spectral distribution of radiation can be predicted from statistical mechanics: One obtains the Planck black body spectrum which depends only on the temperature of the sample and which has its peak at a wavelength of $\lambda_{PEAK} = 0.3$ cm/T(K). This dependence makes the apparent color a sensitive measure of the object's temperature; for example, an experienced blacksmith can glance at a hot slab of iron and determine its temperature to a repeatable accuracy of ±2 K). Even an inexperienced worker can easily measure the temperature to good precision by comparing the color of the hot object to the color of a filament in a calibrated incandescent light bulb. This is the basis of optical pyrometry.

The relationship between apparent color and thermodynamic temperature assumes that the object is in thermal equilibrium. This is at least approximately true for to objects that are simply heated to incandescence, but it is certainly not true for many common light sources such as fluorescent lamps (color temperature typically 4000K, well above the melting point of any material known) or metal (mercury or sodium) vapor lamps .

The concept of color temperature has been extended to the other regions of the spectrum. For example, using sensitive microwave radiometers, we can measure the curve even for cold systems; indeed this is the basis of precision (±0.001 K) measurements of the angular dependence of the 2.7 K temperature of deep space. Another example is provided by the inexpensive ($75) clinical thermometers that measure a human's temperature very quickly and to good accuracy by pointing an infrared radiometer into the ear.

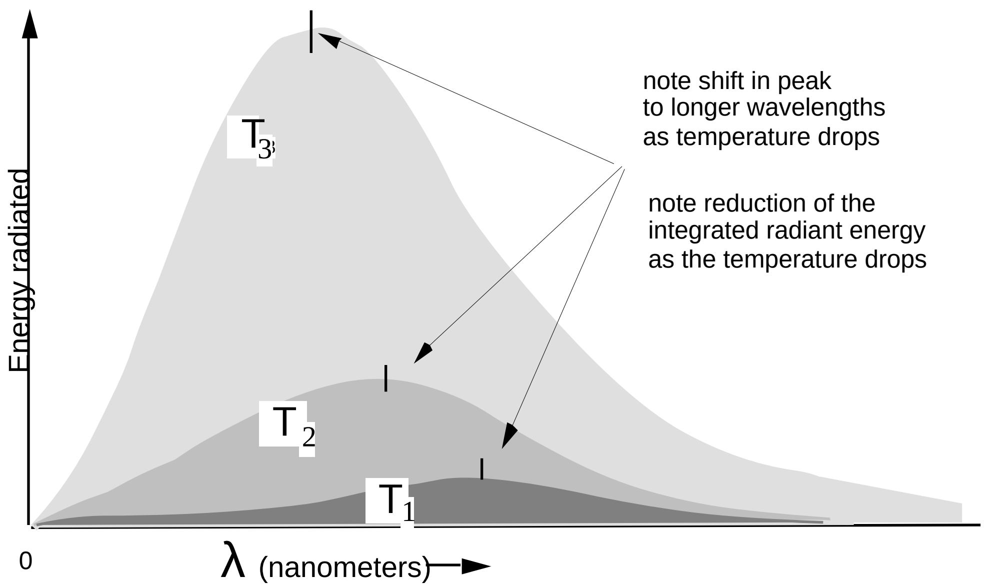


Fig 7.5 Spectrum of a thermal (*black body*) radiator at three different temperatures $T_3>T_2>T_1$

The shape of the spectrum from a hot object was described by Planck:

$$I(\lambda, T) = \frac{C_1}{\lambda^5}\left(\frac{1}{e^{C_2/\lambda T}-1}\right) \qquad \text{where} \quad C_1 = 8\pi\, h \quad \text{and} \quad C_2 = \frac{hc}{k} \qquad (7.1)$$

The total area under the curve represents the total energy radiated and is proportional to the fourth power of the temperature; this the Stefan-Boltzmann law and it helps us understand why it is so difficult to get objects to really high temperatures. The peak of the radiant energy spectrum occurs at a wavelength that is inversely proportional to (or at a frequency directly proportional to) the absolute temperature (Wein Law).

$$\underbrace{P = \sigma\ T^4}_{Stefan-Boltzmann\ Law} \qquad \underbrace{\lambda_{peak} \approx \frac{0.3\ cm}{T_{(Kelvins)}} \qquad f_{peak} \approx T_{(Kelvins)} \times 10^{11}\ Hz}_{Wein's\ Law} \qquad (7.2), (7.3)$$