

9.2: Oscillator Strength. (die Oszillatorenstärke)

The concept of oscillator strength arises from a classical electromagnetic model of the absorption of radiation by an atom. While a detailed understanding of each step in the derivation requires an understanding and recall of some results from classical mechanics and electromagnetic theory, it is not at all difficult to understand qualitatively the meaning of oscillator strength and at least the general gist of the argument that follows.

An atom consists of a nucleus surrounded by electrons - but not all of the electrons are equally strongly bound. We are going to think of an atom as having, for the purposes of this model, just two parts of interest, namely an outer loosely bound electron, and the rest of the atom. If this system is set into vibration, we'll suppose that it has a natural frequency ω_0 , but that the oscillations are damped. An oscillating dipole does, of course, radiate electromagnetic waves. That is to say, it loses energy. That is to say, the oscillations are damped. If the atom is placed in an oscillating electric field (i.e. if you shine a light on the atom) given by $\hat{E} \cos \omega t$ the electron will experience a force per unit mass $\frac{e\hat{E}}{m} \cos \omega t$. The Equation of motion is

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \frac{e\hat{E}}{m} \cos \omega t. \quad (9.2.1)$$

This is the differential Equation that describes forced, damped oscillations. The solutions to this Equation are well known, but I shall defer detailed consideration of it until the chapter on line profiles. Suffice it to say, for our present purposes, that it is possible to determine, from analysis of this Equation, how much energy is absorbed.

If a periodic force is applied to a mass attached to a fixed point by a spring, and the motion is damped, either by viscous forces (for example, if the mass were immersed in a fluid) or by internal stresses in the spring, not all of the work done by the periodic force goes into setting the mass in motion; some of it is dissipated as heat. In a way, we are imagining the atom to consist of an electron attached by some sort of force to the rest of the atom; not all of the work done by the forcing electromagnetic wave goes into setting the electron in motion. Some of the work is absorbed or degraded into a non-mechanical form. Perhaps the energy is lost because the accelerating electron radiates away energy into space. Or perhaps, if you believe in discrete energy levels, the atom is raised to a higher energy level. It does not matter a great deal what you believe happens to the energy that is "lost" or "absorbed"; the essential point for the present is that Equation 9.2.1 allows us to calculate (and I do promise to do this in the chapter on line profiles) just how much energy is lost or absorbed, and hence, if the atom is irradiated by a continuum of wavelengths, it enables us to calculate the equivalent width of the resulting spectrum line. The result obtained is

$$W = \frac{\mathcal{N} e^2 \lambda^2}{4 \epsilon_0 m c^2}. \quad (9.2.2)$$

W = equivalent width in wavelength units.

\mathcal{N} = column density (number per unit area in the line of sight) of absorbing atoms.

λ = wavelength of the line.

ϵ_0 = permittivity of free space.

e, m = charge and mass of the electron.

c = speed of light.

The reader should, as ever, check that the above expression has the dimensions of length. If every quantity on the right hand side is expressed in SI units, the calculated equivalent width will be in meters.

The reader may well object that s/he is not at all satisfied with the above argument. An atom is not at all like that, it will be said. Besides, Equation 9.2.2 says that the equivalent width depends only on the wavelength, and that all lines of the same wavelength have the same equivalent width. This is clearly nonsense. Let us deal with these two objections in turn.

First: Atoms are not at all like that. For a start, an atom is an entity that can exist only in certain discrete energy levels, and the only atoms that will absorb radiation of a given frequency are those that are in the lower level of the two levels that are involved in a line. Thus \mathcal{N} in Equation 9.2.2 must be replaced by \mathcal{N}_1 , the column density (number per unit area in the line of sight) of just those atoms that are in the lower level of the line involved. Thus Equation 9.2.2 should be replaced by

$$W = \frac{\mathcal{N}_1 e^2 \lambda^2}{4 \epsilon_0 m c^2}. \quad (9.2.3)$$

Second: The equivalent width of a line obviously does not depend only on its wavelength. Many lines of very nearly the same wavelength can have almost any equivalent width, and the equivalent width can vary greatly from line to line. We therefore now come to the *definition of oscillator strength*:

Definition

The absorption oscillator strength f_{12} of a line is the ratio of its observed equivalent width to the equivalent width (wrongly) predicted on the basis of the classical oscillator model and given by Equation 9.2.3.

Thus the expression for the equivalent width becomes

$$W = \frac{\mathcal{N}_1 f_{12} e^2 \lambda^2}{4 \epsilon_0 m c^2}. \quad (9.2.4)$$

The oscillator strength for a given line must be determined either experimentally or theoretically before the column density of a particular atom in, for example, a stellar spectrum can be determined from the observed equivalent width of a line. In principle, the oscillator strength of a line could be measured in the laboratory if one were able, for example, to measure the equivalent width of a line produced in an absorbing gas in front of a continuum source, and if one were able independently to determine \mathcal{N}_1 . Other experimental methods can be devised (see section 9.3 on Einstein coefficients), and theoretical methods are also available (see section 9.5 on line strengths).

It should be emphasized that Equation 9.2.4 applies only to an optically thin layer of gas. As far as I can see, there is no reason why Equation 9.2.4 is restricted either to a homogeneous layer of gas of uniform temperature and pressure, or to a gas in thermodynamic equilibrium - but it does require the layer to be optically thin.

We shall now restrict ourselves to an optically thin layer that is in *thermodynamic equilibrium* and of *uniform temperature* throughout. In that case, \mathcal{N}_1 is given by Boltzmann's Equation (see Equation 8.4.18):

$$\frac{\mathcal{N}_1}{\mathcal{N}} = \frac{\varpi_1 e^{-E_1/(kT)}}{u}. \quad (9.2.5)$$

Here \mathcal{N} is the total number of atoms per unit area in all levels, ϖ_1 is the statistical weight $2J+1$ of the lower level, and u is the partition function. Thus Equations 9.2.4 and 9.2.5 combined become

$$W = \frac{\mathcal{N} e^2 \lambda^2 \varpi_1 f_{12} e^{-E_1/(kT)}}{4 \epsilon_0 m c^2 u}. \quad (9.2.6)$$

In the above Equations I have used slightly different fonts for e , the electronic charge, and e , the base of natural logarithms.

The quantity f_{12} is called the *absorption oscillator strength*. An *emission oscillator strength* f_{21} can be defined by

$$\varpi_1 f_{12} = \varpi_2 f_{21}, \quad (9.2.7)$$

and either side of this Equation is usually given the symbol ϖf . Indeed, it is more usual to tabulate the quantity ϖf than f_{12} or f_{21} alone. I should also point out that the notation seen in the literature is very often gf rather than ϖf . However, in chapter 7 I went to considerable trouble to distinguish between statistical weight, degeneracy and multiplicity, and I do not wish to change the notation here. In any case, the value of ϖ (a form of the Greek letter pi) for an atomic energy level is $2J+1$. (We pointed out in chapter 7 why it is not usually necessary to include the further factor $2I+1$ for an atom with nonzero nuclear spin.) Equation 9.2.6 is usually written

$$W = \frac{\mathcal{N} e^2 \lambda^2 \varpi f e^{-E_1/(kT)}}{4 \epsilon_0 m c^2 u}. \quad (9.2.8)$$

If we take the common logarithm of Equation 9.2.8, we obtain

$$\log \frac{W}{\varpi f \lambda^2} = \log \frac{e^2}{4 \epsilon_0 m c^2} + \log \mathcal{N} - \log u - \frac{e V_1}{k T} \log e. \quad (9.2.9)$$

If everything is in SI units, this is

$$\log \frac{W}{\varpi f \lambda^2} = -14.053 + \log \mathcal{N} - \log u - \theta V_1. \quad (9.2.10)$$

I'd be happy for the reader to check my arithmetic here, and let me know (jtatum at uvic dot ca) if it's not right. Here W and λ are to be expressed in meters and N in atoms per square meter. V_1 is the excitation potential of the lower level of the line in volts, and θ is $5039.7/T$, where T is the excitation temperature in kelvin. *Thus, if we measure the equivalent widths of several lines from an optically thin gas, and plot $\log \left(\frac{W}{\varpi f \lambda^2} \right)$ versus the excitation potential of the lower level of each line, we should get a straight line whose slope will give us the excitation temperature, and, provided that we know the partition function, the intercept will give us the column density of the neutral atoms (in all levels) or of a particular ionization state.*

Often it will happen that some points on the graph fall nowhere near the regression line. This could be because of a wildly-erroneous oscillator strength, or because of a line misidentification. Sometimes, especially for the resonance lines (the strongest lines arising from the lowest level or term) a line lies well below the regression line; this may be because these lines are not optically thin. Indeed, Equation 9.2.10 applies only for optically thin lines.

Equation 9.2.10 shows how we can make use of Boltzmann's Equation and plot a straight-line graph whose slope and intercept will give us the excitation temperature and the column density of the atoms. We can go further and make use of Saha's Equation. If we plot $\log \left(\frac{W}{\varpi f \lambda^2} \right)$ versus the lower excitation potential for atomic lines and do the same thing separately for ionic lines, we should obtain two straight lines of the same slope (provided that the gas is in thermodynamic equilibrium so that the excitation temperatures of atom and ion are the same). From the difference between the intercepts of the two lines we can get the electron density. Here's how it works.

If we set up Equation 9.2.9 or Equation 9.2.10 for the atomic lines and for the ionic lines, we see that the difference between the intercepts will be equal to $\log \left(\frac{\mathcal{N}_a u_i}{\mathcal{N}_i u_a} \right)$, and, if the gas is optically thin, this is also equal to $\log \left(\frac{n_a u_i}{n_i u_a} \right)$. Here the subscripts denote atom and ion, \mathcal{N} is column density and n is particles per unit volume. Then from Equation 8.6.7 we see that

$$\log \left(\frac{n_a u_i}{n_i u_a} \right) = \text{difference between intercepts} = 27.24 - \frac{3}{2} \log \theta - \theta(V - \Delta V) - \log n_e \quad (9.2.11)$$

Here θ is $5039.7/T$, where T is the ionization temperature and, in assuming that this is the same as the excitation temperatures obtained from the slopes of the lines, we are assuming thermodynamic equilibrium. V is the ionization potential of the atom. Thus we can obtain the electron density n_e – except for one small detail. ΔV is the lowering of the excitation potential, which itself depends on n_e . We can first assume it is zero and hence get a first approximation for n_e ; then iterate to get a better V in the same manner that we did in solving Problem 4 of section 8.6.

So far we have discussed the equivalent width of a *line*. A line, however, is the sum of several Zeeman *components*, with (in the absence of an external magnetic field) identical wavelengths. It is possible to define an oscillator strength of a Zeeman *component*. Is the oscillator strength of a line equal to the sum of the oscillator strengths of its components? The answer is *no*. Provided the line and all of its components are optically thin, the *equivalent width* of a line is equal to the sum of the equivalent widths of its components. Thus Equation 9.2.8 shows that the ϖf value of a line is equal to the sum of the ϖf values of its components. A further point to make is that, for a component, the statistical weight of each state of the component is unity. (A review from chapter 7 of the meanings of line, level, component, state, etc., might be in order here.) Thus, for a component there is no distinction between absorption and emission oscillator strength, and one can use the isolated symbol f with no subscripts, and the unqualified phrase "oscillator strength" (without a "absorption" or "emission" prefix) when discussing a component. One can accurately say that the ϖf value of a line is equal to the sum of the f values of its components. In other words, $\varpi f(\text{line}) = \Sigma f(\text{components})$, so that one could say that the oscillator strength of a line is the *average* of the oscillator strength of its components. Of course, this doesn't tell you, given the ϖf value of a line, what the f -values of the individual components are. We defer discussion of that to a later section of this chapter.

The phrase " f -value" is often used instead of "oscillator strength". I was rather forced into that in the previous paragraph, when I needed to talk about ϖf values versus f -values. However, in general, I would discourage the use of the phrase " f -value" and would encourage instead the phrase "oscillator strength". After all, we never talk about the "evaluate" of the electron or the " M -value" of the Sun. I suppose "weighted oscillator strength" could be used for ϖf .

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