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CHAPTER

Physical Basics of Spectroscopy

1.1 Photons: Carriers of Information and Energy

1.1.1 Photons: Carriers of Information

Photons are extremely important for all astronomy because they carry information about the observed object to our recording devices. Some of them finally end up in the pixel field of our CCD camera. It is therefore worthwhile to take some time to consider this absolutely most important link in the transmission chain.

It was on the threshold of the twentieth century, when the discovery of the photon with its seemingly odd properties, caused tremendous "headaches" to the entire community of top physicists. This huge intellectual effort finally culminated in the development of quantum mechanics. The list of participants reads substantially like the *Who's Who* of physics at the beginning of the twentieth century: Werner Heisenberg,

Albert Einstein, Erwin Schrödinger, Max Born, Max Planck, Wolfgang Pauli, Niels Bohr, just to name a few. Quantum mechanics became, besides the theory of relativity, the second revolutionary theory of the twentieth century. For the rough understanding about the formation of the photons and finally of the spectra, the necessary knowledge may be reduced to some very basic key points of this theory.

1.1.2 The Wave–Particle Duality

Electromagnetic (EM) radiation exhibits both wave and particle nature. This principle applies to the entire spectrum. Starting with the long radio waves, it remains valid on the domains of infrared radiation, visible light, up to the extremely short-wave ultraviolet, X-rays and gamma rays (Figure 1.1). For our present technical applications, both properties are indispensable. For the entire telecommunications, radio, TV,



Figure 1.1 Electromagnetic spectrum

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mobile telephony, as well as the radar and microwave grill it is the wave nature that is utilized. However, CCD photography, light metering on cameras, gas discharge lamps (e.g. for energy saving light bulbs and street lighting) and last but not least spectroscopy all require the particle nature to work.

1.1.3 The Quantization of Electromagnetic Radiation

It was one of the pioneering discoveries of quantum mechanics that electromagnetic radiation is not emitted continuously but rather quantized (or quasi "clocked"). Simplified explained a minimum "dose" of electromagnetic radiation is generated, called "photon," which belongs to the bosons within the "zoo" of the elementary particles. The term "photon" derives from the Greek " $\varphi \tilde{\omega} \varsigma$ " or "phôs," which means light.

1.1.4 Photons: Carriers of Energy

Each photon has a specific frequency (or wavelength), which proportionally determines the transported energy – the higher the frequency, the higher the energy of the photon (see Section 1.3.3).

1.1.5 Other Properties of Photons

Without any external influences photons exhibit an infinitely long life expectancy. Their generation and "destruction" takes place in a variety of physical processes. Chiefly relevant for astronomical spectroscopy is the broadband generation of photons by hot stars and the narrow-band emission and absorption due to electron transitions between different atomic orbitals.

A photon carrying a specific amount of energy always moves with speed of light. Therefore, according to the special theory of relativity (STR), it has no rest mass. However, based on the mass-energy equivalence a photon, moving with light speed, has a kind of "relativistic mass" causing an actual measurable momentum.

1.2 The Electromagnetic Spectrum

1.2.1 The Usable Spectral Range for Amateurs

Professional astronomers nowadays study the objects in nearly the entire electromagnetic spectrum – including the domain of radio astronomy (see Figure 1.1). Furthermore, space telescopes are used which are increasingly optimized for the infrared domain in order to record the extremely redshifted spectra of objects from the early days of the Universe. For the ground-based amateur, equipped with standard telescopes and spectrographs, only a modest fraction of this domain is reachable. In addition to the specific design features of the spectrograph, the usable range is limited here mainly by the spectral characteristics of the camera, including any filters. So, for example, the camera Atik 314L+ combined with the DADOS spectrograph, achieves useful results in the range of approximately $\lambda\lambda$ 3800–8000, i.e. throughout the visible domain and the near infrared part of the spectrum. Here also the well known lines are located, such as the H-Balmer series and the Fraunhofer absorptions.

1.2.2 The Selection of the Spectral Range

For high-resolution spectra, the choice of the spectral range is normally determined by a specific monitoring project or an interest in particular lines. Perhaps also the emission lines of the calibration light source may be considered in the planning of the recorded section. For low-resolution, broadband overview spectra, mostly the range of the H-Balmer series is preferred. Hot O and B stars can be taken rather in the short-wave part, because their radiation intensity is very strong in the UV range. Only in special cases it makes sense here to include an area on the red side of H α . Between approximately $\lambda\lambda 6200$ and 7700 [1] it is swamped with atmospheric related (telluric) H₂O and O₂ absorption bands. Apart from an undeniable aesthetic aspect they are interesting only for the atmospheric physicist. For astronomers, they are usually only a hindrance, unless the fine water vapor lines are used to calibrate the spectra! Anyway, there exist methods to extract these absorptions from the profile, for example, with the Vspec software or with the freeware program SpectroTools [73].

However, with the late spectral types of K and the entire M class [1] it makes sense to record the near infrared range. The radiation intensity of these stars is very strong here and displays interesting stellar molecular absorption bands. Also, the reflection spectra of the large gas planets show particularly here the impressive molecular gaps in the continuum. Further, the *Spectral Atlas* [1] is an aid to find the appropriate interesting spectral domain for all object classes.

Useful guidance for setting the wavelength range of the spectrograph is the calibration lamp spectrum or the daylight (solar) spectrum. At night the reflected solar spectrum is available from the Moon and the planets. A striking marker on the blue side of the spectrum is the impressive double line of the Fraunhofer H and K absorption.

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Table	1.1	Terminology	in t	the o	optical	range	(UBVRI	λλ3300-	10.000)
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Center wavelen	egth		
λ [μm]	λ [Å]	Astrophysical wavebands	Required instruments
0.35	3500	U band (UV)	
0.44	4400	B band (blue)	
0.55	5500	V band (green)	Most optical telescopes
0.65	6500	R band (red)	
0.80	8000	I band (infrared)	

Further in use is also the Z band, $\sim\lambda\lambda8000-9000$ and the Y band, $\sim\lambda\lambda9500-11,000$ (ASAHI Filters).

Table 1	1.2	Terminology	in t	the infrared	range	(λλ10,000-2,000,000)
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Center wavelen	gth		
λ [μm]	λ [Å]	Astrophysical wavebands	Required instruments
1.25	12,500	J band	
1.65	16,500	H band	Most optical and dedicated
2.20	22,000	K band	
3.45	34,500	L band	Composition land
4.7	47,000	M band	dedicated infrared
10	100,000	N band	telescopes
20	200,000	Q band	
200	2,000,000	Submillimeter	Submillimeter telescopes

Source: Wikipedia page on infrared astronomy

1.2.3 Terminology of the Spectroscopic Wavebands

Terminology for wavebands is applied inconsistently in astrophysics [7] and depends strongly on the context. Furthermore many special fields of astronomy, various satellite projects etc. often use different definitions. Tables 1.1 and 1.2 give a summary according to [7] and Wikipedia (infrared astronomy). Indicated are either the center wavelength λ of the corresponding photometric band filters, or their approximate passband. The original passband of these broadband filters, applied for the photometric UBVRI system, have been defined by Johnson, Bessel and Cousins.

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Table	1.3 Terminology	predominantly	applied by	ground-based
observ	atories			

Far Ultraviolet (FUV)	$\lambda < 3000$	Satellite based special telescopes
Near Ultraviolet (NUV)	λ 3000-3900	
Optical (VIS)	λ 3900-7000	
Near Infrared (NIR)	λ 6563 (Hα)– 10,000	
Infrared or Mid- Infrared	λ 10,000-40,000	(J, H, K, L band 1–4 μm)
Thermal Infrared	λ 40,000-200,000	(M, N, Q band 4–20 μm)
Submillimeter	$\lambda > 200,000$ (200 μ m)	

1.3 Wavelength and Energy

1.3.1 Preliminary Remarks

According to the recommendations of the International Astronomical Union (IAU) among others, the cgs system (centimeter, gram, second) along with the units [erg], angstrom [Å] and gauss [G] should no longer be applied. However, the angstrom for the wavelength is still in use (and not only in the amateur sector). Furthermore in astrophysical papers, for example, the surface gravity g and many other applications are still expressed in cgs units and the magnetic flux density in gauss [G].

1.3.2 Units for Energy and Wavelength Applied in Spectroscopy

It is still very common for many applications to use the erg rather than the joule [J] and 1 erg = 10^{-7} J. Thus for the line flux the unit [erg s⁻¹ cm⁻²] is widely in use (see Section 9.1.3). For the extremely low energies of electron transitions instead of joule [J] almost always the unit electronvolt [eV] is applied, in accordance with the IAU recommendations and $1eV = 1.602 \times 10^{-19}$ J.

Furthermore, in the optical spectral domain the wavelengths are extremely small and in astronomy they are usually measured in angstroms [Å] or nanometers [nm]. One should be aware that 1 Å roughly corresponds to the diameter of an atom, including its electron shells! In the infrared range the

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micron [μ m] is also in use: 1 Å = 10⁻¹⁰ m, 1 nm = 10 Å, 1 μ m = 1000 nm = 10,000 Å.

Sometimes, the wavelength λ is also expressed as "wavenumber *k*," which is the reciprocal value of λ . Here we mainly see *k* expressed in number of waves within 1 cm [cm⁻¹], a further example of the cgs system has obviously still "survived."

$$k = \frac{1}{\lambda} = \frac{\nu}{c} \left[\text{cm}^{-1} \right]$$
 {1.1}

1.3.3 Planck's Energy Equation

For each individual line the corresponding photon energy E can be calculated. This is enabled by the simple equation of the German physicist and Nobel Prize winner Max Planck (1858–1947):

$$E = hv \tag{1.2}$$

Here, E = photon energy in joule [J], h = Planck's constant (the quantum of action 6.626 × 10⁻³⁴ J s, v Greek "nu") = frequency [s⁻¹] of the photon of the spectral line.

The frequency v is simply related to the wavelength $\lambda[m]$ (c = speed of light $3 \times 10^8 \text{ m s}^{-1}$):

$$v = \frac{c}{\lambda}$$
 {1.3]

Inserting Equation {1.3} into {1.2} yields:

$$E = \frac{hc}{\lambda} \tag{1.4}$$

The most important statement of Equations {1.2} and {1.4}: The energy of a photon *E* is proportional to its frequency *v* and inversely proportional to the wavelength λ .

The following simple equations, suitable for pocket calculators, allow converting the wavelength λ [Å] into energy *E* [eV] and vice versa:

$$\lambda[\text{Å}] = \frac{12403}{E[\text{eV}]}$$
 {1.5}

$$E[eV] = \frac{12403}{\lambda[\mathring{A}]}$$
 {1.6}

1.4 The Continuum and Blackbody Radiation

1.4.1 The Blackbody as a Physical Model for Stellar Radiation

Heating up an object raises its temperature, which determines the movements of the atoms inside the object. When the temperature becomes higher than the environment, the object starts to emit electromagnetic radiation. Objects around us, inclusive ourselves, also reflect radiation, which is noticeable in the visible or infrared wavelength range.

Stars, like our Sun behave differently in that they do not reflect radiation which falls on them, but rather absorb all incident radiation. Therefore, as an approximation, but with some exceptions, we can consider the Sun as a blackbody.

A perfect blackbody absorbs all radiation that falls on it, does not reflect any radiation nor is transparent to it. This means that blackbody radiation, i.e. the emitted radiation of a blackbody, is exclusively determined by its temperature. As a result of this approximation, measurement of the emitted radiation of a star lets us determine its temperature through the specific distribution of the blackbody radiation (see Figure 1.3).

The physical model of the blackbody applies well to the non-transparent part of the stellar photosphere. Other parts of the stellar atmosphere show a different behavior as the atoms present absorb photons at certain wavelengths. This represents a highly important source of information, included in the generated spectrum of the star. In contrast to the distribution of the blackbody radiation the analysis of the star's spectrum gives us insight into the chemical composition.

1.4.2 Planck's Radiation Law and Course of the Continuum Level

The curve in Figure 1.2, hereafter referred to as continuum level $I_C(\lambda)$, corresponds to the course of the spectral flux density (see Section 9.1.2), sometimes abbreviated as intensity I. It is plotted over the wavelength, which increases from left to right. In the original, undisturbed profile it represents very roughly the exclusively temperature dependent blackbody radiation characteristics $B_{Teff}(\lambda)$ of the star. As a fit to the continuum it is cleaned from any existing absorption or emission lines. The entire area between the horizontal wavelength axis and the continuum level $I_C(\lambda)$ is called "continuum." This blackbody model is quite useful for rather cool stars exhibiting a maximum radiation in the green to red part of the spectrum, but excluding the M class with the strong and very uneven TiO absorptions [1]. For hot stars, as shown in Figure 1.2, radiating mainly in the blue up to the UV range, it gets significantly overprinted by the Balmer jump of the hydrogen series (see also Figures 2.4 and 2.5).

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Figure 1.2 Continuum, continuum level and approximate blackbody radiation $B_{Teff}(\lambda)$



Figure 1.3 Planck radiation and Wien's displacement law

1.4.3 Wien's Displacement Law

Figure 1.3 shows the theoretical blackbody radiation distribution of different stars, exhibiting bell-shaped curves $B_{Teff}(\lambda)$. With increasing temperature their peak intensities get shifted to shorter wavelength, and respectively to higher frequency (Planck's radiation law). With Wien's displacement law and the given wavelength [Å] of the maximum radiation intensity $\lambda_{I \max}$ [Å] it is theoretically possible to roughly estimate the "effective temperature," T_{eff} [K], of a star (Wilhelm Wien (1864–1928) was a German physicist and Nobel Prize winner):

$$\lambda_{I\max} \left[\text{\AA} \right] \approx \frac{28,978,200}{T_{\text{eff}}}$$
 $\{1.7\}$

$$T_{\rm eff}[{\rm K}] \approx \frac{28,978,200}{\lambda_{I\,{\rm max}}}$$
 {1.8}

Examples of the wavelengths of maximum blackbody radiation:

Alnitak	$T_{\rm eff} \approx 25000~{\rm K}$	$\lambda_{I \max} \approx 1160 \text{ Å}$ (ultraviolet range)
Sun	$T_{\rm eff} \approx 5800~{\rm K}$	$\lambda_{I{ m max}} pprox 4996$ Å (green range)
Betelgeuse	$T_{\rm eff} pprox 3450 \ { m K}$	$\lambda_{I{ m max}} pprox 8400$ Å (infrared range)

1.4.4 Effective Temperature *T*_{eff} and Stefan–Boltzmann Law

The effective temperature, $T_{\rm eff}$, is the temperature required for a blackbody radiator with the same size of the star, in order to generate the identical bolometric energy flow $F_{\rm Bol}$ [erg cm⁻² s⁻¹]. However, $F_{\rm Bol}$ is not limited to the visual spectral range but the radiation energy per unit time and unit area corresponds to the total area under the Planck radiation curve. It is obtained by integration of the spectral flux density $I(\lambda)$ over the entire electromagnetic spectrum from $\lambda = 0$ to infinity (∞):

$$F_{\rm Bol} = \int_{0}^{\infty} I(\lambda) d\lambda \qquad \{1.9\}$$

Further, according to the law of Stefan–Boltzmann, $F_{\rm Bol}$ is proportional to the fourth power of the effective temperature $T_{\rm eff}$

$$F_{\rm Bol} = \sigma \, T_{\rm eff}^4 \tag{1.10}$$

where σ is the Stefan–Boltzmann constant: 5.67 × 10⁻⁵ erg s⁻¹ cm⁻² K⁻⁴. However, it must never be confused with the Boltzmann constant $k_{\rm B}$, applied in statistical mechanics (see Section 14.2.3). The Stefan–Boltzmann law is named after the Austrian physicist and mathematician Josef Stefan (1835–1893) together with his compatriot, the

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physicist and philosopher Ludwig Boltzmann (1844–1906). If F_{Bol} of a star with the radius *R* is multiplied with its supposed spherical surface $4\pi R^2$, it yields the entire bolometric luminosity *L* in [erg s⁻¹], under the assumption that the emission takes place evenly distributed:

$$L = 4\pi R^2 \sigma T_{\rm eff}^4$$
 {1.11]

For example the bolometric luminosity of the Sun with a temperature of ~5780 K and a radius of ~695,800 km, yields $L \approx 3.846 \times 10^{33} \,\mathrm{erg s^{-1}}$, corresponding to 3.846×10^{26} W. The solar flux density finally reaching the surface of the Earth is defined as the solar constant $E_0 = 1368 \,\mathrm{W m^{-2}}$ (from the World Meteorological Organization, WMO).