

SPECTRA, IMAGES, SIMPLE FUNCTIONS, AND DENSITY FUNCTIONS

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ABSTRACT

When working with spectra that represent optical power or photon number, we must be very careful with our units. Since most spectral transformations are nonlinear, the transformation Jacobian produces a nonlinear distortion of the spectrum. A surprising number of researchers ignore these issues and misrepresent their spectra in their publications.

Index Terms— spectrum, nonlinear transformation, density functions, distortion, Jacobian

1. INTRODUCTION

Most researchers, even in our field where they really should know better, think of a spectrum as a simple graph. One can point to a location on a reflectivity spectrum curve and say something like “look here — the reflectivity at $\lambda = 600$ nm is 0.5.” If light reflects first from one surface and then another, then we can simply multiply the two reflectance spectra together to get the overall reflectance of the combination. However, we cannot do this for an irradiance spectrum. We cannot place a finger on a irradiance spectrum and say something like “see, the irradiance here at $\lambda = 600$ nm is 10 W m^{-2} ”. Unlike the reflectance spectrum, the irradiance spectrum does not define the irradiance at a single point. Rather, it defines the differential irradiance with respect to the wavelength, as implied by the units $10 \text{ W m}^{-2} \text{ nm}^{-1}$, so that the irradiance value is given by integrating the spectrum over a specified range. As a result, it also makes no sense to multiply two irradiance functions together.

While the distinction between these two forms of spectra can be ignored in many circumstances, there are also many situations in which they cannot, and inattention to this detail has produced errors in work published throughout our field. It is, for example, partly responsible for the surprisingly persistent fallacy that the human eye’s sensitivity is matched to the peak of the Sun’s radiance spectrum.[1] The fields of physics and engineering that use measurements of optical spectra, like most other areas of physics, sometimes forget to make clear distinctions between simple functions and density functions. Very few textbooks even discuss the issue,[2] despite its fundamental importance in explaining the

meaning of optical measurement. As a result, the relevance to spectrometry of the distinction between simple functions and density functions may not seem immediately obvious, but we will show that while it can often be ignored in standard 2D imaging, it often cannot be ignored in spectrometry without causing severe errors.

One field where this distinction is introduced early on to students, and hammered into their heads regularly in the curriculum, is probability theory, where the two are labelled as mass functions and density functions. Here I will refer to them as simple functions and density functions. While mathematicians who work in probability theory have a habit of saying that measure theory, Stieltjes integrals, and similar 20th century tools of mathematics are *required* tools in order to work with density functions,[3] these are unnecessary for practical work. Physicists have been working with density functions long before measure theoretic tools were developed, and realize that one need only pay close attention to units and to the physical meaning of the quantities being manipulated.

2. WAVELENGTH \leftrightarrow WAVENUMBER TRANSFORMATIONS

The Planck blackbody function provides a useful demonstration for how the units we use can affect the shape of the spectra we draw. The most common representation for the function is to calculate the spectral radiance in flux units of Watts on a wavelength axis, using the expression

$$L_e(\lambda) = \frac{2hc^2}{\lambda^5} \left(\frac{1}{e^{hc/(\lambda k_B T)} - 1} \right).$$

Here, L is the spectral radiance [$\text{W m}^{-2} \text{ sr}^{-1} \mu\text{m}^{-1}$], with the subscript “e” indicating the use of energy-based flux units. The constants are the speed of light c [m/s], k_B Boltzmann constant [J/K], and Planck constant h [J s], while T [K] is the temperature parameter, and λ [μm] is the wavelength. For the Planck blackbody function represented in a different domain such as wavenumber or frequency, see Tab. 1.

Next we look at what happens when we try to transform the blackbody spectrum from a wavelength basis to a wavenumber basis. Here we will use the definition of wavenumber as $\sigma = 1/\lambda$. (A common alternative definition of wavenumber is $k = 2\pi/\lambda$.) Any legitimate transformation of the spectrum must preserve the overall energy (or

This work was supported by JSPS KAKENHI Grant JP20K04516 Grant-in-Aid for Scientific Research.

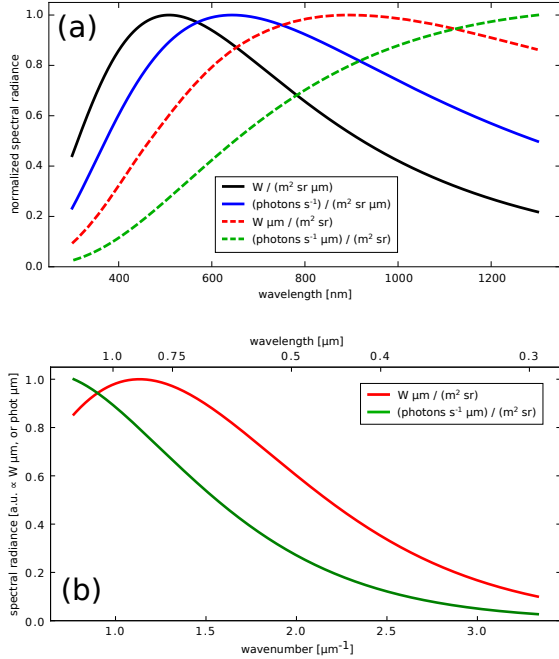


Fig. 1. (a) The Planck blackbody spectrum for a 5770 K source (an approximation to the above-atmosphere solar radiance spectrum), normalized to a peak value of 1. The black and blue curves are calculated in wavelength space, while the red and green curves are calculated in wavenumber space, then re-sampled onto a linear wavelength grid in order to demonstrate the change in shape. (b) The red and green curves calculated in a linear wavenumber space.

photon number) of the integrated spectrum. With this constraint, we can either work directly with infinitesimals to write $d\sigma = -d\lambda/\lambda^2$ or equivalently work with the integral directly to write

$$\begin{aligned} \int_{\lambda_1}^{\lambda_2} L(\lambda) d\lambda &= \int_{\sigma(\lambda_1)}^{\sigma(\lambda_2)} L(\lambda(\sigma)) \left| \frac{d\lambda}{d\sigma} \right| d\sigma \\ &= \int_{\sigma(\lambda_1)}^{\sigma(\lambda_2)} L(\lambda(\sigma)) (-\lambda^2) d\sigma = \int_{\sigma_1}^{\sigma_2} L(\sigma) \lambda^2 d\sigma \end{aligned}$$

where the last line uses the negative sign to swap the order of integration. The factor of λ^2 inside the integral tells us that the resulting curve will have a different shape, as we see in Fig. 1, where the above transformation is indicated by the black and red curves. Since the two curves are plotted together on the same linear wavelength abscissa, one might justifiably feel that doing this for the wavenumber-space representation is illegitimate. Indeed, drawing the curve this way does not preserve the energy of the integral. It does, however, preserve the shape of the function, so that we can demonstrate changes in the location of the peak.

In addition to the wavelength and wavenumber axes, other common representations of optical spectra use abscissae of

frequency [THz] or energy [eV]. Since these units are proportional to wavenumber, however, they only change the axis labels and not the shape of the curve. These four options for the abscissa are what we can call the “density units” of the spectrum. Table 1 gathers together a set of Planck function representations for each different choice of domain.

3. POWER ↔ PHOTON NUMBER TRANSFORMATIONS

While the wavelength-wavenumber transformation of the spectrum is widely recognized, and mistakes regarding it are not so common in the literature, the transformation of flux units from power (Watts) or photon number is abused almost everywhere. Since the energy of a photon is wavelength dependent, transforming the ordinate of the spectrum from Watts to photons/sec causes a shift in the shape of a spectrum. As a result, it matters very much which ordinate we choose. In Fig. 1, two of the curves are representations for the Planck blackbody curve using an ordinate proportional to photon number rather than Watts. Since the number of photons per unit energy is larger at longer wavelengths, the transformation from Watts to photons lifts up the long-wavelength end of the spectrum — shifting the peak of the curve to the red.

The majority of detectors that we use in research these days are integrating sensors, such as the CCD and CMOS detector arrays used in imaging and spectrometry, as well as cryo-cooled infrared detector arrays. The digital number that these sensors return is proportional to the number of photoelectrons collected by the sensor during the integration period. As a result, if we plot data from a digital spectrometer, we should almost always choose the spectrum ordinate to be proportional to photon number and not Watts.

The second category of detectors are flux sampling sensors, which include photodiodes and bolometers (among others). The digital number returned by these detectors is proportional to the instantaneous optical power incident on the face of the sensor. Thus, if we plot data from a spectrometer using a microbolometer detector array, the appropriate ordinate would be proportional to Watts.

The largest number of mistakes occur when authors draw a spectrum measurement and write “intensity [a.u.]” for the ordinate of the plot. If the abscissa is labelled as wavelength (or wavenumber), then we can infer that the intensity must also be represented in wavelength (or wavenumber) space. If the writer is discussing a modern detector array as the source of the measurements, then we can also infer that the ordinate must be proportional to photon number. In older publications, especially before the 1990s, almost all sensors were flux-sampling, and so we can infer that the ordinate will be proportional to optical power. However, the momentum of history has been such that many modern authors persist in discussing radiometric units of optical power while using CCD and CMOS integrating sensor arrays. The result is a misla-

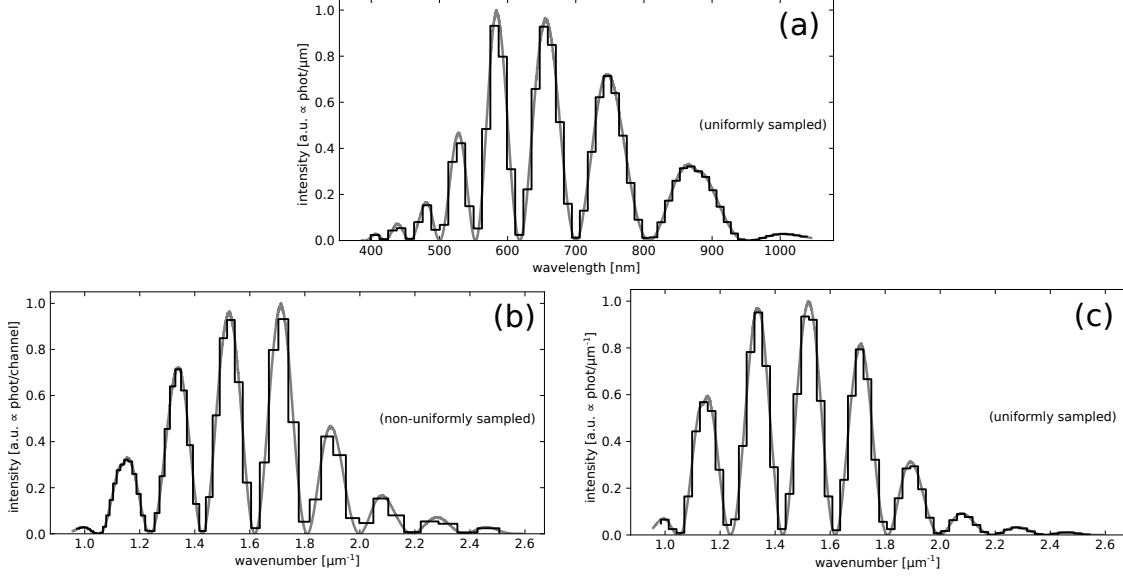


Fig. 2. (a) A spectrum measured with a modern grating spectrometer, so that the appropriate units for the ordinate are proportional to $\text{phot}/\mu\text{m}$. A low-resolution discrete spectrum is superimposed over the measured spectrum. (b) The spectrum shown in (a) resampled onto a nonuniform wavenumber grid. The nonuniform sampling is not clear when the samples are tightly spaced (grey curve) but are obvious in the low-resolution discrete spectrum (black lines). (c) If we interpolate the spectrum from (a) onto a uniformly-sampled wavenumber grid, we need to rescale the individual channel bins in order to conserve overall photon count.

Table 1. Planck blackbody expressions in different domains.[6]

Spectrum variable	Quantum flux	Optical power
Wavelength λ :	$L_q(\lambda) = \frac{2c}{\lambda^4} \left(\frac{1}{e^{hc/(\lambda k_b T)} - 1} \right)$ [photon $\text{s}^{-1} \text{m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$]	$L_e(\lambda) = \frac{2hc^2}{\lambda^5} \left(\frac{1}{e^{hc/(\lambda k_b T)} - 1} \right)$ [W $\text{m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$]
Frequency $\nu = c/\lambda$:	$L_q(\nu) = \frac{2\nu^2}{c^2} \left(\frac{1}{e^{h\nu/(k_b T)} - 1} \right)$ [photon $\text{s}^{-1} \text{m}^{-2} \text{sr}^{-1} \text{Hz}^{-1}$]	$L_e(\nu) = \frac{2h\nu^3}{c^2} \left(\frac{1}{e^{h\nu/(k_b T)} - 1} \right)$ [W $\text{m}^{-2} \text{sr}^{-1} \text{Hz}^{-1}$]
Wavenumber $\sigma = 1/\lambda$:	$L_q(\sigma) = \frac{2c\sigma^2}{e^{hc\sigma/(k_b T)} - 1}$ [photon $\text{s}^{-1} \text{m}^{-2} \text{sr}^{-1} \text{cm}$]	$L_e(\sigma) = \frac{2hc^2\sigma^3}{e^{hc\sigma/(k_b T)} - 1}$ [W $\text{m}^{-2} \text{sr}^{-1} \text{cm}$]
Wavenumber $k = 2\pi/\lambda$:	$L_q(k) = \frac{ck^2}{4\pi^3} \left(\frac{1}{e^{hck/(k_b T)} - 1} \right)$ [photon $\text{s}^{-1} \text{m}^{-2} \text{sr}^{-1} \text{cm}$]	$L_e(k) = \frac{hc^2k^3}{4\pi^3} \left(\frac{1}{e^{hck/(k_b T)} - 1} \right)$ [W $\text{m}^{-2} \text{sr}^{-1} \text{cm}$]
Energy $E = hc/\lambda$ (eV):	$L_q(E) = \frac{2E^2}{c^2 h^3} \left(\frac{1}{e^{E/(k_b T)} - 1} \right)$ [photon $\text{s}^{-1} \text{m}^{-2} \text{sr}^{-1} \text{eV}^{-1}$]	$L_p(E) = \frac{2E^3}{c^2 h^3} \left(\frac{1}{e^{E/(k_b T)} - 1} \right)$ [W $\text{m}^{-2} \text{sr}^{-1} \text{eV}^{-1}$]

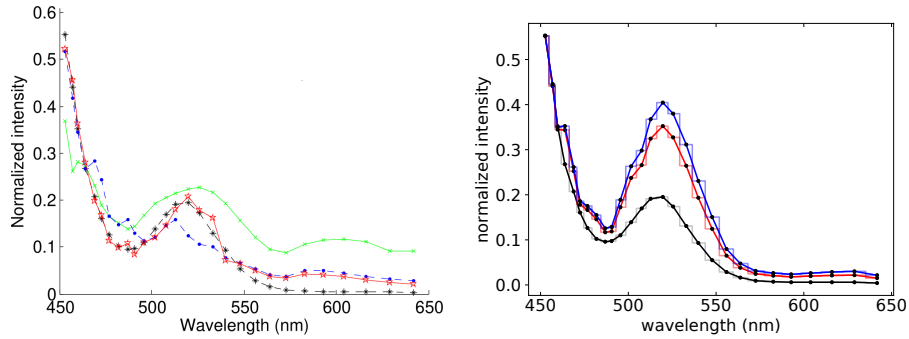


Fig. 3. (a) Original figure from Ref. [7]. (b) The black curve copied and (red, blue) transformed.

belling of the axes, or a distortion of the spectrum shape.

Even Soffer & Lynch, who have written the article [1] most often cited regarding the fallacy of the eye’s optimization to green, focus their discussion almost entirely on the wavelength-wavenumber transformation rather than the energy-photon transformation, even though the meaning of the abscissa transformation is unclear in the case of the eye. It is clear, however, that the *ordinate* of the radiance spectrum should be represented in photons rather than energy, since the retina is a quantum detector and not a power detector.[4, 5]

So far the discussion has focused on continuous representations of spectra. For laboratory measurements, however, what we obtain are discrete functions. Discrete representations give us extra flexibility because the spectra have already been integrated across the passband of the individual spectral channel. If we transform the spectrum from one domain to another, we need only change the width of each individual channel by the appropriate amount without having to rescale the measured data. Figure 2 gives an example of this. Figure 2(a) shows a spectrum measured with a grating spectrometer, so that the individual spectral channels are approximately uniformly sampled in wavelength — that is, the channel bins are all approximately the same width. As a result, the ordinate of the figure can be written with units proportional to $\text{phot}/\mu\text{m}$ or $\text{phot}/\text{channel}$, whichever the user prefers. Figure 2(b) shows the same spectrum in which the edges of the spectral channels have been translated to the wavenumber domain, while the values of the bins have been left unchanged. This of course preserves the overall photon number, but it produces nonuniform sampling — the individual channels are no longer the same width. Here the only appropriate way to write the ordinate would be with units proportional to $\text{phot}/\text{channel}$. If we want to interpolate this spectrum onto a uniformly sampled grid, then we need to re-scale the heights of the individual discrete channels according to the Jacobian of the transformation ($d\lambda \rightarrow -\lambda^2 d\sigma$), the result of which is shown in Fig. 2(c). Here the ordinate can now be written with units proportional to $\text{phot}/\mu\text{m}^{-1}$ or $\text{phot}/\text{channel}$.

Although it is perhaps unfair to single out any single author for violating these rules, it is useful to have an example demonstrating how normalization errors affect published data. Figure 3(a) shows a figure taken from the literature, using a normalized ordinate, and nonuniformly sampled points on the abscissa.[7] The authors use this figure to compare their reconstructed spectra to measurements with a standard laboratory spectrometer, and state that they scale the measurements from the lab spectrometer by normalizing them with the “energies” at each point. This is not the correct way to transform data taken with a photon integrating detector in order to compare to another photon-integrating sensor, but perhaps the authors meant only normalization by the areas. Figure 3(b) replicates the black curve from (a) but rescales it according to the channel widths (red curve) and total channel energies (blue curve), followed by normaliza-

Table 2. The Wien displacement law for peak wavelength, expressed in different domains.[8, 9]

Spectrum variable	Quantum flux	Optical power
Wavelength λ :	$\lambda_w = \frac{3669.7 \mu\text{m K}}{T}$	$\lambda_w = \frac{2897.8 \mu\text{m K}}{T}$
Frequency $\nu = c/\lambda$:	$\lambda_w = \frac{9028.4 \mu\text{m K}}{T}$	$\lambda_w = \frac{5099.4 \mu\text{m K}}{T}$
Wavenumber $\sigma = 1/\lambda$:	$\lambda_w = \frac{9028.4 \mu\text{m K}}{T}$	$\lambda_w = \frac{5099.4 \mu\text{m K}}{T}$
Wavenumber $k = 2\pi/\lambda$:	$\lambda_w = \frac{9028.4 \mu\text{m K}}{T}$	$\lambda_w = \frac{5099.4 \mu\text{m K}}{T}$
Energy $E = hc/\lambda$ (eV):	$\lambda_w = \frac{9028.4 \mu\text{m K}}{T}$	$\lambda_w = \frac{5099.4 \mu\text{m K}}{T}$

tion such that the highest channel value in the spectrum is unchanged. Each curve is also drawn together with its implied channel rectangles. Whereas the correct transformation cannot be determined from the authors’ original figure, using channel rectangles preserves the concept that any transformation will preserve the integral under the curve, and makes it easier to choose the correct transformation. As we can see from the figure, the difference in shapes between the three spectra is clear enough to indicate a visible color difference to our eyes, and a significant difference in any error metric used to compare results. Note that the sudden difference between the original curve and transformed curves at the third point from the left is due to an odd change in the sampling distance between the points there.

4. THE EFFECT OF DOMAIN CHOICE ON WIEN’S LAW

As illustrated in Fig. 1, one of the striking changes caused by a change in the flux units or density units in which we represent a spectrum is that the peak of the blackbody spectrum. For a spectrum represented in $\text{W}/\mu\text{m}$, the expression governing the location of this peak is

$$\lambda_w = (2897.8 \mu\text{m K}) T^{-1} .$$

Thus, when we approximate the solar spectrum with a blackbody spectrum of a 5770 K object, we find that the Wien peak is located at a wavelength of 502 nm. Table 2 gives expressions for the Wien law for blackbody spectra expressed in other domains. For a spectrum represented in photons/ μm , the solar Wien peak shifts to 636 nm. If we switch to wavenumber densities, then the solar Wien peaks become 884 nm (for $\text{W}/\mu\text{m}$) and 1565 nm (for photons μm). Figure 4 illustrates the changes in the spectral shapes and peak locations as a function of temperature and domain.

5. NONLINEAR TRANSFORMS IN IMAGING DATA

While spectral transformations are often nonlinear, such as the wavelength-wavenumber and energy-photon transforms, most image transformations are linear. When distorting images, or mapping 3D surfaces onto 2D, the transformations

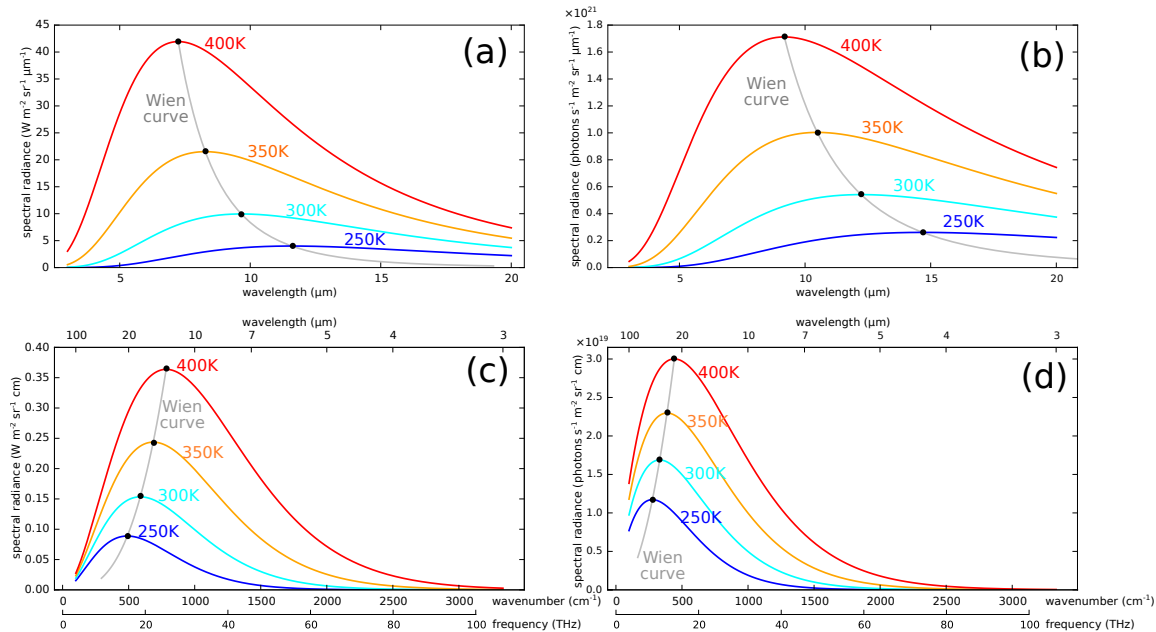


Fig. 4. The Planck blackbody function and Wien law, for various temperatures, in the domains proportional to (a) $W/\mu\text{m}$, (b) photons/ μm , (c) $W\text{ cm}$, and (d) photons cm .

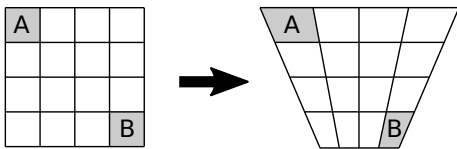


Fig. 5. Distortion of images is a nonlinear transform.

are often nonlinear, so that the same warnings that we discussed above for spectra apply for images as well. Figure 5 gives a simple example of a distortion mapping. In the case of images, the ordinate is typically irradiance [W/m^2], and so it is the 2D integral over the spatial dimension that gives us the energy value, or photon number, that we must conserve in order to retain the correct brightness everywhere in the image.

6. CONCLUSION

Although it is rare for textbooks to call attention to the distinction between simple functions and density functions (Ref. [2] being a rare exception), we should be aware of the distinction between the two, and for most of us, we should make an effort to move away from using Watts when discussing measurements taken with integrating sensors. For prism spectrometers or tunable filter spectrometers, in which the spectral bins are nonuniformly spaced, being careful with these transformations is a necessity.

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