

Electromagnetic Radiation

The main part of this textbook deals with spectroscopy utilizing electromagnetic (EM) radiation. Thus, we will first review the most important properties of this particular probe. We will start with the idealized description of a plane wave within Maxwell's theory and continue with an explicit description of more realistic fields, such as radiation from a dipole and from an arbitrarily accelerated charge. In Sects. 2.3 and 2.4 Fourier transforms are discussed and applied to the important case of radiation from sources with limited emission time. These sections are rather short since the readers should be familiar with such subjects. For those who need a tutorial or a review, a more detailed treatment of the subject can be found in Appendix B.

2.1 Electromagnetic Waves and Maxwell's Theory

As long as its wavelength is not too short radiation can be characterized by the classical description of a plane EM wave in the form

$$E = E_0 \cos(kx - \omega t) , \quad (2.1)$$

or

$$E = E_0 e^{i(kx - \omega t)} . \quad (2.2)$$

E is the electric field of the wave with the amplitude E_0 , wave vector k , and angular frequency $\omega = 2\pi f$ where f is the frequency. The complex form of the electric field (2.2) is often very convenient, but it should be kept in mind that only its real part has a physical meaning. Thus, in order to be correct, the complex conjugate must be added in all calculations. The real field is then obtained as $(E + E^*)/2$. The sign of the imaginary symbol i is arbitrary. It serves to describe the actual phase of the field. Only a consistent sign convention is needed. Different sign conventions can lead to different signs in relations derived from the field. This is the reason why formulas found in the literature often deviate slightly from each other. By convention, a positive sign is used throughout this book.

The correlation between the wave vector k , the wavelength λ , the wave number ν , and the quantum energy ϵ of the radiation are given as follows:

$$k = \frac{2\pi}{\lambda} = 2\pi\nu = \frac{n\omega}{c_0} = \frac{n\epsilon}{\hbar c_0} . \quad (2.3)$$

Here, $n = c_0/c$ is the (real) index of refraction expressed as the ratio between the velocity of light in vacuum and in the solid. Using these relations the calculated value of the wave vector for visible light is of the order of 10^5 cm^{-1} . This value is very small compared to typical wave vectors of quasi-particles excited in the first Brillouin zone of real crystals, or as compared to wave vectors of this zone in general. Typical values for the latter two quantities are $q \approx 10^8 \text{ cm}^{-1}$. This fact is of fundamental importance for solid-state spectroscopy and often plays a dominating role in the selection rules of spectroscopic transitions.

Occasionally, general complex numbers $A = A_c + iA_s$ are used to describe EM waves. A_c and A_s are called the components of a *phasor*, and A is the complex amplitude of the wave. A_c and A_s are defined as the coefficients of the cosine term and the sine term if a harmonic oscillation of the general form

$$E(x, y, z, t) = E(x, y, z) \cos(\omega t - \phi)$$

is separated in its cosine and sine component. Phasors are useful if, for instance, a linear superposition of waves is studied. The resulting wave is then obtained as a summation of complex numbers.

The energy of EM waves is characterized by different quantities depending on the spectral ranges. Often used are the wavelength λ given in Å, nm or μm , the frequency f given in Hz, (the angular frequency in s^{-1}), the wave number ν given in cm^{-1} , or the quantum energy $\hbar\omega$ given in eV. For example, lasers are usually characterized by their wavelength, electronic transitions by their energy in eV, and vibrational excitations by wave numbers. The use of different units is not as confusing as it may appear at a first glance since usually only one type of them appears within a particular field of spectroscopy. Thus, in this book the traditional units for the description of radiation and transition energies will be used. It is nevertheless important to keep in mind the quantitative relations between the various units for the description of the energy as they are given in (2.3) or in Table A.2. For practical use it is convenient to remember that

1 meV corresponds to about 8 cm^{-1} $1 \mu\text{m}$ wavelength corresponds to 1.24 eV and 1 K corresponds to about 0.7 cm^{-1} .

A summary of the energy units commonly used in the various ranges of the EM radiation is given in Table 2.1. This table also lists the spectroscopic techniques applied in the various spectral ranges. Abbreviations are explained in the corresponding sections of this book.

Table 2.1. The electromagnetic spectrum

	Wavelength	Wave number (cm ⁻¹)	Frequency (s ⁻¹)	Energy (eV)	Spectroscopic techniques
Electric waves	∞-0.03 cm		0-E12		ESR, EPR, NMR
Far infrared	3000-40 μm	3-400		(0.4-50)E-3	FTIR, abs., refl.
Infrared	40-0.8 μm	250-12 500	(7-400)E12	0.03-1.6	IR, FTIR
Visible light	0.8-0.4 μm	(12-25)E3		1.6-3	abs., refl., ellipsom.
Ultraviolet	400-10 nm			3-120	abs., UPS
x-ray	10-0.01 nm			50-120E3	XPS, XAFS
γ radiation	10-0.1 pm			(2-1200)E4	MB, PAC

The other characteristic quantities of EM radiation, like the electric field E , the magnetic excitation H , the induction B , the vector potential A , etc. can be expressed most conveniently in the SI units V, A, m, and s. These quantities are listed in Table 2.2, together with descriptors for the radiation intensity. Note that in the latter case we critically discriminate between the “intensity” of a radiation source and the “intensity” of an irradiated object (last line in the table). For the sake of generality the older cgs units are also given.

Table 2.2. Characteristic quantities of the electromagnetic field

Quantity	SI (VAm _s)	cgs (cm g s)	relations
Electric field (E)	Vm ⁻¹	g ^{1/2} cm ^{-1/2} s ⁻¹	1 Vm ⁻¹ = (1/3)cgs
Magnetic excitation (H)	Am ⁻¹	g ^{1/2} cm ^{-1/2} s ⁻¹	1Am ⁻¹ =0.0256Oe
Magnetic induction (B)	Vsm ⁻²	g ^{1/2} cm ^{-1/2} s ⁻¹	1Vsm ⁻² =10 ⁴ G
Vector potential (A)	Vsm ⁻¹	g ^{1/2} cm ^{1/2} s ⁻¹	
(Radiant) power (P)	VA	erg s ⁻¹	
Energy density (W)	VAsm ⁻³	erg cm ⁻³	1VAm ⁻² =10 ³ cgs
Intensity (radiant) (Φ) ^{a,b}	VA ster ⁻¹	erg s ⁻¹ ster ⁻¹	
Radiance (brightness) (L) ^a	VAm ⁻² ster ⁻¹		
Intensity (irradiance) (I) ^{a,b}	VAm ⁻²	erg cm ⁻² s ⁻¹	1VAm ⁻² =10 ³ cgs

^a I , L and Φ can be normalized to unit band width. In this case the symbols are supplied with an index labeling the variable used for the normalization.

^b To follow intuition and to avoid confusion with the assignment of the electric field the symbols I and Φ are used as given in the table in contrast to the often used symbols E and I for irradiance and for radiant intensity.

In addition to the above quantities, which were derived from the definition of the EM wave, photometric (or physiological) quantities such as *candela*, *lumen*, and *lux* are important. According to the most recent definition the photometric quantities are based on the unit of the luminous intensity candela (cd). It is defined as the light emitted from a source radiating at 540 nm with a radiant intensity of $1/683 \text{ W/ster}^1$. Thus the quantitative relation between luminous intensity I_{li} (in candela) and radiant intensity I_{ri} (in W/ster) is

$$I_{\text{li}}(\lambda) = 683.002 y(\lambda) I_{\text{ri}}(\lambda), \quad (2.4)$$

where $y(\lambda)$ is the luminosity function given in Fig. 2.1 and I_{ri} is taken from the black body radiation (3.4), expressed in λ and averaged over the visible spectral range. Even though in this way candela is related to watts it is considered as an SI unit by itself. The luminous flux or luminous power F is measured in lumen (lm) and defined as candela \times ster (or $1 \text{ cd} = 1 \text{ lm/ster}$). $K_{\text{m}} = 683.002 \text{ lm/W}$ is the photometric radiation equivalent which relates the above given definition of candela to the older definition of candela as the emission (and detection by the human eye) of a $1,67 \times 10^{-6} \text{ m}^2$ sized black body at the temperature of melting Pt which is 2042 K. Appendix B.1 has the details of these relations.

The luminous intensity decreases rapidly for wavelength longer or shorter than 540 nm due to the loss of sensitivity of the human eye. This sensitivity is depicted in Fig. 2.1 in relative units for the day light adapted eye (photopic luminosity function, $y(\lambda)$). According to the definitions above and the luminosity function 1 W green light (540 nm), red light (650 nm), and blue light (450 nm) correspond to 683 lm, 73 lm, and 26 lm, respectively. For the

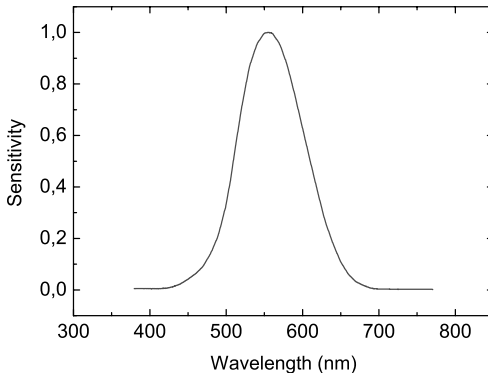


Fig. 2.1. Relative sensitivity of the human eye for daylight adaption (luminosity function)

dark adapted eye (scotopic vision) the luminosity function is redshifted. The irradiant intensity (illuminance) is measured in lux (lx); $1 \text{ lx} = 1 \text{ lm/m}^2$.

¹ ster (from *steradian*) is the unit for the solid angle $\bar{\Omega}$; $1 \text{ ster} = 1/4\pi$; $d\bar{\Omega} = \sin\theta d\theta d\phi$; θ and ϕ are the nutation angle and the precession angle which can extend from 0 to π and from 0 to 2π , respectively.

The relationships between the quantities listed in Table 2.2 are obtained from Maxwell's equations, and the well known relationship between the vector potential and the field B . For plane waves (2.2) and (B.3) yield

$$\mathbf{B} = \frac{1}{\omega}(\mathbf{k} \times \mathbf{E}_0)e^{i(\mathbf{k}\mathbf{r}-\omega t)} \quad \text{with} \quad \mathbf{H} = \frac{\mathbf{B}}{\mu\mu_0} . \quad (2.5)$$

For example, for a wave propagating in the x direction with $\mathbf{E} \parallel \mathbf{z}$, the vector \mathbf{B} is $\parallel -\mathbf{y}$ and has the form

$$\mathbf{B} = -\frac{k}{\omega}E_0e^{i(kx-\omega t)}\mathbf{e}_y .$$

Similarly, the vector potential (Appendix B.3) is given by

$$\mathbf{A} = \frac{i}{\omega}E_0e^{i(\mathbf{k}\mathbf{r}-\omega t)} \quad (2.6)$$

and, for a wave propagating in the x direction, it has the form

$$\mathbf{A} = \frac{i}{\omega}E_0e^{i(kx-\omega t)}\mathbf{e}_z .$$

From these results the energy density of the radiation becomes

$$W = \frac{1}{2}(\mathbf{E}\mathbf{D} + \mathbf{H}\mathbf{B}) = \frac{\varepsilon\varepsilon_0E^2}{2} + \frac{\mu\mu_0H^2}{2} . \quad (2.7)$$

where ε_0 and μ_0 are the dielectric constant and permeability of vacuum, and E, D, H , and B have been assumed as real. ε_0 and μ_0 are related to the light velocity and to the impedance of vacuum by

$$\frac{1}{\sqrt{\varepsilon_0\mu_0}} = c_0, \quad \sqrt{\frac{\mu_0}{\varepsilon_0}} = 377 \text{ Ohm}.$$

The numerical values for ε_0 and μ_0 are compiled in Table A.1.

Since the energy spreads perpendicular to \mathbf{E} and \mathbf{H} and is equally distributed to the electric and to the magnetic field, the intensity I (irradiance) is obtained from

$$I = Wc = \varepsilon\varepsilon_0E^2 \frac{c_0}{\sqrt{\varepsilon\mu}} = \sqrt{\varepsilon\varepsilon_0}E\sqrt{\mu\mu_0}H \cdot \frac{c_0}{\sqrt{\varepsilon\mu}} = EH . \quad (2.8)$$

Written as the Poynting vector \mathbf{I} and for $\mu = 1$

$$\mathbf{I} = \mathbf{E} \times \mathbf{H} = \mathbf{E} \times (\mathbf{k} \times \mathbf{E}) \frac{1}{\omega\mu_0} = \frac{E^2\mathbf{k}}{\omega\mu_0} = E^2c_0\sqrt{\varepsilon\varepsilon_0}\mathbf{e}_k , \quad (2.9)$$

where \mathbf{e}_k is the unit vector in the direction of the wave propagation.

In the above equations W , I , and \mathbf{I} are time-dependent (with a term $\cos^2(\mathbf{k}\mathbf{r} - \omega t)$ for plane waves). To obtain the time average a proper averaging procedure must be performed. In the simple case of plane waves the values of E^2 and B^2 are then replaced by their time average $E_0^2/2$ and $B_0^2/2$.

Using a complex notation for the fields, products of the vectors have to be replaced by the product of one vector with the complex conjugate of the other vector. In this way the sum of the squared components of the vectors represent the square of the magnitude of the field.

The intensity of radiation is very often evaluated for complex fields E from $I = c_0 \epsilon_0 E E^*$. Since in this case the time dependence is lost only the time-average intensity is obtained and its magnitude is two times the magnitude of a real field with the same amplitude.

2.2 Radiation from Accelerated Charges

Even though plane waves are a good example to illustrate electromagnetic theory and are indeed very often useful to describe the EM field locally, they are not a very realistic form of the radiation. In reality EM radiation always originates from accelerated electric charges. The mode of acceleration determines the wave field. Vibrating electric dipoles, such as a vibrating molecule with a finite electric dipole moment, or excited molecular or solid systems provide realistic acceleration and emission patterns. We will therefore first discuss the basic properties of the Hertzian dipole and then make some general remarks about radiation from arbitrarily accelerated charges.

2.2.1 The Hertzian Dipole

The radiation from an oscillating dipole is emitted by moving charges in a pattern shown schematically in Fig. 2.2. A dipole with the length l , charge $\pm Q$ and oscillation amplitude Δl emits radiation in directions \mathbf{r} defined by the unit vector \mathbf{e}_r . Thus, at an arbitrary point \mathbf{r} a field $\mathbf{E}(\mathbf{r})$ will be observed. If the oscillation is harmonic with angular frequency ω the time dependent part of the dipole has the form

$$P_D = P_{D0} \cos \omega t = Q \Delta l \cos \omega t. \quad (2.10)$$

A Hertzian dipole corresponds to the approximation $\Delta l \approx l$ and $\lambda = 2\pi c_0/\omega \gg l$. Its amplitude is therefore $P_{D0} = Ql$. In order to obtain the emitted field we need to evaluate either the potential Φ from a Poisson equation or the vector potential \mathbf{A} from the time-retarded charges or time-retarded currents as outlined in B.3. Since the vector potential by itself is enough to obtain the B field, it is more convenient to calculate the current distribution for the Hertzian dipole and use its time-retarded value in (B.9) rather than

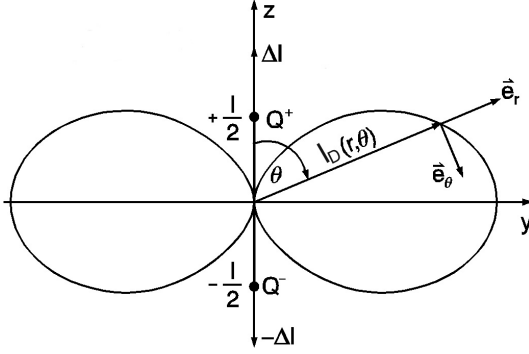


Fig. 2.2. Polar diagram for the emission of electromagnetic radiation from a dipole. $I_D(r, \theta)$ is the intensity observed at distance r under the angle θ . It has rotational symmetric around the dipole axis. e_ϕ looks into the plane of the paper

to calculate Φ directly from the retarded charge distribution. \mathbf{A} is obtained from

$$\mathbf{A}(\mathbf{r}, t) = \frac{\mu\mu_0}{4\pi} \int \frac{\mathbf{j}(\mathbf{r}', t - |\mathbf{r} - \mathbf{r}'|/c)}{|\mathbf{r} - \mathbf{r}'|} d^3x', \quad (2.11)$$

where \mathbf{r}' and $t' = |\mathbf{r} - \mathbf{r}'|/c$ represent the coordinates and the time of the current density distribution and \mathbf{r} the coordinates of the field distribution.²

The time-dependent current distribution for the Hertzian dipole may be derived from the time-dependent charge distribution. If the dipole is very short and oriented in the z direction as in Fig. 2.2 we may consider the time-dependent charge $Q(t) = Q \cos \omega t$ as a source for a current in the z direction. This current then has the form

$$\mathbf{i}(t) = \frac{dQ}{dt} \mathbf{e}_z = -\omega Q \sin \omega t \mathbf{e}_z. \quad (2.12)$$

To evaluate \mathbf{A} we need to integrate over the current density. Even though the latter nearly diverges locally because of the small size of the electron its integral is certainly finite. In a simplified form the integration along x' and y' yields the current \mathbf{i} of (2.12), and the integration along z' yields the length of the dipole l . Here it is assumed that $\mathbf{r}' \ll \mathbf{r}$ for all points of interest so that we can use the expression $t - r/c$ for the retarded time and neglect \mathbf{r}' in the denominator of (2.11). With these approximations the vector potential becomes

$$\mathbf{A}_D = \frac{\mu\mu_0 Q l \omega \sin(\mathbf{k}\mathbf{r} - \omega t)}{4\pi r} \mathbf{e}_z, \quad (2.13)$$

² Note that here and for the remainder of the book limits for the integration extend from $-\infty$ to ∞ if not specified otherwise.

or more generally

$$\mathbf{A}_D = \frac{\mu\mu_0 Q l \omega \sin(\mathbf{k}\mathbf{r} - \omega t)}{4\pi r} \mathbf{e}_D, \quad (2.14)$$

where \mathbf{e}_D is the direction of the dipole moment and \mathbf{k} is the wave vector (ω/c) \mathbf{e}_r . The curl of \mathbf{A}_D yields the field \mathbf{B}_D

$$\mathbf{B}_D = \text{curl } \mathbf{A}_D = -\frac{\mu\mu_0 Q l \omega^2 \sin \theta \cos(\mathbf{k}\mathbf{r} - \omega t)}{4\pi c r} \mathbf{e}_\phi, \quad (2.15)$$

or more generally

$$\mathbf{B}_D = \text{curl } \mathbf{A}_D = -\frac{\mu\mu_0 Q l \omega^2 \cos(\mathbf{k}\mathbf{r} - \omega t)}{4\pi c r} (\mathbf{e}_D \times \mathbf{e}_r), \quad (2.16)$$

where in the first equation spherical polar coordinates \mathbf{e}_r , \mathbf{e}_θ , and \mathbf{e}_ϕ have been used as shown in Fig. 2.2. The result for \mathbf{B}_D in (2.16) has been obtained by retaining only the term proportional to $1/r$. This term dominates for large distances as compared to a terms $\propto 1/r^2$. This approximation is therefore only valid in the far field called the *wave* or *radiation zone*. For a more general solution (static or intermediate zone) see [2.1, 2.2]. Results for the wave zone are, in general, good enough for applications in spectroscopy.

The B field is independent of ϕ , perpendicular to \mathbf{e}_r and \mathbf{e}_θ , and decreases as $1/r$ with distance r from the radiating dipole. These proportions are evident from the second part of (2.16) where $\sin \theta \mathbf{e}_\phi$ was replaced by $(\mathbf{e}_D \times \mathbf{e}_r)$.

The other characteristic quantities for the field follow immediately from the equations given in Sect. 2.1 and Appendix B.2. The electric field is calculated from Maxwell's equations

$$\begin{aligned} \mathbf{E}_D &= -\frac{c^2}{\omega} (\mathbf{k} \times \mathbf{B}_D) = -\frac{\mu\mu_0 Q l \omega^2 \sin \theta \cos(\mathbf{k}\mathbf{r} - \omega t)}{4\pi r} \mathbf{e}_\theta \\ &= -\frac{\mu\mu_0 Q l \omega^2 \cos(\mathbf{k}\mathbf{r} - \omega t)}{4\pi r} (\mathbf{e}_r \times (\mathbf{e}_D \times \mathbf{e}_r)). \end{aligned} \quad (2.17)$$

The power per unit area reaching point \mathbf{r} (irradiance) is given by the Poynting vector evaluated from (2.8) and (2.9)

$$\mathbf{I}_D = \frac{\mathbf{E}_D \mathbf{B}_D}{\mu\mu_0} = \frac{\mu\mu_0 (Ql)^2 \omega^4 \sin^2 \theta \cos^2(\mathbf{k}\mathbf{r} - \omega t)}{16\pi^2 c r^2} \mathbf{e}_r. \quad (2.18)$$

The time average of this function is plotted in Fig. 2.2. The radiation per differential solid angle $d\bar{\Omega}$ is immediately obtained from this by

$$dP = |\mathbf{I}_D| dF = |\mathbf{I}_D| r^2 d\bar{\Omega} \quad (\text{in W}). \quad (2.19)$$

All quantities given above are time-dependent. To obtain time-average values for the radiation power the \cos^2 functions in (2.18) and (2.19) have to be replaced by their average value of $1/2$. Finally, the total average power emitted by the dipole is obtained from (2.19) by integration over the solid angle

$$P_{\text{tot}} = \frac{P_{D0}^2 \mu \mu_0 \omega^4}{12\pi c_0} = \frac{\mu \mu_0 (Ql)^2 \omega^4}{12\pi c} \quad (\text{in W}) . \quad (2.20)$$

If more than two charges oscillate the radiation field becomes more complicated and is described by electric multipole radiation. For modern spectroscopic techniques quadrupole radiation is important. It has still a simple structure. The magnitude of the quadrupole moment for an arrangement of charges symmetric with respect to the z axis is³

$$(P_Q)_{zz} = P_Q = \sum_i Q_i (3z_i^2 - r_i^2) . \quad (2.21)$$

Charges arranged as shown in Fig. 2.3a therefore have a finite quadrupole moment (but no dipole moment). If the positive and negative charges oscillate 180° out of phase and with equal frequency, they establish a time-dependent quadrupole moment of the form $P_Q(t) = P_{Q0} \cos \omega t$. As a consequence they will emit a quadrupole radiation. The emitted electric field and magnetic

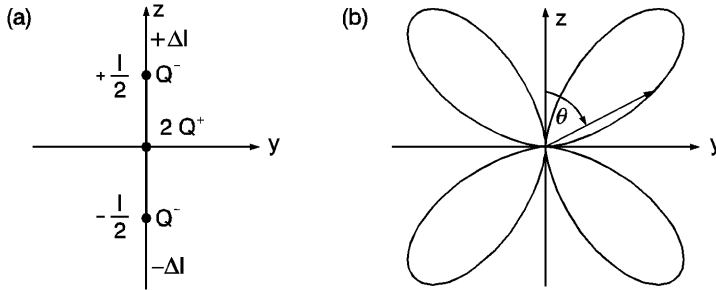


Fig. 2.3. Linear arrangement of charges, Q , with a finite quadrupole moment $-l^2 Q$ (a), and the radiation pattern for a harmonic time dependence of Q (b). The pattern is rotationally symmetric about z

induction are given for the arrangement in the figure as

$$\begin{aligned} E_Q &= -e_\theta \frac{\mu \mu_0 \omega^3 P_{Q0} \sin \theta \cos \theta}{16\pi c r} \cos(\mathbf{k}\mathbf{r} - \omega t) \\ B_Q &= -e_\phi \frac{\mu \mu_0 \omega^3 P_{Q0} \sin \theta \cos \theta}{16\pi c^2 r} \cos(\mathbf{k}\mathbf{r} - \omega t) . \end{aligned} \quad (2.22)$$

³ For the definition of multipole moments, see Appendix B.4.

As a result of these relations the emitted power is proportional to $\sin^2 \theta \cos^2 \theta$ where θ is the direction between the z axis and the direction of emission. The radiation pattern for this geometry of the charges is depicted in Fig. 2.3b.

2.2.2 Emission from Arbitrarily Accelerated Charges

The Hertzian dipole described above may be considered as a special case of radiation from an accelerated point charge Q . The emission from an arbitrarily accelerated charge moving along $\mathbf{r}'(t)$ is also important. It is the basis for the description of black-body radiation, x-ray *bremssstrahlung* or synchrotron radiation. General expressions for the potential Φ and the vector potential \mathbf{A} for this charge are known as Lienard–Wiechert potentials and given in Appendix B.6. From \mathbf{A} and Φ the electric field \mathbf{E} and the magnetic induction \mathbf{B} for arbitrarily accelerated charges can be derived. If the distance between the field point P and the emitting charge is very large ($\mathbf{s} = \mathbf{r} - \mathbf{r}' \approx \mathbf{r}$ in Fig. B.1 or in Fig. 2.4) and the particle is nonrelativistic [$(v/c_0)r = (\dot{r}'/c_0)r \ll r$] the radiation intensity observed at distance r (irradiance) under the angle θ with respect to the direction of acceleration \mathbf{e}_a is given, for Q equal to the elementary charge e , by

$$I(r, \theta) = \frac{e^2 \sin^2 \theta}{16\pi^2 \epsilon_0 c_0^3 r^2} |\mathbf{a}|^2 \quad (\text{in W/m}^2), \quad (2.23)$$

where $\mathbf{a} = d^2\mathbf{r}'/dt^2$ is the acceleration of the particle in Fig. B.1 or in Fig. 2.4. The radiation pattern for this particle is exhibited in the latter figure. The

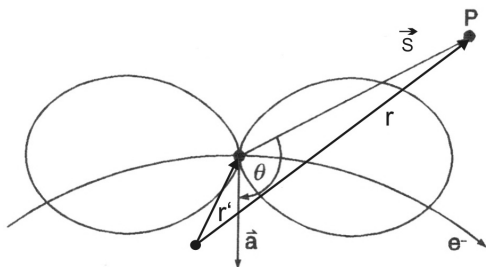


Fig. 2.4. Radiation characteristic for a particle moving with an arbitrary acceleration \mathbf{a}

emission of radiation is strongest perpendicular to the direction of the acceleration, but it is independent of the direction of the particle velocity. The radiation pattern is, of course, directly related to the dipole radiation shown in Fig. 2.2.

The total power (in watts) radiated from the particle is obtained by integrating over the full angular space. This yields

$$P = \frac{e^2}{6\pi\epsilon_0 c_0^3} |\mathbf{a}|^2. \quad (2.24)$$

This well-known formula for radiation emission from nonrelativistic, accelerated charged particles had already been derived by Larmor at the end of the 19th century.

2.3 Fourier Transforms

The radiation pattern described above for a plane wave and for an oscillator are still unrealistic as they assume a single value for the angular frequency ω (or do not give any explicit frequency, as in the case of radiation from an arbitrarily moving point charge). Realistic fields always encompass a frequency spectrum with a given radiation energy per frequency interval. This means a realistic radiation field can be described either by a function of time such as $E(t)$ or by the distribution of the radiation energy over frequencies determined by the field $E(\omega)$. The relation between these two descriptions is given by the Fourier transform (FT) of one type of function into the other. Since FT is fundamental to modern spectroscopy we will review the basic concepts of this mathematical technique in this section. More details are given in Appendix B.7. Nearly all spectroscopic techniques described in the following chapters use this mathematical tool in one way or another. One of the main reasons for the importance of FT is the dramatic development in computer technology. Even personal-size computers can perform a Fourier analysis of very large numbers of data points in a very short time.

2.3.1 Fourier Theorem

In the usual terminology the Fourier theorem consists of two parts.

- a) Any function $h(u)$ periodic in u as $h(u) = h(u+w) = h(u+2\pi/v)$ with the period $w = 2\pi/v$ can be represented by a sum of harmonic functions of the form $\sin(nuv)$ and $\cos(nuv)$ or $\exp(inuv)$ with the fundamental angular frequency v and overtone number n . The coefficients of the harmonic functions in the sum can be evaluated in a unique way from the original function $h(u)$.
- b) Statement (a) also holds for non periodic functions in the sense that the sum is converted into an integral and the frequency range extends now from $-\infty$ to ∞ . In other words, in this case, FT gives a rule for a well defined transform converting a function $h(u)$ in u -space to a corresponding function $g(v)$ in v -space. $h(u)$ and $g(v)$ are called Fourier pairs.

Since statement (b) actually includes periodic functions, it can be expected to cover statement (a). Indeed, it is not very difficult to show that this is true.

Fourier transforms are utilized in various disciplines of science such as optics, spectroscopy, communications, stochastic processes, solid-state science, etc. In spectroscopy u usually represents the time t and v the frequency f or ω .

However, the use of space coordinate x for u and the wave numbers ν for v is also common. In solids FT is usually three-dimensional with space coordinate \mathbf{r} for u and the unit vector of the reciprocal lattice \mathbf{G}_0 for v .

The mathematical expressions for the Fourier theorem, as they will be used in this text are:

- a) A function $E(t)$ periodic in time with period T which means $E(t + T) = E(t)$, where $1/T = f$, and $2\pi f = \omega$ can be expressed by

$$\begin{aligned} E(t) &= \sum_{n=-\infty}^{\infty} c_n e^{i2\pi n f t} \\ &= C_0 + \sum_{n=1}^{\infty} [A_n \cos(2\pi n f t) + B_n \sin(2\pi n f t)] \end{aligned} \quad (2.25)$$

with

$$c_n = \frac{1}{T} \int_{t_0}^{t_0+T} E(t) e^{-i2\pi n f t} dt .$$

The coefficients c_n are complex with $c_{-n} = c_n^*$, and t_0 is arbitrary. The relation between the complex representation and the real representation given in (2.25) is obtained from a straight forward calculation and is left to the reader as an exercise.

- (b) For non-periodic functions $E(t)$

$$\begin{aligned} E(t) &= \int E(f) e^{i2\pi f t} df \quad \text{with} \\ E(f) &= \int E(t) e^{-i2\pi f t} dt . \end{aligned} \quad (2.26)$$

$E(t)$ and $E(f)$ are the Fourier pairs. When $E(t)$ is even or odd in t , the transform can be obtained using only sine or cosine functions, respectively.

2.3.2 Examples of Fourier Transforms

In general FTs used in spectroscopy are rather simple. Advanced computer programs such as *Mathematica* can quite easily calculate FTs analytically on personal computers. We will give here two examples which may serve as a guide for related problems, and summarize some general properties of the Fourier pairs in Appendix B.7.

Let $E(t)$ be of the form $A|\cos 2\pi f t|$ with $f = 1/T$. A graph of this function is shown in Fig. 2.5a. Since the period of this function is $T/2$ the Fourier

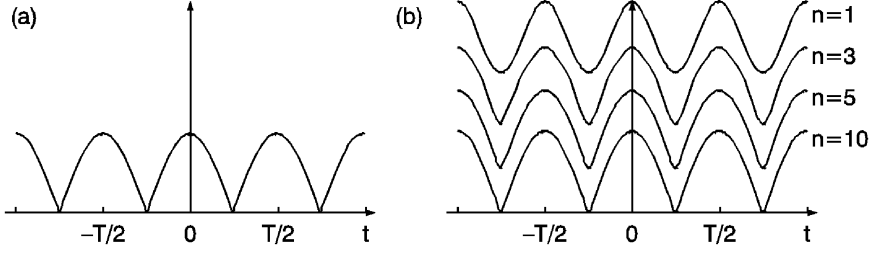


Fig. 2.5. Graph of the function $A|\cos 2\pi t/T|$ (a), and representation of the function by an increasing number of harmonic overtones (b). For clarity, curves for $n = 1$ to 5 are shifted in (b)

coefficients can be calculated from

$$c_n = \frac{2A}{T} \int_{-T/4}^{T/4} \cos(2\pi t/T) e^{-i2\pi n2t/T} dt. \quad (2.27)$$

The integration is performed by replacing the exponential by sine and cosine functions, and using the appropriate trigonometric relationships. c_0 is always the time average of the periodic function. It is equal to $2/\pi$ in our case. Since $E(t)$ is even only the real parts of the coefficients c_n are non zero. Consequently, $c_{-n} = c_n^* = c_n$. The explicit value of c_n is

$$c_n = \frac{A \sin[\pi(2n+1)/2]}{\pi(2n+1)} + \frac{A \sin[\pi(2n-1)/2]}{\pi(2n-1)}. \quad (2.28)$$

Using these values, replacing $2\pi f$ by ω and recalling that the period of $|\cos 2\pi ft|$ is $T/2$ (2.25) yields

$$E(t) = A|\cos 2\pi ft| = A|\cos \omega t| = \frac{2A}{\pi} + \sum_{n=1}^{\infty} \frac{4A}{\pi} \frac{(-1)^{n-1}}{4n^2 - 1} \cos 2n\omega t. \quad (2.29)$$

Figure 2.5b displays $|\cos \omega t|$ represented by an increasing number of harmonic contributions. Obviously, the first ten contributions already represent the function $E(t)$ very well.

The two-sided exponential decay of a sine wave (wave packet) is a good example for FT of a non-periodic function. The function is given by

$$E(t) = Ae^{-\gamma|t|} \sin \omega_0 t. \quad (2.30)$$

From this expression, $\tau = 1/\gamma$ is the lifetime of the oscillation. To obtain the FT we separate the Fourier integral into two parts

$$\begin{aligned} E(f) &= A \int_{-\infty}^{\infty} e^{-\gamma|t|} \sin \omega_0 t e^{-i2\pi ft} dt \\ &= A \left(- \int_0^{\infty} e^{\gamma t} \sin \omega_0 t e^{-i2\pi ft} dt + \int_0^{\infty} e^{-\gamma t} \sin \omega_0 t e^{-i2\pi ft} dt \right) \end{aligned} \quad (2.31)$$

Substituting $-t$ for the integration variable t in the first integral we are left with two integrals which can be solved straightforwardly. We obtain for $E(f)$

$$E(f) = \frac{iA\gamma}{\gamma^2 + 4\pi^2(f + f_0)^2} - \frac{iA\gamma}{\gamma^2 + 4\pi^2(f - f_0)^2} . \quad (2.32)$$

The inverse transform according to (2.26) must give the original time function for the whole time space. The frequency spectrum (2.32) is imaginary and odd. In general, FTs of arbitrary functions $E(t)$ are complex. This is not really a problem. As we will see below, the distribution of the energy in the spectra is given by the square of the magnitude of $E(f)$ which is always real. Since the energy distribution for negative frequencies does not contain any new information products such as $E(f)E^*(f)$ must always be even. This is indeed the case in our example since the absolute square of any odd function is even.

The frequency spectra of harmonic functions are the δ functions. It is easy to show that FT of $E(t) = A \cos \omega_0 t$ is $(A/2)[\delta(f - f_0) + \delta(f + f_0)]$. A similar, but odd and imaginary FT is obtained for $E(t) = A \sin \omega_0 t$. The FT of a time-independent function is $\delta(f)$.

More details about FTs, several examples and useful general rules for the relations between Fourier pairs are given in Sect. 2.4 and Appendix B.7.

2.4 Radiation with a Finite-Frequency Spectrum

Let us return to radiation and apply a Fourier analysis to realistic radiation fields. A strictly monochromatic field, as described in Sects. 2.1 or 2.2, is only possible for waves which propagate fully undamped and extend in time from $-\infty$ to $+\infty$. This is unrealistic. In reality radiation is either damped (at least on an atomic scale) or switched on and off at certain points of time. The consequences of these experimental constraints will be discussed in this section for a damped harmonic oscillator and for a plane wave switched on and off at times $t = 0$ and T , respectively.

2.4.1 Damped Harmonic Oscillator

In a classical description, the time-dependence for the emission of an electric field E from a damped harmonic oscillator is given by

$$\ddot{E} + \gamma \dot{E} + \omega_0^2 E = 0 \quad (2.33)$$

The eigenvalues for this differential equation are

$$\alpha_{1,2} = -\frac{\gamma}{2} \pm i\sqrt{\omega_0^2 - \gamma^2/4} \quad (2.34)$$

so that the general complex solution is a linear combination of the terms $\exp \alpha_1 t$ and $\exp \alpha_2 t$ with complex coefficients. Since we are only interested in the real part of the field we take as the general solution

$$\operatorname{Re}\{E\} = C_1 e^{-\gamma t/2} \cos \omega t + C_2 e^{-\gamma t/2} \sin \omega t \quad (2.35)$$

where ω is the detuned frequency $\sqrt{\omega_0^2 - \gamma^2/4}$. As long as the damping $\gamma/2$ remains smaller than ω_0 , this is a damped harmonic oscillation, where the coefficients C_i serve to satisfy boundary conditions. If we want a maximum field and a zero derivative of the field at $t = 0$, the solution has the form

$$E(t) = E_0 e^{-\gamma t/2} [\cos \omega t + (\gamma/2\omega) \sin \omega t]. \quad (2.36)$$

We can also find a simpler special solution for (2.33):

$$\begin{aligned} E(t) &= E_0 e^{-\gamma t/2} \cos \omega t & \text{for } t \geq 0 \\ &= 0 & \text{for } t < 0. \end{aligned} \quad (2.37)$$

In this case we have applied a more restrictive boundary condition which shuts the oscillator off for $t < 0$. A graph for this solution is displayed in Fig. 2.6.

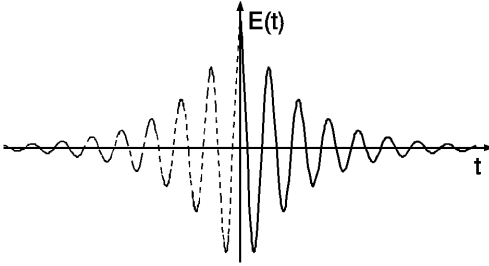


Fig. 2.6. Damped harmonic oscillation for $t > 0$ (—) and symmetrized form (---)

The function in (2.37) describing the damped wave field is often extended to negative values of time and, as we will see later, also to negative values of the frequencies. Also, a symmetric version with respect to $t = 0$ (replace t by $|t|$ for all values of t) is often used. Note that this new function is not a solution for (2.33). It is, however, convenient for mathematical treatments and therefore often used to describe the frequency spectrum of damped oscillations or wave packets.

The frequency spectrum for any time-dependent function is obtained from its FT as shown in the last subsection. Unfortunately the damped oscillation of (2.37) has a rather complicated frequency spectrum because of the abrupt change of the function at $t = 0$. The complex solution for the damped oscillator which may be written as

$$\begin{aligned} E &= E_0 e^{-\gamma t/2} e^{i\omega t} & \text{for } t \geq 0 \\ &= 0 & \text{for } t < 0 \end{aligned} \quad (2.38)$$

gives a more simple but instructive frequency spectrum. Renaming the tuned frequency of the damped oscillator ω_0 , for convenience, and applying FT yields for the frequency spectrum

$$\begin{aligned}
E(f) &= \int_0^\infty E_0 e^{-\gamma t/2} e^{i\omega_0 t} e^{-i2\pi f t} dt \\
&= \frac{E_0}{\gamma/2 + i2\pi(f - f_0)} .
\end{aligned} \tag{2.39}$$

As will be shown in detail in Sect. 2.4.3, the experimentally observed frequency distribution is obtained from the spectral intensity $S(f)$ given by the square of the magnitude of the frequency spectrum. Thus, returning to angular frequencies, we obtain the spectral intensity for the emission from the damped oscillator by

$$\boxed{S(\omega) = E(\omega)E^*(\omega) = \frac{E_0^2}{(\gamma/2)^2 + (\omega - \omega_0)^2}} . \tag{2.40}$$

This particular shape of the intensity spectrum is called a *Lorentzian line*. Its spectral width is obviously determined by the magnitude of γ . The full width half maximum (FWHM) in ω space is exactly equal to γ in the present case.

Frequency and intensity spectra for the real solution of (2.33) are similar to (2.39) and (2.40).

Since γ is the spectral width (uncertainty in frequency) of the line as well as the reciprocal lifetime τ of the oscillation in intensity ($\gamma = 2\pi/\tau$) the relationship between these two quantities is an expression of the uncertainty relation in the following sense. The oscillator energy ϵ is only determined to the accuracy $\delta\epsilon = \hbar\delta\omega = \hbar\gamma$. Thus, the relationship between τ and $\delta\epsilon$ is

$$\tau\delta\epsilon = \tau\hbar\delta\omega = \tau\hbar\gamma = h . \tag{2.41}$$

The relation between life time, or pulse length, and bandwidth is quite general and very important. Pulses with a shorter lifetime have broader frequency spectra. If, for example, the life time of the oscillation is 1 fs the band width of the power spectrum is about 4.1 eV.

2.4.2 Frequency Spectrum for Electromagnetic Waves with a Finite Radiation Time

The frequency analysis of a plane wave oscillating only in a time interval from $t = 0$ to $t = T$ is a straight forward extension of the discussion above. Considering only the time-dependent part of the wave we have to study

$$\begin{aligned}
E(t) &= E_0 \cos \omega_0 t \quad \text{for} \quad 0 \leq t \leq T \\
&= 0 \quad \text{otherwise,}
\end{aligned} \tag{2.42}$$

or its exponential analog. The latter is again more convenient. With FT, as demonstrated above, we obtain for the frequency spectrum

$$\begin{aligned}
E(f) &= \int_0^T E_0 e^{i2\pi f_0 t} e^{-i2\pi f t} dt \\
&= \frac{E_0 \sin[\pi T(f_0 - f)]}{\pi(f_0 - f)} e^{i\pi(f_0 - f)T} .
\end{aligned} \tag{2.43}$$

The exponential term in this result is obviously a phase factor, since we did not start with a packet symmetric about $t = 0$. The intensity spectrum should, of course, not depend on this phase. This is indeed true as the product $E(\omega)E^*(\omega)$ yields for $S(\omega)$

$$S(\omega) = \frac{4E_0^2 \sin^2(\omega_0 - \omega)T/2}{(\omega_0 - \omega)^2} . \quad (2.44)$$

The graph for the real part of the wave packet and the intensity spectrum (for its complex form) are shown in Fig. 2.7. From (2.44) the width of the spectral

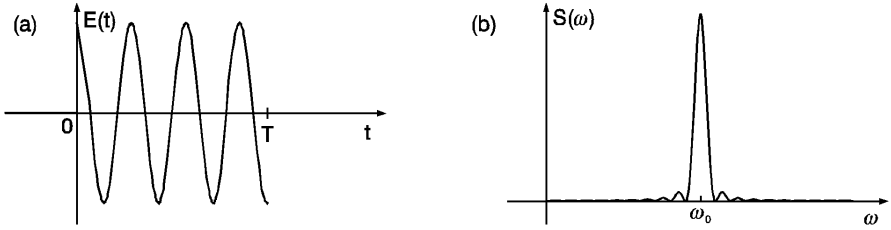


Fig. 2.7. Wave packet for a plane wave starting at time $t = 0$ and extending to $t = T$ (a) and intensity spectrum for its complex representation in time (b)

distribution is determined by the length T of the wave packet. For very large values of T it approaches a monochromatic structure which can be described by a delta function of the form $\delta(\omega_0 - \omega)$. This function is a very useful tool for the mathematical treatment of spectroscopic problems. Appendix B.8 lists some of its most important properties. The FWHM for the frequency spectrum of the wave packet is obtained from (2.44) by $\Delta\omega \approx 5.54/T$. As in the case of the damped waves shorter pulses have broader frequency spectra. A pulse of one femtosecond duration has an approximate bandwidth $\hbar\Delta\omega = 3.65 \text{ eV}$.

2.4.3 Frequency Spectrum and Power Spectrum

As mentioned above, we do not have to worry about complex frequency spectra. The physically meaningful quantity is the intensity or power spectrum given as

$$S(f) = |E(f)|^2 . \quad (2.45)$$

From the above definition it is not obvious that $S(f)$ is the relevant quantity to describe the spectral intensity. Alternately one could have used the intensity $|E(t)|^2$ from any of the time functions given above and taken the FT. The result would not be equal to $E(f)E^*(f)$. The experimentally observed

quantity is indeed $S(f)$. The physical reason for this is that the electric field of the radiation interacts with the electrons of the detector, not its “power”.

Note that the spectral intensity defined in (2.45) is not given in $\text{W}/\text{m}^2\text{Hz}$. We need to prove that $E(f)E^*(f)$ is proportional to the intensity of the radiation, and the factors of proportionality must be evaluated. For a stationary field the intensity as measured with a detector over a period of time $2T$ is

$$I(T) = \varepsilon_0 c_0 \frac{1}{2T} \int_{-T}^T E(t)E^*(t)dt \quad (T \text{ arbitrary}) . \quad (2.46)$$

The rationale for this measurement is illustrated in Fig. 2.8. The quantity

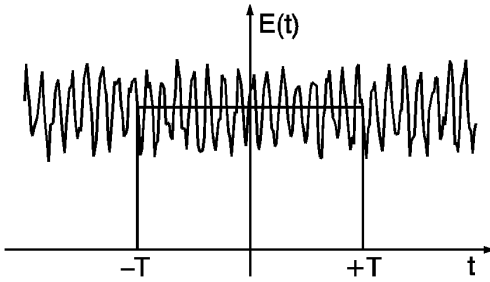


Fig. 2.8. Measurement of radiation intensity for a stochastic field

actually measured is zero for $|t| \geq T$ and originates from a field $E(t, T)$ with a Fourier transform $E(f, T)$. For T large enough $I(T)$ does not depend on T , and (2.46) can be written as

$$\begin{aligned} I &= \lim_{T \rightarrow \infty} \frac{\varepsilon_0 c_0}{2T} \int_{-T}^T E(t, T) \int E^*(f, T) e^{-i2\pi ft} df dt \\ &= \lim_{T \rightarrow \infty} \frac{\varepsilon_0 c_0}{2T} \int \int_{-T}^T E(t, T) e^{-i2\pi ft} dt E^*(f, T) df \\ &= \lim_{T \rightarrow \infty} \frac{\varepsilon_0 c_0}{2T} \int E(f, T) E^*(f, T) df = \frac{\varepsilon_0 c_0}{2T} \int S(f, T) df , \end{aligned} \quad (2.47)$$

where we have dropped the limits of integration in the last line, but understand that T is large enough to have no influence on the measurement of the power. The second Fourier transformation in (2.47) is exact since we are considering a time function for the field E which is only finite between $-T$ and T . The derivation shows that $S(f, T)$ is indeed a spectral power and the intensity per unit frequency range is obtained by multiplying it with $\varepsilon_0 c_0 / 2T$. We may define a spectral intensity $I(f)$ explicitly as

$$I_f(f) = \frac{\varepsilon_0 c_0}{2T} E(f, T) E^*(f, T) \quad (\text{in } \text{W}/\text{m}^2\text{Hz}) . \quad (2.48)$$

For a pulse-like E field, the spectral intensity given in $\text{W}/\text{m}^2\text{Hz}$ may not be very useful since, for example, in a damped oscillation, the intensity changes continuously with time. In this case a more meaningful description is obtained by considering the total energy W_T of the pulse.

$$W_T = \varepsilon_0 c_0 \sigma \int E^2(t) dt \quad (\text{in Joule}) ,$$

where σ is the cross section of the pulse. The spectral energy density in J/Hz is then obtained from

$$W(f) = W_T \frac{|E(f)|^2}{\int |E(f)|^2 df} = \varepsilon_0 c_0 \sigma |E(f)|^2 , \quad (2.49)$$

where Parseval's theorem was used in the form

$$\int |E(t)|^2 dt = \int |E(f)|^2 df . \quad (2.50)$$

The physical meaning of Parseval's theorem is that energy is conserved whether the total energy is expressed in time or in frequency space.

As we have seen, the intensity spectra are always real but we must still address the question of negative frequencies. They are understood as frequencies corresponding to negative times. This imposes a definite constraint on the intensity functions. If the field $E(t)$ is real, they must be even which is indeed always the case. (Note that the intensity spectrum in Fig. 2.7 is not even because the time function was complex.) Of course, the interpretation of negative frequencies does not mean that the reverse transform of $E(-f)$ gives the part of the time function with negative values of t . In fact, the part of $E(f)$ or $S(f)$ with negative f does not give any new information about the intensity spectrum and is, in this sense, useless.

2.5 Coherence and Correlation

For the application of EM fields in spectroscopy some more of their properties must be discussed. This section will summarize the concepts of coherence and correlation in order to provide a basic knowledge of these quantities. It will be sufficient for understanding the following chapters. Specialists in laser spectroscopy or correlation spectroscopy will need to study these subjects in greater depth.

2.5.1 Periodic and Non-Periodic Electromagnetic Fields

In Sect. 2.1 we discussed EM fields with periodic oscillations of infinite duration. This discussion was extended in Sect. 2.4 to non-periodic functions, most of which vanish for $t \rightarrow \infty$. Real radiation fields are different as the phases and

amplitudes of the wave trains have a certain statistical or stochastic character. This character exists for laser radiation as well as for black-body emission even though it is much less prominent in the former. For convenience, we will distinguish four different types of EM fields

- (a) fully periodic fields, to be described by harmonic functions,
- (b) quasi-periodic non-stationary fields which vanish for $t \rightarrow \infty$, to be described by damped oscillator functions, as discussed in Sect. 2.4,
- (c) quasi-stochastic fields where amplitude and phase vary statistically with time but the variations are weak. Such fields may be described by the real part of

$$E(t) = A(t)e^{i\alpha(t)} \quad \text{with} \quad \alpha(t) = 2\pi f_0 t + \phi(t), \quad (2.51)$$

- where the usual time-independent amplitude E_0 and phase ϕ have been replaced by more or less rapidly varying functions in time $A(t)$ and $\phi(t)$,
- (d) highly stochastic fields like those from black-body radiation or from a stochastic generator.

A highly stochastic field may be visualized as a statistically emitted train of damped oscillations as shown in Fig. 2.9. The coherence time for this light is given by the lifetime of the wave.

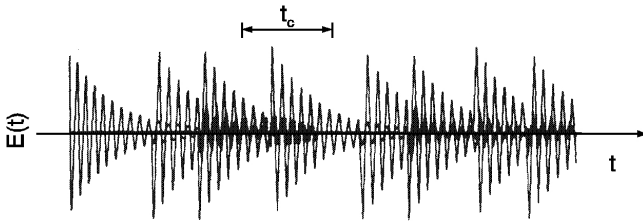


Fig. 2.9. Stochastic light consisting of randomly generated trains of oscillations with a life time t_c

2.5.2 Coherent and Non-Coherent Superposition

The coherence of components in a wave field is of fundamental importance for their superposition. This superposition may be coherent or incoherent. The results are different and need careful consideration. The intensity of the radiation field is proportional to E^2 and is given by

$$\langle E^2 \rangle = \frac{1}{2T} \int_{-T}^T E^2(t) dt \quad (2.52)$$

for an arbitrary function of time. $2T$ is the duration of the measurement, as discussed in (2.46). For two superposed harmonic waves E_1 and E_2 with

amplitudes, frequencies and phases given by $E_{01,2}$, $f_{1,2}$ and $\phi_{1,2}$, respectively, the intensity is

$$\begin{aligned}\langle E^2 \rangle &= \langle (E_1 + E_2)^2 \rangle = \langle E_1^2 \rangle + \langle E_2^2 \rangle + 2\langle E_1 E_2 \rangle \\ &= \frac{E_{01}^2}{2} + \frac{E_{02}^2}{2} + 2E_{01}E_{02}\langle \cos \alpha_1 \cos \alpha_2 \rangle ,\end{aligned}\quad (2.53)$$

where $\alpha_{1,2} = 2\pi f_{1,2}t + \phi_{1,2}$. The first two terms in the equation represent the intensities of the individual waves and the third term describes the interference.

For $\alpha_1 \neq \alpha_2$ the interference term vanishes from the time average, as it can be expressed by cos-functions of the phase difference $\alpha_1 - \alpha_2$ and sum $\alpha_1 + \alpha_2$. Then, the intensities of the two individual fields simply add.

For fields with equal amplitude and α the situation is different. Since the amplitudes add to $2E_0$ the intensity increases from $2 \times (E_0^2/2)$ to $2E_0^2$. This result is also a direct consequence of (2.53), since the time average in the interference term becomes $1/2$. This surprising increase in energy seems to violate energy conservation. In practice, energy is, of course, conserved even in an interference experiment of this type. Coherent and collinear superposition of two equal waves is indeed only possible for beams oriented perpendicular to each other and split into two equal parts each by inserting a beam splitter of 45° . In this case each of the original waves propagates, after leaving the splitter, in two mutually perpendicular partial beams with field amplitude $E_0/\sqrt{2}$. The constructive interference can then only occur for one of the partial beams, and superposition leads to an intensity of $\langle (2E_1/\sqrt{2})^2 \rangle = E_0^2$ at maximum. Since in this case the intensity in the other superposed beam will be zero due to destructive interference, energy is conserved.

2.5.3 Temporary Coherence and Correlation

A discussion of coherence needs a more precise definition of this concept. Comparing one field with a second one which is shifted in space or time, is probably a good example. Coherence as we understand it from this is a phase correlation in time or space. In other words, we ask how well is $E(r_2, t_2)$ known for a general EM field $E(r, t)$ if we know $E(r_1, t_1)$. For small Δr and Δt the question can often be answered but this will become harder as the two functions move further apart in space and time. A good indicator to describe the problem could be the *mutual coherence* or *mutual correlation function* defined as

$$G(r_1, r_2, \tau) = \langle E^*(r_1, t)E(r_2, t + \tau) \rangle , \quad (2.54)$$

where $\langle \rangle$ refers to a time average. Spatial coherence is relevant for interference experiments with light from extended sources. Since this will not be discussed in the frame of this book, we will restrict ourselves to temporal coherence. In this case coherence at the same point r in space is considered and the argument

r for the coordinates can be dropped in (2.54). Then we obtain from (2.54) the *temporal coherence function* or *autocorrelation function* explicitly

$$G(\tau) = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T E^*(t) E(t + \tau) dt . \quad (2.55)$$

The autocorrelation function is maximum for $\tau = 0$ and may go to zero for $\tau \rightarrow \infty$. The autocorrelation function for a partially or highly stochastic light field vanishes for $\tau \rightarrow \infty$ since eventually $E(t)$ and $E(t + \tau)$ become random in phase and all contributions cancel due to the time averaging. The autocorrelation functions do not have to become zero for $\tau \rightarrow \infty$. For example the autocorrelation function for a constant $E(t) = E_0$ is $E_0^2 \neq 0$ for all values of τ . The autocorrelation function for a sin- or cos-wave is given by a cos-wave, and remains oscillating for all values of τ .

Note that the definition of the autocorrelation function in (2.55) cannot be used for non stationary fields like wave packets, etc. $G(\tau)$ would be identically zero. In this case we have to define it as

$$G(\tau) = \lim_{T \rightarrow \infty} \int_{-T}^T E^*(t) E(t + \tau) dt . \quad (2.56)$$

For the case of a wave packet this function is indeed maximum for $\tau = 0$ and approaches 0 for $\tau \rightarrow \infty$. Since the only interesting behavior of $G(\tau)$ is its dependence on the time shift τ , a normalized autocorrelation function of the form

$$g(\tau) = G(\tau)/G(0) \quad (2.57)$$

is often used. In this case discrimination between stationary and non-stationary fields is not required.

The decay time of the autocorrelation function gives the coherence time $\Delta\tau$ and the coherence length $\Delta l = c_0 \Delta\tau$. There are several possible definitions for the decay time of $G(\tau)$. The FWHM is one. Another straight forward definition is related to the variance (mean square deviation) of the autocorrelation function or to the second moment of the absolute square of this function. In the latter case the coherence time is defined by

$$(\Delta\tau_v)^2 = \frac{\int \tau^2 |G(\tau)|^2 d\tau}{\int |G(\tau)|^2 d\tau} . \quad (2.58)$$

This definition may be paralleled by a definition for the spectral bandwidth of the function $E(t)$ as the variance of the absolute square of the power spectrum.

$$(\Delta f_v)^2 = \frac{\int (f - f_0)^2 |S(f)|^2 df}{\int |S(f)|^2 df} . \quad (2.59)$$

The expressions for $\Delta\tau$ and Δf allow us to study the product of the two quantities. As might be expected, there is a fundamental connection between them. This connection can be investigated in a very general way through an analysis of a field with a quasi-stochastic fluctuation given by (2.51). Splitting the complex exponent $\alpha(t)$ into a harmonic part oscillating with the frequency f_0 and a fluctuating phase $\phi(t)$ we have

$$E(t) = \int E(f) e^{i2\pi f t} df = A(t) e^{i\phi(t)} e^{i2\pi f_0 t},$$

where $E(f)$ is the Fourier transform of $E(t)$. This expression can be used to study explicitly the relationship between the fluctuation of $E(t)$ in time and its bandwidth. Multiplying both sides with $\exp(-i2\pi f_0 t)$ yields

$$A(t) e^{i\phi(t)} = \int E(f) e^{i2\pi(f-f_0)t} df. \quad (2.60)$$

A very small bandwidth of $E(t)$ allows only substantial values for $E(f)$ if f is very close to f_0 , which means $(f-f_0)$ very small or very slow fluctuations with a long coherence. On the other hand, if $E(f)$ gives substantial contributions to the integral even for large values of $(f-f_0)$ rapid fluctuations with a short coherence exist. Thus, bandwidth Δf and coherence Δt are inversely related. The fundamental relationship

$$\Delta t \Delta f = \text{constant} \approx 1 \quad (2.61)$$

is quite general. The constant is determined by the particular type of the field as well as by the actual definition used for the bandwidth and for the coherence. There are numerous examples for this relationship in the literature. We will give only one and leave others as problems.

Let the field be the damped, one-sided complex exponential wave $E(t) = \exp(-\gamma t/2) \exp(i2\pi f_0 t)$ where we assumed $E_0 = 1$, for convenience. We evaluate the autocorrelation function $G(\tau)$ from (2.56) and use (2.58) and (2.59) for the definition of $\Delta\tau_v$ and Δf_v , respectively. This yields

$$\begin{aligned} G(\tau) &= \int E^*(t) E(t+\tau) dt = \int_0^\infty e^{-\gamma t/2} e^{-\gamma(t+\tau)/2} e^{i2\pi f_0 \tau} dt \\ &= e^{-\gamma\tau/2} e^{i2\pi f_0 \tau} \int_0^\infty e^{-\gamma t} dt \\ &= \frac{1}{\gamma} e^{-\gamma\tau/2} e^{i2\pi f_0 \tau} \quad \text{for } \tau \geq 0, \quad \text{and 0 otherwise} \end{aligned} \quad (2.62)$$

Note that for negative τ the integration must be performed from $-\tau$ to ∞ . The power spectrum $S(f)$ for the field under consideration was already evaluated in (2.40) so that we can immediately calculate the correlation time $\Delta\tau_v$ and the band width Δf_v from

$$\begin{aligned}
(\Delta\tau_v)^2 &= \frac{\int \tau^2 |G|^2 d\tau}{\int |G|^2 d\tau} = \frac{(1/\gamma^2) \int_0^\infty \tau^2 e^{-\gamma\tau} d\tau}{(1/\gamma^2) \int_0^\infty e^{-\gamma\tau} d\tau} \\
&= \frac{4/\gamma^5}{2/\gamma^2} = \frac{2}{\gamma^2}
\end{aligned} \tag{2.63}$$

and

$$\begin{aligned}
(\Delta f_v)^2 &= \frac{\int (f - f_0)^2 |S|^2 df}{\int |S|^2 df} \\
&= \int \frac{(f - f_0)^2 df}{[(\gamma/2)^2 + (2\pi)^2 (f - f_0)^2]^2} \bigg/ \int \frac{df}{[(\gamma/2)^2 + (2\pi)^2 (f - f_0)^2]^2} \\
&= \frac{1}{(2\pi)^2 2\gamma} \frac{\gamma^3}{2} .
\end{aligned} \tag{2.64}$$

The square root of the product of the two quantities yields the well known result

$$\Delta\tau_v \Delta f_v = \frac{1}{2(2\pi)^2} \tag{2.65}$$

Note that the relationship we had in (2.41) between the life time of an oscillation and its bandwidth is very similar to (2.65). Physically these relationships are indeed based on the same fundamental principle of uncertainty but conceptually they are very different. The result from (2.65) can be compared with the simple product of the decay time $\tau = 2/\gamma$ and the FWHM $\Delta f = \gamma/2\pi$ of the Lorentz line which yields

$$\tau \Delta f = 1/\pi \tag{2.66}$$

2.5.4 The Wiener–Khinchin Theorem

In many applications both functions, the Fourier transform $E(f)$ and the correlation function $G(\tau)$ of a fluctuating field $E(t)$ are needed. An example was just given. It turns out that the two functions are not independent but are correlated in a rather simple way known as the *Wiener–Khinchin* theorem. This theorem states that the Fourier transform of the correlation function $G(\tau)$ equals the power spectrum $S(f)$ of a field $E(t)$, and vice versa. In mathematical terms this means that

$$\begin{aligned}
\int G(\tau) e^{-i2\pi f\tau} d\tau &= S(f) \quad \text{and} \\
\int S(f) e^{i2\pi f\tau} df &= G(\tau) .
\end{aligned}$$

(2.67)

The proof of the theorem is rather simple for non stationary fields. Using the definition for the Fourier transform of $G(\tau)$ and writing it as

$$\begin{aligned}
\int G(\tau)e^{-i2\pi f\tau}d\tau &= \int E^*(t)E(t+\tau)e^{-i2\pi f\tau}(e^{-i2\pi ft}e^{i2\pi ft})dtd\tau \\
&= \int E^*(t)e^{i2\pi ft}E(t+\tau)e^{-i2\pi f(t+\tau)}dtd(t+\tau) \\
&= E^*(f)E(f) ,
\end{aligned} \tag{2.68}$$

which is exactly the power spectrum $S(f)$. The proof for stationary fields is similar but more laborious. The Wiener–Khinchin theorem is fundamental in coherent signal processing.

Problems

2.1 Show that the relation between the E field and the B field for an electromagnetic plane wave is given as $\mathbf{B} = (1/\omega)(\mathbf{k} \times \mathbf{E}_0) \exp i(\mathbf{k}\mathbf{r} - \omega t)$.

(Purpose of exercise: use of Maxwell's equations)

2.2 Show that the wave equation, as derived from Maxwell's equations for a conducting system, is given by

$$\Delta \mathbf{E} = \frac{\varepsilon\mu}{c_0^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \mu\mu_0\sigma \frac{\partial \mathbf{E}}{\partial t}$$

Discuss the equation for a good metal and study the behavior of \mathbf{E} for a plane wave solution by performing a back substitution.

(Purpose of exercise: use of Maxwell's formalism)

2.3 Calculate the magnetic induction and the Poynting vector for a Hertzian dipole of the radiation zone from the vector potential.

Hint: Use spherical polar coordinates and neglect terms $\propto 1/r^2$.

(Purpose of exercise: use of spherical polar coordinates.)

2.4 Two positive and two negative charges are linearly arranged with the two negative charges coinciding at $z = 0$ and the two positive charges at $z = \pm l$. Calculate the electric dipole moment, the electric quadrupole moment and the quadrupole radiation field if the charges vary harmonically as $Q = Q_0 \cos \omega t$.

Hint: For the evaluation of the field add the contributions from the two oppositely oriented dipole radiators.

(Purpose of exercise: multipole radiation; Pick the right approximation.)

2.5 Show that $E = \exp(-\gamma t/2) \cos \omega t$ for $t > 0$ and $E = 0$ for $t < 0$ is a solution for the damped harmonic oscillator but $E = \exp(-\gamma|t|/2) \cos \omega t$ is not a solution.

(Purpose of exercise: understanding damped oscillation.)

2.6* Show that the integral form of the Fourier theorem includes the representation of periodic functions as a sum of harmonic functions and evaluate the coefficients in the sum from the integral theorem.

Hint: Separate the integral from $-\infty$ to ∞ into a sum of integrals over the range equal to the period.

(Purpose of exercise: get a feel for the Fourier theorem.)

2.7* Evaluate the relationships between the complex Fourier coefficients c_n and the coefficients for the real representation A_n and B_n in (2.25). Show that

$$\begin{aligned} c_0 &= \frac{1}{T} \int_{t_0}^{t_0+T} E(t) dt, & A_n &= \frac{2}{T} \int_{t_0}^{t_0+T} E(t) \cos n\omega t dt, \\ B_n &= \frac{2}{T} \int_{t_0}^{t_0+T} E(t) \sin n\omega t dt, \end{aligned} \quad (2.69)$$

(Purpose of exercise: equivalence of real and complex formalism of Fourier transforms.)

2.8 Calculate the difference in the Fourier transform of two functions generated from each other by an arbitrary shift in time.

(Purpose of exercise: get an understanding for the spectroscopic meaning of a time shift.)

2.9 Show that the FT of the intensity $I(t) \propto |E(t)|^2$ for an asymmetric exponential decay $E(t) = Ae^{-\gamma t}$ is different from the power spectrum $S(\omega)$.

(Purpose of exercise: get convinced of the difference between the two quantities.)

2.10* Calculate the Fourier transform for the exponential decay $E(t) = Ae^{-\gamma t}$ for $t \geq 0$, $E(t) = 0$ otherwise and show that the inverse Fourier transform gives the correct time function.

Hint: Use integration in the complex plane for the inverse transformation.

(Purpose of exercise: to prove that the full details of the time spectrum are retained when the inverse transform is taken.)

2.11 Calculate the autocorrelation function for a sin-wave and for a cosine-wave.

(Purpose of exercise: use correlation functions.)

2.12 Calculate the product of the coherence time $\Delta\tau$ and the bandwidth Δf for a Gaussian line with the definitions of (2.58) and (2.59).

(Purpose of exercise: verify the relation between coherence length and bandwidth.)



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