

Selected Topics in Advanced Experimental Physics

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Part I

Concept: Fourier Transformation

Chapter 5

Mössbauer Spectroscopy [WIP]

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Overview

We close the part on oscillations and Fourier transforms by the Mössbauer effect, which describes the recoil-less emission and absorption of a gamma photon by a atomic nucleus. It leads to the most narrow spectral lines in physics with $\Delta E/E \approx 10^{-18}$ XXX check.

During his PhD thesis work in Munich and Heidelberg in the years 1955 – 1958, Rudolf Mössbauer investigated the emission and reabsorption of gamma radiation by ^{191}Ir . He discovered an unexpected increase in absorption when cooling both the emitter and the absorber material. This observation and its explanation led to his receiving the Nobel Prize in 1961 at the age of 32. Today, Mössbauer spectroscopy is a common tool used to study materials. One example is the Mars rovers, which use Mössbauer spectroscopy to search for water.

The structure of this chapter follows that of the Nobel Prize lecture by Rudolf Mössbauer (see reference Mössbauer, 1961, reprinted in Kalvius and Kienle, 2012). Other good sources are Schatz, Weidinger, and Deicher, 2010 and Wegener, 1966.

Resonance fluorescence

At room temperature, the fluorescence emission peak of dye molecules is displaced from the absorption peak due to the Stokes shift. The molecules lose energy between absorption and emission, for example, through the reorientation of the surrounding solvent or matrix molecules.

This is different for atoms in the gas phase. When yellow light from a sodium lamp shines on sodium vapor, the atoms in the vapor absorb the light and re-emit it a few nanoseconds later. The emission of photons by the sodium atoms in the lamp and the absorption of photons by the sodium atoms in the vapor occur at the same energy or wavelength. This process is called resonance fluorescence. It is fluorescence, not scattering, because an excited state is populated.

The width of the transition in emission and absorption is determined by



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several processes: the natural linewidth is given by the decay rate to the ground state via Fourier transform. This is the ultimate limit. The line can be broadened by other processes, for example by collisions with other atoms, by Doppler shifts due to thermal motion, or by saturation due to high excitation rate. A typical relative linewidth is $\Delta E/E \approx XXX$ with $E \approx 2$ eV and ΔE given by a decay rate of 1 ns^{-1} .

Recoil in resonance absorption

When a photon of frequency ν is emitted, it carries a momentum $\hbar k = h\nu/c$ with it. If the atom was at rest before emission, then momentum conservation requires that also the atom must move afterwards. This movement carries kinetic energy ΔE_{recoil} , which has to be taken from the transitions energy E_0 . We find

$$\Delta E_{\text{recoil}} = \frac{|p_{\text{atom}}|^2}{2M} = \frac{E_0^2}{2Mc^2} \quad (5.1)$$

with the mass of the atom M and c the velocity of light. For the D-line of sodium, this is about $\Delta E_{\text{recoil}} \approx XXX$, i.e. much smaller than the natural linewidth of the transition. For an optical transition involving atoms or molecules, the recoil effect can be neglected.

This is different for atomic nuclei that emit gamma radiation. After a nuclear reaction such as an alpha- oder beta-decay, the nucleus will most likely end up in an excited state. It can decay to its ground state by emission of a gamma photon with an energy in the range of a few keV to MeV. E_0 and thus ΔE_{recoil} are much larger than for visible light emission. Since metastable nuclear states have lifetimes of nanoseconds or longer, the natural linewidth is comparable to that of dye molecules

The recoil acts twice. First, the spectrum of the emitted gamma photon shifts to lower energies because some energy remains at the emitting nucleus. Second, absorption requires an additional amount of energy, equal to the recoil energy, because the absorbed photon must supply the energy necessary for the nucleus to move afterward. Thus, there is a $2\Delta E_{\text{recoil}}$ mismatch between the emitted photon and gamma absorption. Depending on thermal broadening, some overlap is found (Fig. 5.1). Unlike resonance fluorescence in the visible spectrum, resonance absorption of gamma radiation should not or only extremely weakly occur when source and absorber are identical.

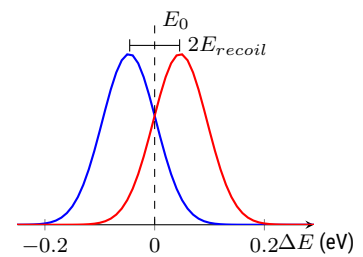


Figure 5.1: Thermal motion causes emission (blue) and absorption (red) lines to broaden. Recoil leads to a relative shift. Only the overlapping region contributes to resonance absorption. The sketch is to scale for the 129 keV transition of ^{191}Ir at room temperature.

¹ Moon, 1951.

Doppler shifting of transitions

Things changed in 1951 when P. B. Moon published¹ an experiment, in which he supplied the missing energy of $2\Delta E_{\text{recoil}}$ through a Doppler shift. One needs an excited nuclear state that decays in the emitter by gamma radiation to the ground state. In the absorber, all nuclei are in the ground state and thus able to absorb a gamma photon when the recoil mismatch is compensated. The tips of a high-speed rotor were coated with gold that had been treated in a nuclear reactor. The ^{198}Au isotope decays into an excited ^{198}Hg which in turn decays by gamma emission of 412 keV into the ^{198}Hg ground

state. At a speed of 630 m/s of the gold tip toward the mercury absorber, the Doppler shift should compensate for $2\Delta E_{\text{recoil}}$. Moon found the expected increase in absorption.

Temperature tuning of transitions

Mössbauer investigated² the isotope ^{191}Ir , which decays by emitting a 129-keV gamma photon to the ground state. This choice simplifies resonance absorption because the nucleus is heavy and the photon has low energy. One can learn something about the linewidth by tuning the temperature of either the emitter or the absorber. In both cases, the overlap region in Fig. 5.1 changes. Mössbauer kept the absorber at room temperature and switched the emitter temperature between 88 K and 303 K. From the difference in absorption he derived a line with in terms of excited state lifetime of $\tau = 360$ ps.

In a second series of experiments, he kept the absorber at 88 K and adjusted the temperature of the source from 370 K to 88 K. One might expect a significant decrease in resonance absorption when both the emission and absorption lines narrow and the recoil remains constant. However, this is not what Mössbauer found. The absorption increased by about a factor of 10. Initially, he considered this to be an experimental flaw, as he mentioned in his Nobel Lecture.

² Rudolf L Mössbauer, 1958b.

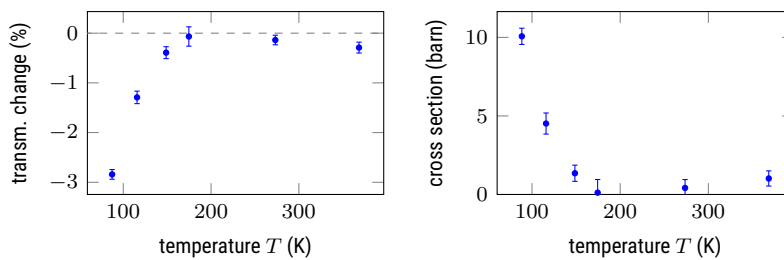


Figure 5.2: Left: Transmission reduction when the source and absorber are both cooled. Right: Absorption cross section calculated from the data on the left. Data from Rudolf L Mössbauer, 1958b

Simple model

How can this observation be explained? The key point is that the atoms are not in a gaseous state. Above, we implicitly assumed a gas phase because the recoil momentum is taken over by just one atom. Additionally, the thermal broadening was calculated assuming a Maxwell velocity distribution. This is not the case in a solid. In a solid, the atoms (and thus the nuclei) are bound by an energy of about 10 eV, which is much stronger than the recoil energy. The atoms vibrate around their equilibrium position. Their vibrational frequencies are described by the photon dispersion relation.

Let's assume the simplest photon dispersion relation: the Einstein model. The only allowed vibrational frequency is Ω . The vibration can absorb energies in integer multiples of $E_{\text{phonon}} = \hbar\Omega$. If the recoil energy, E_{recoil} , is much larger than Ω , this quantization has only a minor effect. However, when $E_{\text{recoil}} \ll \hbar\Omega$, no phonon is emitted when a gamma photon is emitted. This is the Mössbauer effect, the recoilless emission (and absorption) of gamma

radiation.

XXX andes First, we will stay with the Einstein model and examine the emission probabilities for different numbers of photons. Next, we introduce the full phonon dispersion. This leads us to the Debye-Waller factor, which also describes the blurring of spots in X-ray diffraction.

Classical model of the Debye Waller factor

We use the classical model of a vibrating atom that continuously emits gamma radiation (Schatz, Weidinger, and Deicher, 2010). A quantum mechanical approach can be found in Czycoll, 2016. The position of the atom oscillates with an amplitude of a .

$$x(t) = a \sin \Omega t \quad (5.2)$$

so that the emitted field at frequency ω_0 is ($k = 2\pi/\lambda$)

$$E(t) = E_0 e^{-i(\omega_0 t + kx(t))} \quad (5.3)$$

$$= E_0 e^{-i\omega_0 t} \left(1 - ika \sin \Omega t - \frac{k^2 a^2}{2} \sin^2 \Omega t + \dots \right) \quad (5.4)$$

The \sin^n terms lead to new³ frequencies in the gamma emission spectrum at $\omega_0 \pm n\Omega$ and the fundamental line at ω_0 is reduced in amplitude. For its amplitude A one finds

³ this is very similar to Raman scattering

$$A = 1 - \frac{k^2 a^2}{4} + \dots = J_0(ka) \simeq \exp\left(-\frac{k^2 a^2}{4}\right) \quad (5.5)$$

with J_0 the zeroth order Bessel function. The *Debye Waller factor* f describes the intensity, i.e. the square of the amplitude

$$f = |A|^2 = J_0(ka)^2 \simeq \exp\left(-\frac{k^2 a^2}{2}\right) \quad (5.6)$$

In a real system (and in quantum mechanics) the amplitude a would not be constant. It is thus convenient to express a by the mean square displacement $\langle x^2 \rangle$ of a 1d or 3d ($\langle u^2 \rangle$) oscillation

$$\langle x^2 \rangle = \frac{a^2}{2} \quad \text{and} \quad \langle u^2 \rangle = 3 \langle x^2 \rangle \quad (5.7)$$

so that we get all together⁴

⁴ the \simeq vanishes in quantum mechanics

$$f = \exp\left(-\frac{k^2 \langle u^2 \rangle}{3}\right) \quad (5.8)$$

Debye model

To find the mean square displacement $\langle x^2 \rangle$ (or $\langle u^2 \rangle$) we start from a single-frequency oscillator at frequency Ω and mass M . Its mean potential energy, i.e., potential energy at the mean square displacement, is half the total energy

$$\frac{1}{2} M \Omega^2 \langle x^2 \rangle_n = \frac{1}{2} \hbar \Omega \left(n + \frac{1}{2} \right) \quad (5.9)$$

when the oscillator is in quantum state n , Thus

$$\langle x^2 \rangle_n = \frac{\hbar}{M\Omega} \left(\frac{1}{2} + n \right) \quad (5.10)$$

and averaging over all possible states n occupied with the probability P_n we get in the Einstein model for the phonon dispersion

$$\langle x^2 \rangle_E = \frac{\hbar}{M\Omega} \left(\frac{1}{2} + \sum n P_n \right) = \frac{\hbar}{2M\Omega} \left(1 + \frac{2}{\exp(\hbar\Omega/k_B T) - 1} \right) \quad (5.11)$$

In the Debye model (i.e. constant velocity of sound), the density of states is

$$D(\Omega)d\Omega = \frac{9N\hbar^3\Omega^2}{k_B^3\Theta_D^3}d\Omega \quad (5.12)$$

with the Debye temperature Θ_D and N the number of unit cells and 3 vibrational degrees of freedom. We now weight $\langle x^2 \rangle_E$ with $D(\Omega)$ to plug in the Debye model

$$\langle x^2 \rangle = \frac{1}{3N} \int_0^{\Omega_D} D(\Omega) \langle x^2 \rangle_E d\Omega \quad (5.13)$$

Without going further into the details here (see, e.g. Schatz, Weidinger, and Deicher, 2010), we get $\langle x^2 \rangle \propto T$ for $T \gg \Theta_D$. At zero temperature, $\langle x^2 \rangle$ remains finite due to the quantum mechanical zero point motion. With increasing temperature, it increases quadratically. In this limit, one can compute the integral and get for the Debye Waller factor in the Debye approximation

$$f_D(T) = \exp \left\{ -\frac{3E_0^2}{4Mc^2k_B\Theta_D} \left[1 + \frac{2\pi^2}{3} \left(\frac{T}{\Theta_D} \right)^2 \right] \right\} \quad (5.14)$$

where we have used $\hbar k = E_0/c$ with the energy E_0 of the gamma quant.

Interpretation

At all temperatures, a fraction $f(T)$ of all emission and absorption events occur without recoil. This fraction increases exponentially as the temperature decreases, but it does not approach one even at $T = 0$. It also increases with the Debye temperature; that is, the Mössbauer effect is more pronounced in harder, stiffer crystals. A lower gamma energy E_0 increases the effect as well.

Although the Mössbauer effect is called "recoilless," momentum must still be conserved. The recoil momentum must remain somewhere. If a phonon—the vibration of an atom in a crystal lattice—does not absorb the momentum, then the crystal as a whole does. The entire crystal then moves slightly in the direction opposite the gamma quantum emission. However, since the crystal is much heavier than an atom, this movement is not observable.

In a classical model without zero-point motion, the spectrum of emitted gamma radiation would be a sharp Lorentzian at the nuclear transition energy. This is depicted as a delta function in Figure 5.4. As temperature increases, crystal vibrations lead to the formation of symmetric sidebands above and below this frequency: the $\omega_0 \pm n\Omega$ terms above. Quantum mechanics introduces two changes. First, the spectrum at $T = 0$ contains a

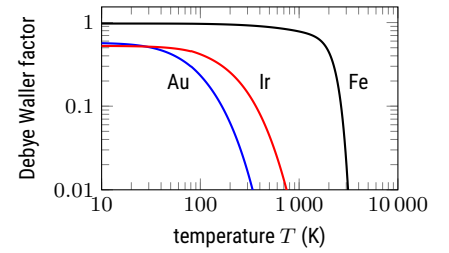


Figure 5.3: Debye Waller factors for the elementary crystals of ^{57}Fe , ^{197}Au and ^{192}Ir with transition energies of 14.3, 77 and 129 keV. Data from Friedrich, 2020.

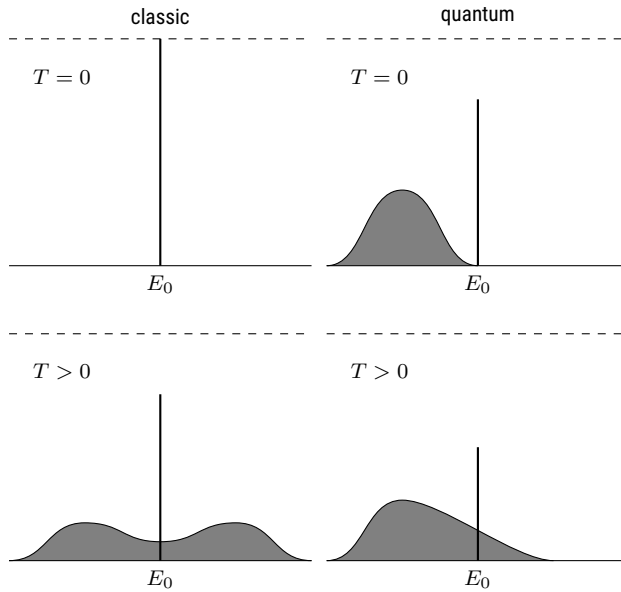


Figure 5.4: Sketch of the classical and quantum mechanical gamma spectrum. Inspired by Fig. 2.2 of Wegener, 1966

phonon band at a lower energy due to zero-point motion. This is because all "+" operations in the above equations and thus $f(T = 0) < 1$ trace back to the " $n + 1/2$ " of the harmonic oscillator. At higher temperatures, the spectrum remains asymmetric because the emission of a phonon is always possible. However, absorption of a phonon, which leads to $E > E_0$, requires a populated phonon state.

The first Mössbauer spectrum

So far, our discussion has covered the situation of Walter Mössbauer when he submitted his first article, Rudolf L. Mössbauer, 1958b. Only upon rereading his own article in the journal, he realized that measuring the gamma emission spectrum as sketched in Fig. 5.4 would be both convincing and technically feasible (Rudolf Mössbauer, 2000). The idea is to use the Doppler shifting technique to scan an isotope's emission line against its own absorption line. Unlike the original experiment discussed above, the energy scale is no longer $E_{\text{recoil}} \approx 0.1$ eV, but rather the lifetime-limited linewidth of about 10 μeV . Thus, the velocity of the source can be about four orders of magnitude slower. Fearing that his competitors would realize this as well, Mössbauer set out to conduct the experiment himself, using toy mechanical gears to rotate the source at a speed of a few centimeters per second. Figure 5.5 shows the data.

This is the first observation of a recoilless transition, i.e. nuclear resonance absorption. The transition has an energy of 129 keV and a line width of just 4.6 μeV . The ratio or relative accuracy is about 10^{10} . In modern experiments, a relative linewidth of 10^{18} can be observed (XXX Ref).

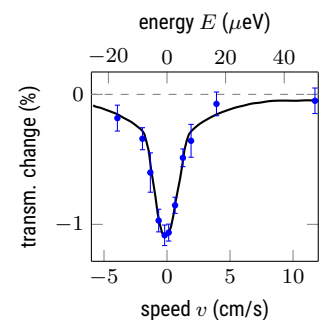


Figure 5.5: First spectrum of the Mössbauer line of ^{192}Ir . Data from Rudolf L. Mössbauer, 1958a

Effects influencing the gamma energy

Several effects influence the position of the gamma absorption line or cause line splitting in high-resolution Mössbauer spectroscopy. In the following discussion, we will examine some of these effects using ^{57}Fe as an example. This isotope is relatively abundant (about 2.5%) and stable in natural iron. Therefore, it is easy to produce gamma absorbers containing ^{57}Fe .

Figure XXX shows the level scheme. The transition to the ground state has an energy of 14.41 keV and a lifetime of 97.8 ns. The ground state has a nuclear spin of $I = 1/2$, while the excited state has $I = 3/2$. We will discuss three effects.

isomeric shift The electron density at the nucleus, combined with the different sizes of nuclei in various isomers (metastable, excited nuclear states), causes a shift. This shift is also called a "chemical shift."

electric quadrupole splitting Line splitting occurs when an electric field gradient is combined with a nuclear quadrupole moment.

magnetic hyperfine splitting In a ferromagnetic material, such as ^{57}Fe , the 'external' magnetic field splits the degenerate lines similar to the Zeeman effect.

The first two have the same origin. Electrons generate an electric potential at the nucleus's position, resulting in Coulomb energy. This potential can be expressed⁵ as a Taylor series and in terms of the electron wave function Ψ . The lowest order contains two contributions: the isomeric shift and the electric quadrupole splitting.

⁵ Schatz, Weidinger, and Deicher, 2010.

The isomeric shift is

$$E_I = \frac{e}{6\epsilon_0} |\Psi(0)|^2 \int \rho(\mathbf{r}) r^2 d\mathbf{r} = \frac{Ze^2}{6\epsilon_0} |\Psi(0)|^2 \langle r^2 \rangle \quad (5.15)$$

where ρ is the nuclear charge distribution and $\langle r^2 \rangle$ the mean square nuclear radius. The energy E_I depends on the state (via $\langle r^2 \rangle$) and the chemical environment of the atom (via $\Psi(0)$). This term allows us to distinguish between chemical environments when source and absorber contain the same isotope.

The electric quadrupole splitting can be written as

$$E_Q = \frac{e}{6} \sum_{i=x,y,z} V_{ii} Q_{ii} = (3m_I^2 - I(I+1)) \hbar\omega_Q \quad (5.16)$$

with the tensor of the electric field gradient V_{ii} and the nuclear quadrupole moment Q_{ii} . This field gradient vanishes when the crystal structure is cubic. The quadrupole moment vanishes when the nucleus is spherical, i.e. for $I = 1/2$. At higher nuclear spin values, one finds a splitting according to $|m_I|$, i.e. into $m_I = \pm 1/2$ and $m_I = \pm 5/2$ in the case of ^{57}Fe .

The magnetic hyperfine splitting results from the energy of the nuclear magnetic moment I in an external magnetic field \mathbf{B} , which can also be produced by a magnetized sample. As usual we have

$$E_{HF} = -\boldsymbol{\mu} \cdot \mathbf{B} = -g_I \mu_N m_I B_z \quad (5.17)$$

with the nuclear magneton $\mu_N = e\hbar/(2m_p) \approx 3 \cdot 10^{-8} \text{ eV/T}$ (proton mass m_p). g_I is the corresponding g-factor.

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Part II

Concept: Hybridization

Part III

Example: All Together

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