SOME SIMPLE ASPECTS OF THE THEORY OF THE MÖSSBAUER EFFECT

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The purpose of this paper is to make some simple remarks about the underlying principles of the Mössbauer effect.

Ever since the effect was first found there have been attempts to give a simple picture. Many of these pictures seem to be in violent contradiction with one another. I should like to point out that the Mössbauer effect is deeply rooted in quantum mechanics, and displays all the well known paradoxes of quantum mechanics, including complementarity and the uncertainty principle. For this reason, it is very often possible to describe the phenomena in ways which seem to be completely different but which can be shown to be equivalent.

One duality which is not quantum mechanical, but enters in an important way, is the presence of two systems, a lattice and radiation. Simple pictures of the Mössbauer effect are very often accurate for one and distorted for the other. From the point of view of radiation, there is a line which is sharp, i.e., it has the very small natural line width and it is unshifted. From the point of view of the lattice, there is an elastic transfer of momentum to the lattice; that is, the emission takes place without changing its internal motions.

Since most of the simple descriptions are classical, we may ask under what conditions a classical description is valid. For any quantum mechanical system, the correspondence principle tells us that the classical picture is valid when the quantum numbers are large. Let us now look at the quantum numbers that describe the system. For the radiation, there is either no photon (before) or one photon (after). The quantum numbers are thus 0 or 1, which are obviously not large, so that the system is far from the classical limit. For the lattice, it is known that the Mössbauer effect occurs at temperatures which are of the order of the Debye temperature or lower. The Debye temperature describes an energy characteristic of the phonon oscillator frequencies, and, therefore, at temperatures near the Debye temperature the lattice excitation quantum numbers are 0, 1 or 2. Again, the system is very far from the classical limit. Thus it may be expected that a classical treatment will perhaps give correct results for some aspects of the problem, but to get all of them it will be necessary to use quantum mechanics.

Wave-particle duality must be considered immediately, since there are two classical limits for any system - the wave-limit and the particle-limit. Furthermore, since the Mössbauer effect involves two systems, the radiation and the lattice, there are essentially four classical limits. Three of these limits have been examined to some extent and all give some insight.

1) The particle-wave description. The lattice is an assembly of particles emitting a classical wave. The picture is of a moving object emitting radiation which is frequency modulated. This gives a sharp line spectrum, whose center remains

the mean value of the kinetic energy equals the mean value of the potential energy equals one half the total energy. We can then take thermal averages and can get the result that

$$\langle P.E.\rangle_T = m\omega^2 \langle x^2\rangle_T/2 = (1/2)(n_T + 1/2)\hbar\omega \quad ,$$

where the subscript T denotes the thermal average.

Then

$$-\log f = k^2 \langle x^2 \rangle_T = k^2 \hbar^2 \, (2n_T + 1)/(2m\,\omega\hbar\,).$$

Now $k^2 \hbar^2/2m$ is just the free recoil energy R, and we get

$$k^2 \;\langle x^2 \rangle_T = R\,(2n_T + 1)/\hbar\omega\;.$$

For a high f, this quantity should be small. It will be small if the recoil energy is small compared to the spacing of the energy levels of the oscillator (this can be loosely identified with the Debye temperature), and also if the temperature is all.

However, we can also use another relation:

$$\langle K.E. \rangle_T = \langle p^2 \rangle_T/2m = \tfrac{1}{2}(n + 1/2)\,\hbar\omega\;.$$

Combining the two, we obtain

$$\langle p^2 \rangle_T \quad \langle x^2 \rangle_T = (n + 1/2)^2\,\hbar^2.$$

This is just the uncertainty principle (exact at zero temperature). Substituting, we find that

$$-\log f = k^2 \;\langle x^2 \rangle_T = \left(p_\gamma^{\,2}/ \;\langle p^2 \rangle_T\right)\left(n_T + 1/2\right)^2\,,$$

where p_γ is the momentum of the gamma ray. $p_\gamma = \hbar k$

Thus at low temperatures, where the n_T factor is negligible, we see that a large f-factor is obtained if the momentum of the zero point motion of the particle is large compared to the momentum of the gamma ray. Physically, this means that if the particle has a large uncertainty in its motion, it can absorb the momentum of the gamma ray without changing its motion very much.

On the other hand, on the wave-wave picture it appeared that to get a large f, the dimensions of the emitting "atom wave" should be small, i.e., that the zero point motion should be small rather than large. This apparent contradiction can be resolved by noting that when zero point motion is large in configuration space, it is small in momentum space and vice versa. This is a manifestation of complementarity.

The process of momentum transfer will now be treated in more detail, since it gives considerable insight into what is happening in the lattice and how the momentum is absorbed. It is of considerable importance that the emission is of one photon, transferred all at once, and not a continuous transfer or emission in a number of little steps.

Let us assume that an atom is oscillating and at some instant there is a change in momentum from $\vec{p}_1$ to $\vec{p}_1 + \Delta\vec{p}$. The final energy E_f is then

$$E_f = E_i + [(2\, \vec{p}_i \cdot \Delta\vec{p})/2m] + \Delta p^2/2m\ ,$$

where E_i is the initial energy ($E_i = p_i^2/2m$).

If the momentum were not transferred all at once, but rather in little pieces, say N pieces, each of magnitude Δp, and if this happened over a time large compared to the period of oscillation, the term linear in p_1 would average out to zero, and the energy transfer could be given by

$$E_f - E_i = N\, (\Delta p)^2/2m = p_\gamma{}^2/2mN\ ,$$

where $p_\gamma = N\Delta p$ is the total momentum transfer, i.e., the momentum of the gamma ray.

If we take the limit where there is a continuous transfer of momentum, $N \to \infty$, and there is zero energy transfer. This is just the adiabatic limit, in which the system must always remain in the same quantum state. There is always a Mössbauer effect, but there is no effect on the lattice. This is in disagreement with the actual situation, where there are always inelastic processes in addition to the Mössbauer line.

The particle-wave picture assumes a continuous adiabatic momentum transfer and is therefore incapable of describing the changes which occur in the lattice as a result of the radiation process.

In the particle-particle picture the momentum transfer happens in one piece, so that

$$E_f - E_i = (2\vec{p}_1 \cdot \vec{p}_\gamma/2m) + (p_\gamma)^2/2m = (2\vec{p}_1 \cdot \vec{p}_\gamma/2m) + R\ .$$

The last term is just the free recoil energy.

Since the first term averages to zero if the lattice is at rest, the average energy transfer is equal to the free recoil energy. This is known to be the case from the quantum mechanical calculation.

This treatment can be generalized by looking at all of the moments of this energy distribution:

$$\langle (E_f - E_i)^n \rangle = \langle [(2\vec{p}_1 \cdot \vec{p}_\gamma/2m) + R]^n \rangle\ .$$

The average must be taken over the distribution of the momentum of the particle. The motion of the particle does not enter into the first moment, but, for the mean square, the motion enters, and gives the usual Doppler broadening. Using the well known result that the probability for transition from an initial state to a final state of a lattice is the square of the matrix element,

$$P_{i\to f} = \left| \langle f \,|\, \exp - (i\, \vec{p}_\gamma \cdot \vec{x}/\hbar) \,|\, i \rangle \right|^2\ ,$$

it is possible to calculate the moments of the energy distribution for the quantum mechanical case. It is then found that an expression can be derived which is the same as that of the classical particle-particle description for the first two moments, i.e., the average plus the mean Doppler width. For the higher moments, which give the shape of the distribution, the quantum mechanical result differs from the classical particle-particle result by terms involving commutators which vanish in the classical limit. Thus in the limit where the lattice can be treated classically, the particle-particle model gives the exact energy distribution.