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The Forced Harmonic Oscillator and the Zero-Phonon Transition of the Mössbauer Effect

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The Heisenberg picture solution of the forced harmonic oscillator is specialized to the case when the force is an impulse, and the result is used to illustrate very simply the zero-phonon feature of the Mössbauer effect.

I. INTRODUCTION

Over the years, the forced harmonic oscillator has received a good deal of attention as a soluble model illustrating various formal techniques as well as various physical processes.[1,2] We wish to show here how it can be used very simply to illustrate the zero-phonon feature of the Mössbauer effect. The phenomenon itself has been extensively reviewed,[3,4] and we therefore only briefly describe a simple version of the problem.

A stationary excited nucleus of excitation energy E decays with the emission of a photon of momentum A. The nucleus thereby acquires a recoil momentum P and a kinetic energy $P^2/2m$. This energy is derived from E and therefore the emitted photon energy A/c is less than E by $P^2/2m$. The situation is different if the nucleus is bound to a crystal lattice. It is then possible for the photon to carry off essentially the entire energy E. The purpose of the present article is to illustrate this feature with the harmonic oscillator. The approach is based on the idea that the effect on the atom due to emission of a photon can be simulated by the application of an impulsive force to the oscillator.[4]

First we shall review the solution of the forced harmonic oscillator in the Heisenberg picture. Then we apply the results to the zero-phonon transition.

II. THE FORCED HARMONIC OSCILLATOR[2]

In standard notation, a linear harmonic oscillator subjected to an external time-dependent force $F(t)$ is described by the Hamiltonian

$$H=(P^2/2m)+\tfrac{1}{2}m\omega^2Q^2-QF(t). \qquad (1)$$

By introducing Boson creation and annihilation operators

$$a^+=-i(2m\hbar\omega)^{-1/2}(P+im\omega Q);$$
$$a=i(2m\hbar\omega)^{-1/2}(P-im\omega Q), \qquad (2)$$

the Hamiltonian can be cast into the more convenient form

$$H=\hbar\omega(a^+a+\tfrac{1}{2})-(a+a^+)K(t), \qquad (3)$$

where $K(t)=(\hbar/2m\omega)^{1/2}F(t)$. The energy of the oscillator, of course, is not H but

$$H_0=(P^2/2m)+\tfrac{1}{2}m\omega^2Q^2=\hbar\omega(a^+a+\tfrac{1}{2}). \qquad (4)$$

It is easily verified from the equation of motion

$$i\hbar\dot{a}=[a,H]=\hbar\omega a-K(t) \qquad (5)$$

that in the Heisenberg picture

$$a(t)=\exp(-i\omega t)[a(0)+\xi(t)], \qquad (6)$$

where

$$\xi(t)=\frac{i}{\hbar}\int_0^t \exp(i\omega\tau)K(\tau)\,d\tau. \qquad (7)$$

Now it is well known, that associated with the operators $a^+(0)$, $a(0)$ is a complete orthonormal set of vectors $\{\phi_m\; m=0, 1, 2\cdots\}$, satisfying

$$a^+(0)a(0)\phi_m = m\phi_m;$$
$$a^+(0)\phi_m = (m+1)^{1/2}\phi_{m+1};$$
$$a(0)\phi_m = (m)^{1/2}\phi_{m-1}. \tag{8}$$

Similarly associated with the pair $a^+(t)$, $a(t)$ is a complete orthonormal set $\{\psi_m\}$, satisfying

$$a^+(t)a(t)\psi_m = m\psi_m;$$
$$a^+(t)\psi_m = (m+1)^{1/2}\psi_{m+1}$$
$$a(t)\psi_m = (m)^{1/2}\psi_{m-1}. \tag{9}$$

In particular, $a(t)\psi_0 = 0$, and hence by (6),

$$a(0)\psi_0 = -\xi(t)\psi_0. \tag{10}$$

Thus ψ_0 is a "coherent" state and we may take[2]

$$\psi_0 = \exp(-\tfrac{1}{2}\mid\xi(t)\mid^2)\sum_{m=0}^{\infty}\frac{[\xi(t)]^m}{(m!)^{1/2}}\phi_m. \tag{11}$$

Using (9) it is then possible to determine ψ_1, ψ_2, etc. ϕ_m and ψ_m are of course eigenstates of $H_0(0)$ and $H_0(t)$, respectively, corresponding to the eigenvalue $\hbar\omega(m+\frac{1}{2})$. In the language of lattice dynamics, such states would be said to contain m "phonons," each phonon being a quantum of energy of magnitude $\hbar\omega$.

III. ILLUSTRATION OF ZERO-PHONON TRANSITION

We now choose $F(t) = A\delta(t-\lambda)$, where $\lambda > 0$ and δ is the Dirac delta function. As mentioned in the Introduction, we suppose this corresponds to the impulsive force exerted on the bound atom by the emission of a photon. We wish to calculate the probability that after the impulse, the oscillator has the same energy as before. For simplicity we assume the oscillator is in its ground state ϕ_0. Thus we require the probability that at time $t>\lambda$, the energy is $\frac{1}{2}\hbar\omega$ or, in other words, that the oscillator be in the ground state ψ_0 of $H_0(t)$. Substituting for F in (3) and then (7) we find $\xi(t) = i(2m\hbar\omega)^{-1/2}A\exp(i\omega\lambda)\,(t>\lambda)$ and hence the required probability is by (11),

$$|(\psi_0, \phi_0)|^2 = \exp(-\mid\xi(t)\mid^2)$$
$$= \exp(-A^2/2m\hbar\omega). \tag{12}$$

Thus there is a nonvanishing probability that the impulse creates no phonons. In terms of photon emission this situation corresponds to the fact that the emitted photon takes with it essentially the whole energy E_0. It must be remembered that in the present model one is dealing with a particle bound to a fixed center and the vectors ϕ_m, ψ_m do not correspond to a definite particle momentum.

We now calculate the average momentum transfer for $t>\lambda$. By inverting (2) we find $P = -i(m\hbar\omega/2)^{1/2}(a-a^+)$. Hence $(\phi_0, P(0)\phi_0) = 0$ and for $t>\lambda$,

$$(\phi_0, P(t)\phi_0) = -i(m\hbar\omega/2)^{1/2}(\phi_0, [a(t)-a^+(t)]\phi_0)$$
$$= A\cos\omega(t-\lambda). \tag{13}$$

Similarly the average transfer of energy for $t>\lambda$ is

$$(\phi_0, [H_0(t)-H_0(0)]\phi_0) = A^2/2m \tag{14}$$

which is just the energy the particle would have if it recoiled freely.

There is of course no inconsistency between Eq. (14) and the remarks following Eq. (12). For a single oscillator it is possible that no change of energy occurs but for an ensemble of oscillators there will be an average increase of $A^2/2m$.

Finally, we should mention that it is possible to calculate exactly the probability of no change in energy when the oscillator is at temperature T, thereby yielding the corresponding Debye–Waller factor. However, as this does not contain any unusual features, we shall not do so here.

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