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Radiation damping in an anharmonic oscillator

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Abstract. The effect of radiation damping in an anharmonic oscillator has been calculated using the technique of Kryloff and Bogoliuboff. It is found that the intensity distribution of the emitted spectral line is asymmetric about its intensity maximum. The index of asymmetry agree with the experimental data on x-ray $K_{\alpha_{1,2}}$ lines.

Keywords. Anharmonicity; radiation damping; Fourier analysis; index of asymmetry and spectral lines.

1. Introduction

The inclusion of the effects due to radiation damping in the classical electronic simple harmonic oscillator gives rise to a symmetrical broadening of the emitted spectral line (Sneddon 1951, Breene 1964, Blokhin 1957). To summarize briefly the governing equation for such an oscillator is

$$x'' = -\omega_0^2 x + 2\sigma x''', \tag{1}$$

where $\sigma = q^2/3mc^3 = 3\cdot 16 \times 10^{-24}$ sec, q and m being the charge and mass of the electron and c the velocity of light, and ω_0 is the frequency of the undamped oscillations. Sneddon (1951) and Breene (1954) simplified the above differential equation on the assumption that the contribution due to the term $2\sigma x'''$ is very small as compared to the other terms so that $x'' + \omega_0^2 x$ itself is negligibly small and subsequently estimated x''' in eq. (1) from $x'' + \omega_0^2 x = 0$ as $x''' = -\omega_0^2 x'$. This assumption leads to

$$x'' + 2bx' + \omega_0^2 x = 0, \tag{2}$$

where $b = \sigma\,\omega_0^2$. It may be noted that for $\lambda = 1$Å, $\omega_0 = 1\cdot 8 \times 10^{19}$ sec^{-1} and $b = 10^{15}$ sec^{-1}. The solution of this equation, under the condition $b \ll \omega_0$ is

$$x = a_0 \exp(-bt) \exp(i\omega_0 t), \tag{3}$$

where a_0 is a constant. A simple Fourier analysis (Breene 1964) of eq. (3) leads to the following expression for the shape of the spectral line:

$$I = \frac{I_m}{1 + \left(\frac{\omega - \omega_0}{b}\right)^2}\ , \tag{4 a}$$

where

$$I_m = \frac{q^2\omega_0^4 a_0^2}{6\pi^2 c^3 b^2} = \frac{3m^2c^3}{2\pi^2 q^2}\, a_0^2. \tag{4 b}$$

Equation (4 *a*) is graphically shown in figure 1 for $b = 10^{15}$ sec^{-1}. It has the maximum of intensity at $\omega = \omega_0$ and half-maximum at $\omega = \omega_0 \pm b$, and is symmetrical in shape.

The object of the present paper is to mathematically investigate the effects due to radiation damping in an anharmonic oscillator and to determine the modified natural shape of the spectral line. The governing equation for the anharmonic oscillator is simplified under the hypothesis of Sneddon, and the resulting nonlinear equation is solved in the first approximation by the Kryloff-Bogoliuboff (1947) technique in section 2. It is shown in section 3 that the intensity distribution of the emitted spectral line is asymmetric about its intensity maximum.

2. The damped anharmonic oscillator

The governing equation for an anharmonic oscillator in the presence of radiation damping is

$$x'' = -\omega_0^2 x - \alpha x^2 - \beta x^3 + 2\sigma x''', \tag{5}$$

where α and β are real anharmonicity parameters. Moreover, we are only interested in those physical situations where the anharmonic terms produce minor quantitative effects (Landau and Lifshitz 1960). Following Sneddon (1951), we assume that the contribution of the term $2\sigma x'''$ is small as compared to other terms in eq. (5), and estimate x''' from the equation

$$x'' = -\omega_0^2 x - \alpha x^2 - \beta x^3, \tag{6}$$

as

$$x''' = -\omega_0^2 x' - 2\alpha x x' - 3\beta x^2 x',$$

so that eq. (5) assumes the form

$$x'' = -\omega_0^2 x - \alpha x^2 - \beta x^3 - 2bx' - 2\sigma(2\alpha x x' + 3\beta x^2 x'), \tag{7}$$

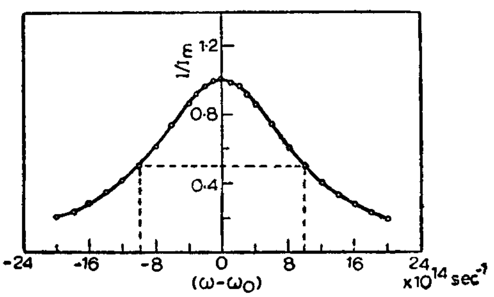


Figure 1. Shape of the spectral line emitted from a harmonic oscillator.

where $b = \sigma\, \omega_0^2$. In essence, the above is roughly equivalent to the assumption that the radiation damping effects perturb the equation of an undamped anharmonic oscillator negligibly so that x''' can be estimated from eq. (6). It is to be noted here that since the contributions of the anharmonic terms is also small we could estimate x''' from the equation $x'' = -\,\omega_0^2 x$ also, though such an estimation is certainly not the most desired one since it does not take care of the anharmonic character of the oscillator.

2.1. *Inadequacy of the method of Landau and Lifshitz*

One may recall that Landau and Lifshitz (1960) solved eq. (6), the equation for an undamped anharmonic oscillator, by the method of successive approximations up to third order and found that the frequency of such an oscillator is amplitude-dependent in general. Their solution for eq. (6) is

$$x = a\cos\omega t + \left(-\frac{\alpha a^2}{2\,\omega_0^2} + \frac{\alpha a^2}{6\,\omega_0^2}\right)\cos 2\,\omega t$$

$$+ \frac{a^3}{16\,\omega_0^2}\left(\frac{\alpha^2}{3\,\omega_0^2} - \frac{\beta}{2}\right)\cos 3\omega t + \ldots \tag{8}$$

with

$$\omega = \omega_0 + \left(\frac{3\beta}{8\omega_0} - \frac{5\alpha^2}{12\omega_0^3}\right) a^2 + \ \ldots \tag{9}$$

However, with the effects of radiation damping included in the mathematical analysis, the amplitude is expected to be time-dependent. Thus the frequency of the damped anharmonic oscillator is also expected to be time-dependent because of the amplitude-dependence of the former. The method of successive approximations is inadequate to meet such situations, for the integration with respect to t of some function of ω and t, say $g\ (\omega, t)$, cannot be performed without prior knowledge of explicit relation between ω and t. Moreover, the convergence of the successive approximations to the actual solution can possibly be guaranteed only in very restricted situations.

For these reasons we have adopted the method of Kryloff and Bogoliuboff (1947) in which the time-dependence of frequency is taken care of.

2.2. *Solution by the method of Kryloff and Bogoliuboff*

We write eq. (7) in the form

$$x'' + \omega_0^2 x + \epsilon f(x, x') = 0, \tag{10}$$

where

$$\epsilon f(x, x') = \alpha x^2 + \beta x^3 + 2bx' + 2\sigma\,(2\alpha x x' + 3\beta x^2 x'). \tag{11}$$

In eq. (10) ϵ is a parameter characterizing the smallness of the deviation of $\omega_0^2 x + \epsilon f(x, x')$ from the purely harmonic term $\omega_0^2 x$. For $\epsilon = 0$, the eq. (10) has the solution

$$x = a\cos(\omega_0 t + \phi), \tag{12}$$

where a and ϕ are constants. For $\epsilon \neq 0$, we consider a and ϕ as new unknown functions of time which are to be so determined that eq. (12) becomes a solution of eq. (10). The Kryloff–Bogoliuboff method leads to the following equations for a and ϕ in the first approximation:

$$\frac{da}{dt} = \frac{\epsilon}{2\pi\omega_0} \int_0^{2\pi} f(a\cos\theta, -a\omega_0 \sin\theta) \sin\theta \, d\theta,$$

$$\frac{d\phi}{dt} = \frac{\epsilon}{2\pi a\omega_0} \int_0^{2\pi} f(a\cos\theta, -a\omega_0 \sin\theta) \cos\theta \, d\theta.$$

For $\epsilon f(x, x')$ given by eq. (11), the above equations lead to

$$\frac{da}{dt} = -b\left(a + \frac{2\kappa}{\omega_0} a^3\right), \tag{13 a}$$

$$\frac{d\phi}{dt} = \kappa a^2, \tag{13 b}$$

where $\kappa = 3\beta/8\omega_0$. The solutions of eqs (13 *a*) and (13 *b*) with the initial conditions of $a = a_0$ and $\phi = 0$ at $t = 0$, are respectively given by

$$a(t) = a_0 \exp(-bt) \left[1 + \frac{2\kappa a_0^2}{\omega_0} (1 - \exp(-2bt)\right]^{-1/2}, \tag{14 a}$$

$$\phi(t) = \frac{\omega_0}{4b} \ln\left[1 + \frac{2\kappa a_0^2}{\omega_0} (1 - \exp(-2bt))\right]. \tag{14 b}$$

The solution of eq. (7) is, therefore,

$$x(t) = a(t) \cos\{\omega_0 t + \phi(t)\},$$

which, for convenience in further calculations, is written in the exponential form as

$$x = a \exp i(\omega_0 t + \phi), \tag{15}$$

where a and ϕ are given by eqs (14 *a*) and (14 *b*) respectively.

The expression (14 *a*) for the amplitude of the oscillator clearly shows that the life-time (Breene 1964) of this oscillator, correct to the order of 10^{-3}, is given by $1/(2b)$ which is the same as that of the corresponding damped harmonic oscillator.

2.3. *Fourier analysis of the solution for the damped anharmonic oscillator*

The motion of the electron as given by eq. (15) is not simple harmonic but can be represented as a superposition of infinite number of continuously varying (in ω) harmonic terms, *i.e.*, as a Fourier integral

$$x(t) = \int_{-\infty}^{\infty} x(\omega) \exp(i\omega t) \, d\omega, \tag{16}$$

The radiation of frequency characteristic of each of these terms is then emitted with an intensity proportional to the square of its amplitude-density, *i.e.*, $|x(\omega)|^2$. The amplitude-density is given as the Fourier transform of eq. (16):

$$x(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} x(t) \exp(-i\omega t)\, dt.$$

Since for $-\infty < t < 0$, $x(t) = 0$; and for $0 \leqslant t < \infty$, $x(t)$ is given by eq. (15), we have

$$x(\omega) = \frac{1}{2\pi} \int_{0}^{\infty} a(t) \exp i\{\omega_0 t + \phi(t)\} \exp(-i\omega t)\, dt$$

$$= \frac{a_0}{2\pi} \int_{0}^{\infty} \exp - \{b + i(\omega - \omega_0)\}\, t$$

$$\times \exp\left(-\frac{1}{2} + \frac{i\omega_0}{4b}\right) \ln\left\{1 + \frac{2\kappa a_0^2}{\omega_0}(1 - \exp(-2bt))\right\} dt. \tag{17}$$

This is the expression for the amplitude-density in the first approximation under the assumptions made above. It is obviously a complicated task to exactly evaluate the value of this infinite integral. Therefore we calculate the value of this integral on the basis of certain physically relevant approximations without essentially loosing any of its characteristics.

In the limiting case when radiation damping is absent, we note that

$$\lim_{b \to 0} a(t) = a_0, \quad \lim_{b \to 0} \psi(t) = \kappa a_0^2 t,$$

so that the solution to undamped anharmonic oscillator is given by

$$x = a_0 \cos(\omega_0 + \kappa a_0^2)\, t.$$

Thus $\omega_0 + \kappa a_0^2$ is the modified frequency of an undamped anharmonic oscillator. In the framework of our analysis, the anharmonic terms produce only minor quantitative effects and so it can be safely assumed that

$$|\kappa a_0^2| \ll \omega_0.$$

Under this condition we expand the logarithm, and retain only first order terms in $\kappa a_0^2/\omega_0$, so that

$$x(\omega) = \frac{a_0}{2\pi} \int_{0}^{\infty} \exp - \{b + i(\omega - \omega_0)\}\, t$$

$$\times \exp\left(-\frac{1}{2} + \frac{i\omega_0}{4b}\right) \left\{\frac{2\kappa a_0^2}{\omega_0}(1 - \exp(-2bt))\right\} dt.$$

The integrand in the above expression converges to zero as $t \to \infty$. Therefore we break up the entire range of integration into two parts: namely (i) from

$t = 0$ to $t = 1/2b$, the life-time of the oscillator, and (ii) from $t = 1/2b$ to $t \to \infty$. In the integrand over part (i) we make the small bt approximation and replace $\exp(-2bt)$ by $(1 - 2bt)$ to simplify the integrand. However, we remark that we do not apply this approximation to the term $\exp(-bt)$ occurring in this part since this integral can now be evaluated without doing so. In the integrand over part (ii) we make large bt approximation and replace $\exp(-2bt)$ by zero. These approximations lead to

$$x(\omega) = \frac{a_0}{2\pi}\left[\int_0^{\frac{1}{2b}} \exp\left[-\left\{\left(b + \frac{2b\kappa a_0^2}{\omega_0}\right) + i(\omega - \omega_0 - \kappa a_0^2)\right)\right\}t\, dt\right.$$
$$+ \exp\left(-\frac{\kappa a_0^2}{\omega_0} + i\frac{\kappa a_0^2}{2b}\right)$$
$$\left.\times \int_{\frac{1}{2b}}^{\infty} \exp\left(-\{b + i(\omega - \omega_0\}\, t\, dt\right)\right]$$

Direct integration yields

$$x(\omega) = \frac{a_0}{2\pi}\left[\frac{b + i(\omega - \omega_0) + \kappa a_0^2\left(\frac{2b}{\omega_0} - i\right)}{\{b + i(\omega - \omega_0)\}}\; \frac{A}{B}\right]$$

where

$$A = \exp\left[-\left\{\left(\frac{1}{2} + \frac{\kappa a_0^2}{\omega_0}\right) + i\left(\frac{\omega - \omega_0 - \kappa a_0^2}{2b}\right)\right\}\right]$$

$$B = \left\{b\left(1 + \frac{2\kappa a_0^2}{\omega_0}\right) + i(\omega - \omega_0 - \kappa a_0^2)\right\}.$$

Under the condition $|\kappa a_0^2|/(\omega_0) \ll 1$, this simplifies to

$$x(\omega) = \frac{a_0}{2\pi}\left[\frac{b + i(\omega - \omega_0) + \kappa a_0^2 \exp\left[-\frac{1}{2}\left(\frac{2b}{\omega_0} - i\right)\right]\; C}{\{b + i(\omega - \omega_0)\}\{b + i(\omega - \omega_0 - \kappa a_0^2)\}}\right] \tag{18}$$

where

$$C = \exp\left[-i\left(\frac{\omega - \omega_0 - \kappa a_0^2}{2b}\right)\right].$$

Separation of real and imaginary parts in eq. (18) followed by simple algebra leads to

$$|x(\omega)|^2 = \frac{a_0^2}{4\pi^2}\,\frac{1}{\{b^2 + (\omega - \omega_0)^2\}\{b^2 + (\omega - \omega_0 - \kappa a_0^2)^2\}}$$
$$\times\left[b^2 + (\omega - \omega_0)^2 + \frac{2\kappa a_0^2\, e^{-\frac{1}{2}}}{\omega_0}\left\{(2b^2 - \omega_0(\omega - \omega_0))\right.\right.$$
$$\times \cos\left(\frac{\omega - \omega_0 - \kappa a_0^2}{2b}\right) - b(2\omega - \omega_0)$$
$$\left.\left.\times \sin\left(\frac{\omega - \omega_0 - \kappa a_0^2}{2b}\right)\right\} + (\kappa a_0^2\, e^{-\frac{1}{2}})^2\left(1 + \frac{4b^2}{\omega_0^2}\right)\right].$$

The power radiated by the oscillating electron is, then (Breene 1964),

$$
\begin{aligned}
I &= \frac{2q^2\,\omega_0^4}{3C^3}\,|x\,(\omega)\,|^2 \\
&= I_m \frac{b^2}{\{b^2+(\omega-\omega_0)^2\}\,\{b^2+(\omega-\omega_0-\kappa a_0^2)^2\}} \\
&\quad \times \Big[b^2+(\omega-\omega_0)^2+\frac{2\kappa a_0^2\,e^{-\frac{1}{4}}}{\omega_0}\Big\{(2b^2-\omega_0(\omega-\omega_0)) \\
&\quad \times \cos\left(\frac{\omega-\omega_0-\kappa a_0^2}{2b}\right)-b\,(2\omega-\omega_0)\sin\left(\frac{\omega-\omega_0-\kappa a_0^2}{2b}\right)\Big\} \\
&\quad +(\kappa a_0^2\,e^{-\frac{1}{4}})^2\left(1+\frac{4b^2}{\omega_0^2}\right)\Big],
\end{aligned} \tag{19}
$$

where I_m is given by eq. (4*b*).

3. Discussion

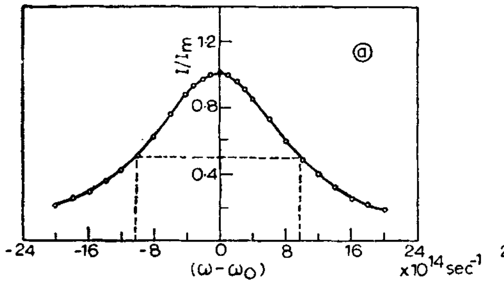
It may be noted that for $\kappa = 0$, *i.e.*, when the anharmonicity is absent, eq. (19) reduces to eq. (4*a*) which represents a symmetrical spectral line. For $\kappa \neq 0$, the right hand side of eq. (19) is a complicated expression and only its graphical analysis can be made.

Let us consider the specific example of a spectral line of wavelength $\lambda = 1$Å, so that $\omega_0 \approx 2 \times 10^{19}$ sec^{-1} and $b = 10^{15}$ sec^{-1} (section 1). The origin of radiation, according to the classical theory, lies in the oscillations of electrons in an atom regarded as a harmonic oscillator. For an atomic anharmonic oscillator, however, no estimates of the values of anharmonicity constants α and β exist in contrast to the molecular anharmonic oscillator on which there is a vast literature. We have, therefore, to make an assumption for the values of these constants keeping consistency with the physical conditions. In a common physical situation it is expected that the values of α and β are such as to make restoring force weaker in the anharmonic oscillator than in the corresponding harmonic oscillator. In fact, at large distances from the equilibrium position, the restoring force is expected to be zero. Hence we expect the frequency of anharmonic oscillations to be smaller than ω_0, the natural frequency of the harmonic oscillations. This leads us to believe that the value of κa_0^2 is negative, its absolute value being much smaller than ω_0. With these considerations in view we have graphically represented eq. (19) in figures (2 *a* and 2*b*) for $\kappa a_0^2 = -10^{14}$ sec^{-1} and -2×10^{14} sec^{-1} respectively.

The most striking feature of the spectral line emitted by the anharmonic oscillator, as is obvious from figures 2*a* and 2 *b*, is that the intensity does not distribute itself symmetrically about the maxima, instead the low frequency tail is slightly stretched out. The index of asymmetry i_a, which is defined as the ratio of the part of the full width at half-maximum on the low-frequency side of the maximum ordinate to the part of the width on the high-frequency side is, for 1Å line, given by

(i) for $\kappa a_0^2 = -10^{14}$ sec^{-1} $\quad i_a = 1{\cdot}04$

(ii) for $\kappa a_0^2 = -2 \times 10^{14}$ sec^{-1} $\quad i_a = 1{\cdot}08$.



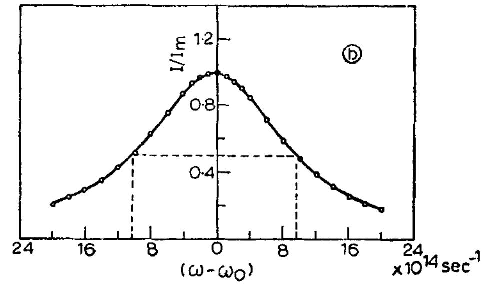


Figure 2. Shape of the spectral line emitted from an anharmonic oscillator, for
(*a*) $\kappa a_0^2 = -10^{14}\,\text{sec}^{-1}$,
(*b*) $\kappa a_0^2 = -2 \times 10^{14}\,\text{sec}^{-1}$.

The x-ray $K_{\alpha_1,2}$ lines emitted by elements having atomic number from $Z = 21$ to $Z = 40$ are asymmetric in shape (Blochin 1957). The wavelengths of the $K_{\alpha_1,2}$ lines emitted by the elements having $Z = 34$ to 36 are in the 1 Å region, and the index of asymmetry for these elements as reported by Blochin (1957) is 1·0 - 1·1. Our values lie fairly close to these experimental observations. The paper thus forms a classical basis for the x-ray spectral line asymmetry.

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