RADIATION OF MULTIPOLES

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Abstract

The radiation of multipoles formed by putting together elementary dipoles is investigated according to the classical theory and wave mechanics. It turns out that the radiations are of two kinds:

The first part has the same frequency as the dipoles and is present only if the multipole structure is present even without vibration.

The second part is always present. If n, the order of the multipole, is even then the frequencies are 2ν, 4ν, up to $n\nu$. If n is odd then the frequencies are ν, 3ν, up to $n\nu$.

The relative intensities of subsequent multipoles are proportional to the square of the ratio: dipole amplitude to wave-length, as has been found in other cases. This calculation would apply to the infrared radiation of molecules.

RECENTLY there have appeared a number of papers on the radiation of higher poles;[1] this radiation seems to explain the presence of forbidden lines.[2] Although e.g. Rubinowicz' paper gives rather complete general formulas for the classical theory, it seems not useless to bring out the physical facts as clearly as possible by considering the case of a combination of linear oscillators, as they are present in molecules like CO_2 (two) or CCl_4 (four).

I. Classical Theory

We consider quadrupoles, but there is no difficulty in generalizing to higher poles. The simplest quadrupole consists of two equal dipoles vibrating in the direction of the line joining them but with opposite phases.

If the direction of vibration is the z-axis, the field of one dipole can best be described by a Hertz-vector Z

$$Z_x = Z_y = 0$$

$$Z_z = Z = a\frac{\cos 2\pi\nu(t - r/c)}{r} \tag{1}$$

$$E = \Delta Z - \frac{1}{c^2}\frac{\partial^2 Z}{\partial t^2}, \quad H = \frac{1}{c}\operatorname{rot}\frac{\partial Z}{\partial t}\cdot \tag{2}$$

If we have now the two dipoles the distance l apart along the Z axis and vibrating with the same amplitude but opposite phase, we will get the re-

[1] I. Placinteanu, Zeits. f. Physik **39**, 276 (1926). A. Rubinowicz, Phys. Zeits. **29**, 817 (1928); Zeits. f. Physik **53**, 267 (1929); **61**, 338 (1930); I. Blaton, Zeits.f.Physik **61**, 263 (1930); I. Bartlett, Phys. Rev. **34**, 125 (1929); A. F. Stevenson, Proc. Roy. Soc. **A128**, 591 (1930); L. Huff and R. W. Houston, Phys. Rev. **36**, 842 (1930).

[2] I. Bowen, Proc. Nat. Ac. **14**, 30 (1928); Astrophys. J. **67**, 1 (1928); R. Frerichs and I. S. Campbell, Phys. Rev. **36**, 1460 (1930).

sultant Hertz vector at any point by taking the difference between the contributions from the two dipoles. The resultant Hertz vector will consist of three parts:

$$Z_2 = -\frac{a \cos 2\pi\nu(t - r/c)}{r} \frac{l}{r} \cos\theta. \tag{3}$$

This part will not contribute to the radiation in distant places on account of the factor l/r

$$Z_2 = 2\pi \frac{a \sin 2\pi\nu(t - r/c)}{r} \frac{l}{\lambda} \cos\theta. \tag{4}$$

This part does give radiation which will represent a spherical wave of the *same frequency* as the one which would be emitted by a dipole, although its intensity varies in a different manner with θ and its amplitude is diminished by the factor $2\pi l/\lambda$. The formula is

$$+ H_\phi = E_\theta = \frac{2\pi l}{\lambda} \cos\theta \left\{ \frac{4\pi^2}{\lambda^2} a \frac{\sin 2\pi\nu(t - r/c)}{r} \sin\theta \right\}. \tag{4a}$$

The total intensity emitted is the fraction $(8\pi^2/5)$ (l^2/λ^2) of that emitted by one dipole.

The third part is the most interesting one; it is always present, even if the two dipoles are not apart ($l = 0$) when at rest, that is to say if there were e.g. two negative charges vibrating on opposite sides of a positive charge with the same position of equilibrium. It arises from the difference of position caused by the vibration itself. That is to say, we have to take r now not as the distance from the point of observation to the dipole, or quadrupole, but to the vibrating charge. If we call the deviation from the equilibrium position in a given moment z', we have to put in (1)

$$r = r_0 + z' \cos\theta \tag{5}$$

and have for the dipole

$$\begin{aligned} Z &= a\frac{\cos 2\pi\nu(t - r_0/c) + 2\pi/\lambda z' \cos\theta \sin 2\pi\nu(t - r_0/c)}{r} \\ &= \frac{a \cos 2\pi\nu(t - r_0/c)}{r} + \frac{2\pi a^2}{\lambda} \cos\theta \frac{\sin 2\pi\nu(t - r/c) \cos 2\pi\nu(t - r/c)}{r} \\ &= \frac{a}{r} \frac{\cos 2\pi\nu(t - r_0/c)}{r} + \frac{2\pi a^2}{\lambda} \frac{\cos\theta}{2} \frac{\sin 2\pi 2\nu(t - r_0/c)}{r}. \end{aligned} \tag{6}$$

If the two dipoles of opposite phase are present, the first member drops out, and we have

$$Z_3 = \frac{2\pi}{\lambda} a^2 \frac{\cos\theta}{r} \frac{\sin 2\pi 2\nu(t - r_0/c)}{r}. \tag{7}$$

That represents a spherical wave, with the same angular distribution as Z_2, but with the *double* frequency and an amplitude proportional to the square of the amplitude of oscillation. The total amount radiated is $(4\pi^2/\lambda_0^2(a^2)2/5)$ times the amount radiated by one dipole.

Generalization to higher poles will give the following result: Assume that we have a pole whose order is n. n is defined in this manner: Let the unit vector $\boldsymbol{p}_i$ indicate the direction of one of the constituent unit dipoles which make up the higher pole. Let $\boldsymbol{r}$ be the unit vector in the direction of observation.

Then a pole of order n is one for which

$$\sum_i (\boldsymbol{p}_i\boldsymbol{r})^{n'} = 0$$

for all $\boldsymbol{r}$ and $n'<n$ and $\sum_i(\boldsymbol{p}_i\boldsymbol{r})^n \neq 0$ for some $\boldsymbol{r}$. In fact the left hand side is a spherical harmonic of order n. With this definition, a dipole has $n=1$, a quadrupole $n=2$, a tetrahedron $n=3$.

Let us now define a vector which will depend only on the orientation of $\boldsymbol{r}$ to a system of coordinates fixed in one pole

$$\boldsymbol{L}_n = \sum_i \boldsymbol{p}_i(\boldsymbol{p}_i\boldsymbol{r})^{n-1}$$

we will need later besides a scalar, defined by

$$\sigma_n = (\boldsymbol{L}_n\boldsymbol{r}')$$

where $\boldsymbol{r}'$ is a unit vector perpendicular to $\boldsymbol{r}$.

We find then two different kinds of radiation.

(1) If there is a "statical" multipole structure of order n and strength p_n present, we get a radiation (Hertz vector) of the same frequency as the frequency of the constituent dipoles, but with the factor

$$\frac{1}{n!}\left(\frac{2\pi}{\lambda}\right)^{n-1} p_n\boldsymbol{L}_n$$

(2) If the multipole has its origin only in the motion (that is if the field in equilibrium corresponds to a pole of higher order), part (1) is absent. But there is always present a radiation with a Hertz vector

$$Z = \frac{1}{n!}\,\frac{a^n}{r}\boldsymbol{L}_n \cos^{n-1}2\pi\nu(t - r/c)\frac{\partial^{n-1}}{\partial r^{n-1}}\cos 2\pi\nu(t - r/c).$$

If n is odd, we have

$$Z = \frac{1}{n!}(-1)^{(n-1)/2}\frac{a^n}{r}\boldsymbol{L}_n\left(\frac{2\pi}{\lambda_0}\right)^{n-1}\cos^n 2\pi\nu(t - (r/c))$$

$$= \frac{(-1)^{(n-1)/2}}{2^{n-1}n!}\,\frac{a^n}{r}\left(\frac{2\pi}{\lambda_0}\right)^{n-1}\boldsymbol{L}_n\left\{\sum_{2s=0}^{2s=n-1}\binom{n}{s}\cos 2\pi(n-2s)\nu(t-(r/c))\right\} \quad (8)$$

If n is even

$$Z = \frac{(-1)^{n/2}}{2^{n-1}n!}\frac{a^n}{r}\left(\frac{2\pi}{\lambda_0}\right)^{n-1} L_n\left\{\sum_0^{2s=n-2}\left(\binom{n}{s}-\binom{n}{s-1}\right)\sin 2\pi(n-2s)\nu(t-(r/c))\right\}. \quad (8a)$$

Accordingly we get radiation which has the frequency $(n-2s)\nu$.

The only similar case where this seems to have been stated explicitly[3] is the case of n equal particles moving equidistant on a circle, which arrangement of course forms a pole of n fold multiplicity.

II. Wave Mechanics

In this case it is simpler to treat absorption instead of emission. The transition to emission is always easily made by using as external field the Landé-Dirac ghost field.

We assume a harmonic oscillator, whose Schrödinger equation is

$$\frac{d^2\psi}{dz^2} - \frac{8\pi^2 M}{h}2\pi^2 M\nu^2 z^2\psi = \frac{4\pi i M}{h}\frac{\partial\psi}{\partial t} \quad (9)$$

with the solution

$$\psi = \sum c_k\psi_k e^{-2\pi i k\nu t}\ \psi_k = e^{-\zeta^2/2}H_k(\zeta)b_n$$

with the abbreviation

$$\zeta = 2\pi\left(\frac{M\nu}{h}\right)^{1/2} z.$$

H_n is a Hermitian polynomial.

$$b_n = \left(2^{-k}\frac{1}{n!}\left(\frac{4\pi M\nu}{h}\right)^{1/2}\right)^{1/2}.$$

If there is now a perturbation function present of the form

$$V = e^{2\pi i s\nu t}v'$$

we find

$$\frac{dc_{k+s}}{dt} = \frac{2\pi i}{h}c_k\int V'\psi_k\psi_{k+s}d\zeta. \quad (10)$$

If we have a light wave polarized parallel to z and propagated parallel to x, its electric field will be

$$E_z = E\cos 2\pi\nu s(t - x/c). \quad (11)$$

The perturbation function is then given in the first case (of a statical multipole structure) by

$$V = \frac{z}{n!}\sigma_n p_n\frac{\partial^{n-1}}{\partial x^{n-1}}E_z$$

[3] J. J. Thomson, Phil. Mag. (VI) **6**, 673 (1903); G. A. Schott, Electromagnetic Radiation, Cambridge 1912, p. 102.

[4] See f. e. E. U. Condon and P. M. Morse, Quantum Mechanics, New York, 1930, p. 47. A. Sommerfeld, Wellenmechanischer Ergänzungsband, Braunschweig 1929 p. 17.

from which we get[5]

$$\frac{dc_{n+s}}{dt} = \frac{2\pi i}{h} c_k \left(\frac{2\pi}{\lambda_0}\right)^{n-1} p_n \sigma_n E \frac{1}{n!} \int z\psi_k \psi_{k+s} dz.$$

The latter integral gives of course the same selection rule as for a dipole $s = \pm 1$ and only modifies the intensity of the absorption by the same factors as in the corresponding classical example.

More interesting is the case arising from the existence of the oscillatory We will put the perturbation function multipole.

$$V = \frac{1}{n!} z^n \sigma_n e \frac{\partial^{n-1}}{\partial x^{n-1}} E_z$$

which leads to

$$\begin{aligned} \frac{dc_{k+s}}{dt} &= \frac{2\pi i}{h} c_k \frac{eE}{n!} \left(\frac{2\pi}{\lambda_0}\right)^{n-1} \sigma_n \left(\frac{1}{2\pi\left(\frac{M\nu}{h}\right)^{1/2}}\right)^{n+1} b_k b_{k+s} I_{k,s}{}^n \\ &= \frac{ic_k}{(\pi M\nu h)^{1/2}} eE \frac{\sigma_n}{n!} \left(\frac{h\nu}{Mc^2}\right)^{(n-1)/2} \frac{1}{2^{k+s/2}(k!(k+s)!)^{1/2}} I_{k,s}{}^n \end{aligned} \tag{12}$$

where

$$I_{k,s}{}^n = \frac{1}{b_k b_{k+s}} \int \zeta^n \psi_k \psi_{k+s} d\zeta = \int \zeta^n e^{-\zeta^2} H_k H_{k+s} d\zeta. \tag{13}$$

To evaluate this integral, we use first the following formula,[6] where an upper index j indicates j fold differentiation in respect to the argument

$$H_k{}^{(1)} = 2kH_{k-1}$$

and therefore

$$H_k{}^{(j)} = 2k\cdot(2k-2)\cdots(2k-2j+2)H_{k-j}. \tag{14}$$

If we write

$$H_k = \sum_i a_i{}^{(k)} \zeta^i$$

we have

$$H_k{}^{(j)}(0) = j!a_j{}^{(k)} = 2^j k(k-1)\cdots(k-j+1)H_{k-j}(0). \tag{15}$$

But on account of the formula[5]

$$H_k = (-1)^k e^{\zeta^2} \frac{d^k}{d\zeta^k} e^{-\zeta^2}$$

[5] Of course, we have been quantizing not the motion of one charge, but of a characteristic vibration (normal coordination). As these are independent (no natural interaction), there are only transitions between different states of the *same* vibration possible, as G. Dieke has kindly pointed out.

we have

$$H_{k-j}(0) = (-1)^{k-j}\left\{\frac{d^{k-j}}{d\zeta^{k-j}}\left(\sum_0^\infty(-1-)^l\frac{\zeta^{2l}}{l!}\right)\right\}_{\zeta=0}$$

$$= 0 \text{ for } k-j \text{ odd}$$

$$= (-1)^{(k-j)/2}\frac{(k-j)!}{\left(\frac{k-j}{2}\right)!} \text{ for } k-j \text{ even}$$

and finally

$$a_i^{(k)} = \frac{k!}{(i!)^2}2^i(-1)^{(k-i)/2}\frac{(k-i)!}{\left(\frac{k-i}{2}\right)!} \text{ for } k-i \text{ even} \tag{16}$$

$$= 0 \text{ for } k-i \text{ odd}.$$

We now use Sommerfeld's method[7]

$$I = \int_{-\infty}^{\infty}\zeta^n\left(\frac{d^{k+s}}{d\zeta^{k+s}}e^{-\zeta^2}\right)H_k d\zeta$$

$$= \int_{-\infty}^{\infty}e^{-\zeta^2}\frac{d^{k+s}}{d\zeta^{k+s}}(\zeta^n H_k)d\zeta$$

$$= \int_{-\infty}^{\infty}e^{-\zeta^2}\frac{d^{k+s}}{d\zeta^{k+s}}\left(\sum_{i=0,1}^{k}a_i^{(k)}\zeta^{i+n}\right)d\zeta$$

$$= 0 \text{ for } k+s > k+n \text{ or } s > n$$

$$= \sum_i \int_{-\infty}^{\infty}a_i^{(k)}(i+n)(i+n-1)\cdots(i+n-k-s)\zeta^{i+n-k-s}e^{-\zeta^2}d\zeta \text{ for } s \leqq n$$

if we now put

$$i+n-k-s = l$$

we have

$$I = \sum_{l=0,1}^{n-s}a_{l+k+s-n}^{(k)}(l+k+s)\cdots l\int_{-\infty}^{\infty}e^{-\zeta^2}\zeta^l ds.$$

The integral is 0 if l is odd and $\pi^{1/2}\frac{(2l)!}{l!2^{2l}}$ if l is even $= 2j$.

Accordingly, we have

$$I_{k,s}^{(n)} = 0 \text{ if } s-n \text{ odd}$$

$$= \pi^{1/2}\sum_{j=0}^{(n-s)/2}\frac{(4j)!}{2^{4j}(2j)!}(2j+k+s)\cdots 2j$$

$$\cdot(-1)^{j+(s-n)/2}2^{2j+k+s+n}k!\frac{(n-s-2j)!}{\left(\frac{n-s}{2}-j\right)!}\frac{1}{(2j+k+s-n)!^2}$$

[6] Condon and Morse, reference 4, p. 50.

[7] Sommerfeld, reference 4, p. 59.

$$= \pi^{1/2}(-1)^{(s-n)/2}2^{k+s-n}\, k!\sum_{j=0}^{q}(-1)^j \frac{(4j)!}{(2j)!^2}\frac{1}{4^j}\,(2j+k+s)!\,\frac{(2q-2j)!}{(q-j)!}\,\frac{1}{(2j+k-q)!^2} \tag{17}$$

with $n-s=2q$.

That means that for n odd the transitions 1, 3, 5 $\cdots n$ and n even the transitions 2, 4, 6, $\cdots n$ are permitted, and accordingly the frequencies ν, 3ν, $5\nu \cdots n\nu$ or 2ν, $4\nu \cdots n\nu$ absorbed and emitted, in analogy to the classical theory. In normal cases, the formula are not as terrible as they look. For example, for $n=2$ (quadrupole) we have $s=2$

$$I_{k,2}{}^{(2)} = (\pi)^{1/2}2^k k!\frac{(k+2)!}{(k!)^2} = (\pi)^{1/2}2^k(k+1)(k+2).$$

If $n=3$ (tetraeder) there are possible two transitions
$s=1$, frequency ν

$$I_{k,1}{}^{(3)} = -(\pi)^{1/2}2^{k+2}k!\left\{\frac{(k+1)!2!}{(k-1)!^2} - \frac{4!}{(2!)^2}\,\frac{1}{4}\,\frac{(k+3)!}{(k+1)!^2}\right\}$$

$$= -(\pi)^{1/2}2^{k+2}\left\{2k^2(k+1) - \frac{1}{4}\,\frac{(k+2)(k+3)}{k+1}\right\}$$

$s=3$ frequency 3ν

$$I_{k,3}{}^{(3)} = (\pi)^{1/2}2^k\frac{k!(k+3)!}{k!^2} = (\pi)^{1/2}(k+1)(k+2)(k+3).$$

In general, we have for $s=n$, frequency $n\nu$

$$I_{kn}{}^{(n)} = (\pi)^{1/2}2^k\frac{k!(k+s)!}{k!^2} = (\pi)^{1/2}2^k(k+1)\cdots(k+2) \tag{18}$$

which will make the factor in (12) proportional to $[k\cdot(k+1)\cdots(k+n)]^{\frac{1}{2}}$ or $k^{n/2}$, if $k \gg n$; this corresponds to the fact that the amplitude of light emitted classically is proportional to a^n as $a^2 \sim k \sim$ the energy of one dipole.

The relative transition probability from $k+s$ to k for a pole of the n order to the same probability of a pole of $(n-1)$ the order is

$$\frac{1}{n}\,\frac{\sigma_n{}^2}{\sigma_n{}^2{}_{-1}}\left(\frac{I^{(n)}{}_{k,s}}{I^{(n-1)}_{k,s}}\right)^2\left(\frac{h\nu}{Mc^2}\right)^{1/2}$$

$h\nu/Mc^2$ is the ratio of the energy of vibration to the intrinsic energy and can be rewritten

$$\frac{M/2\, v_{\max}^2}{Mc^2} = \frac{1}{2}\left(\frac{v_{\max}}{c}\right)^2 = \frac{1}{2}\left(\frac{2\pi\nu a}{c}\right)^2 = 2\pi^2\left(\frac{a}{\lambda_0}\right)^2.$$

Rubinowicz[2] has found a similar result for atoms.