Electromagnetic radiation and matter

What is an electromagnetic wave?

Electromagnetic waves are produced by the motion of electrically charged particles. These waves are called electromagnetic radiation because they radiate from electrically charged particles. They can travel through vacuum, air, as well as other substances.

\[ \lambda \nu = c \]

\[ \tilde{\nu} = 1/\lambda \]

\[ E = h\nu \]

\[ c = 3 \times 10^8 \text{ m.s}^{-1} \]

http://www.colorado.edu/physics/2000/waves_particles/
Can one use radiowaves to look at proteins? How about x-rays?
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An electromagnetic wave depends on both the electric and magnetic field strength, i.e. as described by Maxwell’s equations

\[ \nabla \times \vec{E}(t) = -\frac{\partial \vec{B}(t)}{\partial t} \]
\[ \nabla \times \vec{H}(t) = \frac{\partial \vec{D}(t)}{\partial t} + \vec{J} \]

\[ \nabla \cdot \vec{D}(t) = \rho \]
\[ \nabla \cdot \vec{B}(t) = 0 \]

\[ \vec{D}(t) = \varepsilon \vec{E}(t) \]
\[ \vec{B}(t) = \mu \vec{H}(t) \]
Electromagnetic quantities:

- $\vec{E}$, Electric Field
- $\vec{H}$, Magnetic Field
- $\vec{D}$, Electric Flux (Displacement) Density
- $\vec{B}$, Magnetic Flux (Induction) Density
- $\vec{J}$, Current Density
- $\frac{\partial \vec{D}}{\partial t}$, Displacement Current

- $\rho$, Charge Density
- $\varepsilon$, Dielectric Permittivity
- $\mu$, Magnetic Permeability
If we model the electron above as a mass on a spring and pull the mass downwards, it will feel a restorative force given by Hooke’s law, namely

$$F = -kx \quad (1.0)$$

where $k$ is the spring constant. The total force will be

$$F = m \frac{d^2x}{dt^2} + kx = 0 \quad (1.1)$$

and the frequency of oscillation is given by

$$\nu = \frac{1}{2\pi} \left( \frac{k}{m} \right)^{1/2} \quad \text{or} \quad \omega = \left( \frac{k}{m} \right)^{1/2} \quad (1.2)$$
Equation 1.1 can be solved to give,

\[ \begin{align*}
    x &= \frac{1}{2} x_0 \left( e^{i\omega(t-t_0)} + e^{-i\omega(t-t_0)} \right) \\
    x &= x_0 \cos[\omega(t-t_0)].
\end{align*} \]  

(1.3)

From this we can calculate the velocity,

\[ v = \frac{dx}{dt} = -\omega x_0 \sin[\omega(t-t_0)] \]  

(1.4)

The total energy of the system is the kinetic energy plus the potential energy,

\[ \begin{align*}
    E &= \frac{1}{2} mv^2 + \frac{1}{2} kx^2 \\
    &= \frac{1}{2} m \left( \omega^2 x_0^2 \sin^2[\omega(t-t_0)] \right) + \frac{1}{2} k x_0^2 \cos^2[\omega(t-t_0)] \\
    &= \frac{1}{2} k x_0^2 \left( \sin^2[\omega(t-t_0)] + \cos^2[\omega(t-t_0)] \right) \\
    &= \frac{1}{2} k x_0^2
\end{align*} \]  

(1.5)

We can also write the energy in terms of momentum \( p = mv \),

\[ E = \frac{p^2 + kx^2}{2m} \]  

(1.6)
For a long time, this classical description was sufficient to describe all observed phenomena. A problem arose when it came time to describe blackbody radiation. In this case, equation 1.6 has to be written in terms of Hamiltonian operators, i.e.

$$E\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + kx^2 \psi = \hat{K}_\psi + \hat{P}_\psi$$

where \(\psi\) is a wavefunction and \(\hbar\) is Planck’s constant. This equation is the Schrödinger equation.

Erwin Schrödinger

Nobel Laureate

1933
As an aside….

What is blackbody radiation? Why can’t it be described classically?

Heated “bodies” radiate – i.e. emit energy
e.g. ring on your stove.

In the previous three slides, we described the generation of electromagnetic waves as an oscillation of the charges. We then modelled this oscillation as a weight on a spring.

\[ F = m \frac{d^2x}{dt^2} + kx = 0 \]

with the frequency of oscillation given by

\[ \nu = \frac{1}{2\pi} \left( \frac{k}{m} \right)^{1/2} \quad \text{or} \quad \omega = \left( \frac{k}{m} \right)^{1/2} \]

This is a harmonic oscillator.
For an example, go to http://www3.adnc.com/~topquark/fun/JAVA/dho/dho.html and run the applet with a damping of zero (and launch). What you see is:

Position $\rightarrow$ cosine function (equation 1.3)

Velocity $\rightarrow$ $\frac{dx}{dt}$ $\Rightarrow$ sine function (equation 1.4)

Energy $\rightarrow$ constant (equation 1.5)
Conclusion:

- The harmonic oscillator can be used to describe EM waves.

Can it describes all types of EM waves? Also those from diatomics, i.e. which arise from the vibration of molecules?
The harmonic oscillator as a model for a diatomic molecule

We can write two equations of motion:

\[ m_1 \frac{d^2 x_1}{dt^2} = k (x_2 - x_1 - l_0) \]  \hspace{1cm} (1.8)

\[ m_2 \frac{d^2 x_2}{dt^2} = -k (x_2 - x_1 - l_0) \]  \hspace{1cm} (1.9)

where \( l_0 \) is the equilibrium length of the spring. These equations indicate that if the spring is stretched, i.e. \( z_2 - z_1 > l_0 \), then the force acting on \( m_1 \) is towards the right and that on \( m_2 \) is towards the left (negative sign).
If we add equations 1.8 and 1.9, we get

$$m_1 \frac{d^2 x_1}{dt^2} + m_2 \frac{d^2 x_2}{dt^2} = 0$$

or

$$\frac{d^2}{dt^2} (m_1 x_1 + m_2 x_2) = 0$$

We can define a center of mass coordinate:

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} = \frac{m_1 x_1 + m_2 x_2}{M}$$

This allows us to write

$$M \frac{d^2 X}{dt^2} = 0$$

which implies that the center of mass moves uniformly in time.
But we are interested in the motion on the two masses, i.e. the relative motion, therefore we need to define a relative coordinate

$$\zeta = x_2 - x_1$$

To write the equation of motion in terms of this relative coordinate, we devide equation 1.8 by $m_1$ and equation 1.9 by $m_2$ and subtract the new equations from each other, i.e.

$$\frac{d^2x_2}{dt^2} - \frac{d^2x_1}{dt^2} = \frac{-k(x_2 - x_1 - l_0) - k(x_2 - x_1 - l_0)}{m_2}$$

$$\frac{d^2x}{dt^2} = \frac{-kx}{m_1 m_2} \left(\frac{1}{m_1} + \frac{1}{m_2}\right) = -kx \left(\frac{m_1 + m_2}{m_1 m_2}\right) = -kx \frac{\mu}{\mu}$$

where $x = \zeta - l_0$ and $\mu$ is the reduced mass. In other words, we have that

$$\mu \frac{d^2x}{dt^2} + kx = 0$$

Reduce a 2 body problem into a 1 body problem
As was done for the harmonic oscillator, we can now determine the potential energy of the system. Recall that previously, we found the potential energy to be $U = \frac{1}{2} kx^2$. We can write a mathematical expansion of the energy for our diatomic molecule by using a Taylor expansion of the potential energy $U(\xi)$ about the equilibrium position $l_0$.

The expansion is:

$$U(\xi) = U(l_0) + \frac{dU}{d\xi}(\xi - l_0) + \frac{1}{2!} \frac{d^2U}{d\xi^2}(\xi - l_0)^2 + \frac{1}{3!} \frac{d^3U}{d\xi^3}(\xi - l_0)^3 + \ldots$$  \hspace{1cm} (2.0)

where each derivative is evaluated at $\xi = l_0$.

To simplify equation 2.0, we can look at the potential energy curve and make a few definitions:

- $\Delta U(\xi) = U(\xi) - U(l_0)$
- $\frac{dU}{d\xi} @ l_0$
As a result, we have

\[ \Delta U(\xi) = \frac{1}{2} k (\xi - l_0)^2 + \frac{1}{6} \gamma (\xi - l_0)^3 + \ldots \] (2.1)

\[ = \frac{1}{2} k x^2 + \frac{1}{6} \gamma x^3 + \ldots \]

If we keep to small displacements of x, we can simplify the equation above to

\[ \Delta U(x) = \frac{1}{2} k x^2 \]

which is a quadratic equation.

As you can see from the graph, this equation is a good estimate for small x.
At this point: We can describe EM waves – but in order to describe e.g. scattering – we need to introduce two more concepts

1- DAMPED

2- DRIVEN
We can now take our weight on a spring and submerge the entire system in a viscous medium:

The force will therefore contain an additional term due to friction,

\[ F = m \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = 0 \]

This is a damped harmonic oscillator.

As before, it can be shown that a solution to this equation is:

\[ x = \exp\left\{-\frac{f}{2m}t\right\} \cos(\omega'(t-t_0)) \]

with \( \omega' = \sqrt{\frac{k}{m} - \left(\frac{f}{2m}\right)^2} \) \hspace{1cm} (1.7)
Proof:

1. \[ \frac{d}{dt}(e^{au}) = a \cdot e^{au} \cdot \frac{du}{dt} \]

2. \[ \frac{d}{dt}(\sin u) = \cos u \cdot \frac{du}{dt} \]

General:

\[ \frac{d}{dt}(\cos u) = -\sin u \cdot \frac{du}{dt} \]

\[ x = e^{-\frac{ft}{2m}} \cos(\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2} + \omega t m) \quad \text{with} \quad \omega = \sqrt{\frac{k}{m} - \left(\frac{F}{2m}\right)^2} \]

\[ \frac{dx}{dt} = \frac{d}{dt} \left\{ e^{-\frac{ft}{2m}} \cdot \cos[\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2} + \omega t m] \right\} + e^{-\frac{ft}{2m}} \frac{d}{dt} \left\{ \cos[\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2}] \right\} \]

\[ = \left( -\frac{f}{2m} e^{-\frac{ft}{2m}} \right) \cdot \cos[\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2}] + e^{-\frac{ft}{2m}} \left\{ -\omega \sin[\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2}] \cdot \omega \right\} \]

\[ \therefore \frac{dx}{dt} = -\frac{f}{2m} e^{-\frac{ft}{2m}} \cdot \cos[\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2}] \cdot \omega - \omega^2 e^{-\frac{ft}{2m}} \sin[\sqrt{\omega^2 - \left(\frac{F}{2m}\right)^2}] \]
\[ \frac{d^2x}{dt^2} = \frac{d}{dt} \left( \frac{dx}{dt} \right) \]

\[ = \left( -\frac{f}{2m} \right) \frac{d}{dt} \left( e^{-\frac{ft}{2m}} \right) \cos \left( \omega \left( t - t_0 \right) \right) \]

\[ - \left( \frac{f}{2m} \right) e^{-\frac{ft}{2m}} \frac{d}{dt} \left\{ \sin \left( \omega \left( t - t_0 \right) \right) \right\} \]

\[ - \omega \frac{d}{dt} \left\{ e^{-\frac{ft}{2m}} \right\} \sin \left( \omega \left( t - t_0 \right) \right) \]

\[ - \omega \frac{d}{dt} \left\{ e^{-\frac{ft}{2m}} \right\} \cos \left( \omega \left( t - t_0 \right) \right) \]

\[ \therefore \frac{d^2x}{dt^2} = \left( -\frac{f}{2m} \right)^2 e^{-\frac{ft}{2m}} \cos \left( \omega \left( t - t_0 \right) \right) + \left( \frac{f}{2m} \right) e^{-\frac{ft}{2m}} \sin \left( \omega \left( t - t_0 \right) \right) \cdot \omega \]

\[ + \omega \cdot f \cdot \frac{d}{dt} \left\{ e^{-\frac{ft}{2m}} \right\} \sin \left( \omega \left( t - t_0 \right) \right) - \omega \cdot e^{-\frac{ft}{2m}} \cos \left( \omega \left( t - t_0 \right) \right) \cdot \omega \]

Putting everything together:

\[ m \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = 0 \]
\[ kx = k \cdot e^{-ft/2m} \cdot \cos[w'(t-t_0)] \]

\[ + \int \frac{dx}{dt} = -\frac{f^2}{2m} e^{-ft/2m} \cdot \cos[w'(t-t_0)] - \frac{1}{2} w' e^{-ft/2m} \cdot \sin[w'(t-t_0)] \]

\[ + \frac{md^2x}{dt^2} = \frac{f^2}{4m} e^{-ft/2m} \cdot \cos[w'(t-t_0)] + \frac{1}{2} w' e^{-ft/2m} \cdot \sin[w'(t-t_0)] \]

\[ + \frac{f}{2} w' e^{-ft/2m} \cdot \sin[w'(t-t_0)] - m(w')^2 e^{-ft/2m} \cdot \cos[w'(t-t_0)] \]

\[ m \cdot \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = e^{-ft/2m} \cdot \cos[w'(t-t_0)] \left\{ k - \frac{f^2}{2m} + \frac{f^2}{4m} - m \left( \frac{k}{m} - \frac{f^2}{2m} \right) \right\} \]

\[ m \cdot \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = e^{-ft/2m} \cdot \cos[w'(t-t_0)] \left\{ k - \frac{f^2}{4m} + k + \frac{f^2}{4m} \right\} \]

\[ m \cdot \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = 0 \]
For an example, go to http://www3.adnc.com/~topquark/fun/JAVA/dho/dho.html and run the applet with a damping of 0.06, 0.12, 0.24, 0.32, 0.5, and 1.8 (using launch after each increase in damping). What you see is:

Position $\rightarrow$ exponential decay $\times$ cosine function  \hspace{1cm} (equation 1.7)

Velocity $\rightarrow$ ???

Energy $\rightarrow$ ???
Driven harmonic oscillators

Up to this point, we have considered both undamped and damped harmonic oscillators. In both cases, no driving (additional) force was applied, i.e.

\[ F = ma + kx = 0 \]  \hspace{1cm} \text{harmonic}

\[ F = ma + fv + kx = 0 \]  \hspace{1cm} \text{damped harmonic}

In the following section, we will see what effect applying a driving force has on the system. We are interested in doing this because the interaction of radiation with matter is described by a driven and damped harmonic oscillator.

Let us consider a driving force of \( F_0 \cos(\omega t) \). What will the equation of force be?

\[
\frac{md^2x}{dt^2} + f\frac{dx}{dt} + kx = F_0 \cos(\omega t)
\]

Example:

http://webphysics.ph.msstate.edu/javamirror/explrsci/dswmedia/drivosc.htm
A solution to this equation is:

\[ x = x' \cos(\omega t) + x'' \sin(\omega t) \]

with

\[ x' = \frac{F_0 \, m \left( \omega_0^2 - \omega^2 \right)}{m^2 \left( \omega_0^2 - \omega^2 \right)^2 + f^2 \omega^2} \]

and

\[ x'' = \frac{F_0 \, f \, \omega}{m^2 \left( \omega_0^2 - \omega^2 \right)^2 + f^2 \omega^2} \]

with \( \omega_0 = \left( \frac{k}{m} \right)^{\frac{1}{2}} \) is the frequency of the mass, and \( \omega \) is the frequency of the driving force (example – the sinusoidal box on web site).
Proof:

\[ x = x' \cos(wt) + x'' \sin(wt) \]

\[ \frac{dx}{dt} = -x'w \sin(wt) + x''w \cos(wt) \]

\[ \frac{d^2x}{dt^2} = -x'w^2 \cos(wt) - x''w^2 \sin(wt) \]

\[ m \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = -mx'w^2 \cos(wt) - mx''w^2 \sin(wt) \]

\[ -fx'w \sin(wt) + fx''w \cos(wt) \]

\[ + kx' \cos(wt) + kx'' \sin(wt) \]

Grouping the terms in \( \sin(wt) \) and \( \cos(wt) \) together yields

\[ m \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = \cos(wt) \left\{ fwx'' + kx' - mx'w^2 \right\} \]

\[ + \sin(wt) \left\{ kx'' - fx'w - mx''w^2 \right\} \]
Expanding \( \alpha \) and using the definition \( k = \omega_0^2 \cdot m \),

\[
f \omega x'' + kx' - mx' \omega^2 = \frac{F_0 (f \omega)^2}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} + \frac{F_0 \omega_0^2 m^2 (\omega_0^2 - \omega^2)}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} \]

\[
- \frac{F_0 m^2 \omega^2 (\omega_0^2 - \omega^2)}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2}
\]

\[
= F_0 \left\{ \frac{f^2 \omega^2 + m^2 (\omega_0^2 - \omega^2)(\omega_0^2 - \omega^2)}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} \right\}
\]

\[
i_1 = F_0
\]

Similarly for \( \omega \):

\[
kx'' - f \omega x' - m \omega^2 x'' = \frac{F_0 f \omega \omega_0^2 m}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} - \frac{F_0 f \omega m (\omega_0^2 - \omega^2)}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} \]

\[
- \frac{F_0 f^2 m \omega^2}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2}
\]

\[
= F_0 f m \left\{ \frac{\omega_0^2 \omega - \omega \omega_0^2 + \omega^3 - \omega^3}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} \right\} = 0
\]

\[
m \frac{d^2x}{dt^2} + f \frac{dx}{dt} + kx = F_0 \cos(\omega t)
\]
Two conditions are important:

Scattering limit:
\[ m^2(\omega_0^2 - \omega^2)^2 >> f^2 \omega^2 \]

\[
\begin{align*}
    x' &= \frac{F_0 m (\omega_0^2 - \omega^2)}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2} \\
    x'' &= \frac{F_0 f \omega}{m^2 (\omega_0^2 - \omega^2)^2 + f^2 \omega^2}
\end{align*}
\]

Resonance limit:
\[ \omega_0 \sim \omega \]

\[
\begin{align*}
    x' &= \frac{F_0 (\omega_0 - \omega) \tau^2}{2m\omega_0 [1 + (\omega_0 - \omega)^2 \tau^2]} \\
    x'' &= \frac{F_0 \tau}{2m\omega_0 [1 + (\omega_0 - \omega)^2 \tau^2]}
\end{align*}
\]

where \( \tau = \frac{2m}{f} \)