The Physical Basis of Spectroscopic Methods

1. Wave Nature of Matter

Diffraction of a wave

X-ray diffraction pattern of DNA (observed by Rosalind Franklin, 1920-1958)

Interaction of waves, e.g. visible light, x-rays, with ordered matter gives rise to scattering and diffraction patterns.

From the pattern produced the structure of the matter can be deduced.
How is a diffraction pattern produced?

a) X-ray scattering from a single electron

\[ \text{Incident light, } I_0 \]

\[ \text{Scattered light, } I_{sca} \]

\[ \text{Interference } \rightarrow \text{ Diffraction Pattern} \]

b) X-ray scattering from two electrons

\[ \text{Incident light, } I_0 \]

\[ \text{Scattered light, } I_{sca} \]

\[ \text{Interference } \rightarrow \text{ Diffraction Pattern} \]
Diffraction pattern of a crystal (yeast phenylalanine tRNA)

Experimental of the measurement of x-ray diffraction from a crystal
Diffraction is a wave phenomenon

Diffraction pattern observed from an electron beam scattered by aluminium foil

→ Electrons behaving as waves (C. J. Davisson, L. H. Germer and G. P. Thomson, 1927)

Matter has wave properties!

Wavelength, $\lambda$, of a matter wave (de Broglie equation),

$$\lambda = \frac{h}{mv} \quad (1.1)$$

$h$ = Planck's constant, $6.6 \times 10^{-34}$ J s
$m$ = mass of the particle (kg)
$v$ = velocity of the particle (m s$^{-1}$)
The amplitude of an electron matter wave is known as the wavefunction, $\psi$ (Schrödinger, 1887-1961).

What is the physical meaning of the wavefunction?

Consider the molecular ion, HeH$^{2+}$.

The electron density at a point, $(x, y, z)$ is given by the square of the wavefunction at that point:

$$[\psi(x,y,z)]^2$$

The probability of finding an electron in a small volume, $\Delta v$, around the point $(x,y,z)$ is:

$$[\psi(x,y,z)]^2 \cdot \Delta v$$
Practical application: Electronmicroscope

The discovery that electrons have wave properties led to the idea of using an electron beam instead of light in a microscope.

Ernst Ruska, inventor of the first electronmicroscope (1931, Berlin). Nobel prize for Physics, 1986.

The maximum resolution of a microscope is approximately equal to the wavelength of the radiation used.

For a light beam, $\lambda \approx 300$-800 nm.

What is the resolution of an electronmicroscope?
Design of a transmission electron microscope (TEM)

The wavelength of the electron beam depends on the magnitude of the electrical potential difference through which the electrons are accelerated.

Decrease in potential energy = eV  
Increase in kinetic energy = $\frac{1}{2} mv^2$
\[ eV = \frac{1}{2}mv^2 \quad (1.2) \]

\[ \Rightarrow \quad v = \frac{\sqrt{2eV}}{m} \quad (1.3) \]

Now the wavelength of the electron beam from the de Broglie equation is given by,

\[ \lambda = \frac{\hbar}{mv} \]

Substituting in the velocity from equation (1.3) yields,

\[ \lambda = \frac{\hbar}{\sqrt{2eVm}} \quad (1.4) \]

\[ m = \text{mass of an electron} = 9.1 \times 10^{-31} \text{ kg} \]
\[ e = \text{charge of an electron} = 1.6 \times 10^{-19} \text{ C} \]

What is the theoretical maximum resolution of an electron microscope when using an "electron gun" with a voltage of 100 V?
Virus particle
Mitochondrion

- Inner Membrane
- Folded into Cristae
- Outer Membrane
- Matrix