University of Babylon
College of Sciences
Department of Chemistry
Course No. Chsc 424

Undergraduate Studies
Physical chemistry
Fourth-year - Semester 1
The scholar year 2024-2025

Lectures of Quantum mechanics of Chemistry

Prof. Dr. Abbas A-Ali Drea

Lecture No. 5: Mechanics of Wave Motion

Introduction:

A wave is an oscillation accompanied by a transfer of energy that travels through a medium (space or mass). Frequency refers to the addition of time. Wave motion transfers energy from one point to another, which displace particles of the transmission medium–that is, with little or no associated mass transport.

Waves have consisted of oscillations or vibrations (of a physical quantity), around almost fixed locations.

There are two main types of waves:-

1-Mechanical waves propagate through a medium, and the substance of this medium is deformed. Restoring forces then reverse the deformation. For example, sound waves propagate via air molecules colliding with their neighbors.

2-Electromagnetic waves, do not require a medium. It is consist of periodic oscillations of electrical and magnetic fields. It is generate by charged particles, and can therefore travel through a vacuum.

1-Wave motion:

A wave can be transverse through oscillations that are perpendicular to the propagation of energy transfer. Consider this wave as travelling

- In the χ direction in space. E.g., let the negative χ direction be to the right, and the positive χ direction be to the left. With constant U (displacement) with constant velocity **v**, where **v** is
- Independent of wavelength (no dispersion).

- Independent of amplitude (linear media, nonlinear).

Therefore the displacement as function to the distance and time of dispersion of energy.

$$U=f(x, t) \quad ----1$$

With constant waveform (shape), this wave can describe by the two-dimensional functions

(Waveform -vt traveling to the right) that's mean U=f(x, -vt)

(Waveform +vt traveling to the left) U=f(x, +vt)

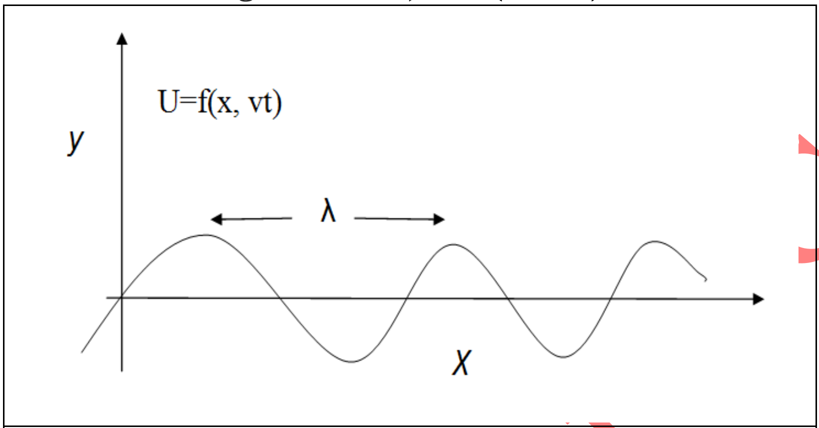


Diagram of wave motion into direction.

When the displacement at maximum value U= A,

So that: $U=f(x, vt) = f(x, -vt) \quad --2$

At constant time (stop, t=0) that's another confirmation for the displacement of the wave

$$U=A.\sin 2\pi \bar{v}\, x \text{ -------3}$$

A is constant value and $\bar{v}$ is wave number that's reciprocal of wavelength.

2-Standing wave motion:

A standing wave does not appear to travel. Each point on the standing wave will oscillate about a point on the axis of the wave. Adjacent points are in phase with each other (sections of the wave flap up and down together), so that points of a particular phase remain at a fixed location as time progresses. Adjacent points each oscillate with a different amplitude. (In a travelling wave, adjacent points all have the same amplitude, but the phase changes along the wave instead). Since adjacent points are in phase, no energy is transferred from one point to the next, unlike a travelling wave.

the same frequency (with the same polarization and the same amplitude) travelling in opposite directions Standing waves are formed by the superposition of two travelling waves of. This is usually achieved by using a travelling wave and its reflection, which will ensure that the frequency is exactly the same.

Antinodes are points on a stationary wave that oscillate with maximum amplitude. Nodes are points of zero amplitude and appear to be fixed.

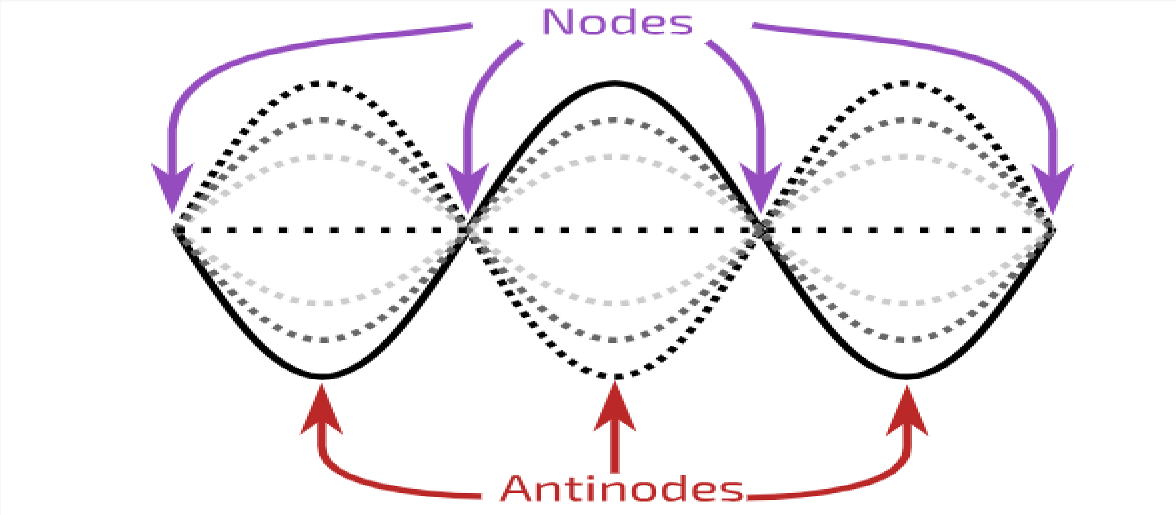


Figure 1: A sinusoidal standing wave.

The different dashed lines show the standing wave at different moments in time. Adjacent nodes and antinodes are always a distance $\lambda/4$ apart, where λ is the wavelength.

3-Derivation of Standing wave

The general differential equation of wave motion in one dimension included two variables (dimension and time), which supposed that the length is unlimited for wave motion.

$$\left(\frac{d^2U}{dx^2}\right) = \frac{1}{V^2}\cdot\left(\frac{d^2U}{dt^2}\right) \quad \text{----1}$$

The standing wave describes the motion behavior of electron in the chemical bond between two atoms, since boundary conditions of motion is represent the limited bond length.

$$0 \le x \le L$$

1-The standing wave is represented the vibrational motion and none wave motion within unlimited dimension length. At this case in general.

2-There is an exchange between the kinetic energy and potential energy of the chemical bound system.

By using the separation method of variables through equation 1. The displacement of wave motion function is divided into two sub-function as in following:-

$$U=f(x, t) =X_{(x)}.\ T_{(t)} \quad \text{-----2}$$

(by differential equation 2 at a constant for each variable.)

At constant variable of time $\frac{dU}{dx} = T_t \cdot \frac{dX}{dx}$, $\frac{d^2U}{dx^2} = T_t \cdot \frac{d^2X}{dx^2}$ -----3

At constant variable of dimension $\frac{dU}{dt} = X_x \cdot \frac{dT}{dt}$, $\frac{d^2U}{dt^2} = X_x \cdot \frac{d^2T}{dt^2}$ -----4

By substitution equation 3 and 4 into 1 equation and rearrangement the resultant equation through divided into T.X products

$$\frac{1}{X} \cdot \frac{d^2X}{dx^2} = \frac{1}{V^2} \cdot \frac{1}{T} \cdot \frac{d^2T}{dt^2} \quad \text{------------5}$$

Equation 5 is a separated variables equation, the mathematical way of solvation by using mathematical separation constant $(-\frac{\omega^2}{v^2})$, therefore equation 5 is separated into two differential equations.

$$\frac{1}{X} \cdot \frac{d^2X}{dx^2} = (-\frac{\omega^2}{v^2}), \text{--------6} \qquad \frac{1}{V^2} \cdot \frac{1}{T} \cdot \frac{d^2T}{dt^2} = (-\frac{\omega^2}{v^2}) \text{ ------7}$$

To solve equation 6

By supposing the following, if $\frac{dX}{dx} = V$ *so that* $\frac{d^2X}{dx^2} = \frac{dV}{dx}$

If $\frac{dV}{dx} \cdot \frac{dX}{dX} = \frac{dV}{dX} \cdot \frac{dX}{dx}$ so that $\frac{d^2X}{dx^2} = V \frac{dV}{dX}$ -----9

By substituted equation 14 into 12 to get on $\frac{1}{X} . V . \frac{dV}{dX} = (-\frac{\omega^2}{v^2})$,*or*

$V . dV = \left(-\frac{\omega^2}{v^2}\right) . XdX$-----10 by integration to get on

$\frac{V^2}{2} = -\frac{\omega^2}{v^2} . \frac{X^2}{2}$ That's mean $V = \pm\frac{\omega}{v} . X$ --------11

By substituting the value of constant V into equation 11 to get on:

$\frac{dX}{dx} = \pm\frac{\omega}{v} . X$ by rearrangement $\frac{dX}{X} = \pm\frac{\omega}{v} . dx$ --------12

Integration of equation 12 for both sides $lnX = \pm\frac{\omega}{v} . x$ this will give

$X = e^{\frac{\pm i\omega x}{v}}$ -----13 and the same mathematic way for T function

$$T = e^{\pm i\omega t} \text{---14}$$

The final solution of equation 1 is represented by substituting the equations 13 and 14 into equation 2 into & equation 1 at last as in following

$$U = e^{\frac{\pm i\omega x}{v}} . e^{\pm i\omega t} \quad \text{------15}$$

Equation 15 can be produced four different solutions according to different signs in the functions.

$$U = e^{\frac{+i\omega x}{v}} . e^{+i\omega t}$$

$$U = e^{\frac{-i\omega x}{v}} . e^{-i\omega t}$$

$$U = e^{\frac{+i\omega x}{v}} . e^{-i\omega t}$$

$$U = e^{\frac{-i\omega x}{v}} . e^{+i\omega t}$$

The solvation of these equations can be done by selecting the significant capacity of the phase. Eq.16, can be written also into sin angle and cos angle wave functions.

$$\begin{pmatrix} \text{U} = Sin\, \omega t \, . \, Sin\, \frac{\omega x}{v} \\ \text{U} = Sin\, \omega t \, . \, Cos\, \frac{\omega x}{v} \\ \text{U} = Cos\, \omega t \, . \, Sin\, \frac{\omega x}{v} \\ \text{U} = Cos\, \omega t \, . \, Cos\, \frac{\omega x}{v} \end{pmatrix} \text{-----16}$$

The capacity of the Standing wave can be achieved depending on the limitation of boundary condition since U=0 at x=0 and $t \geq 0$.

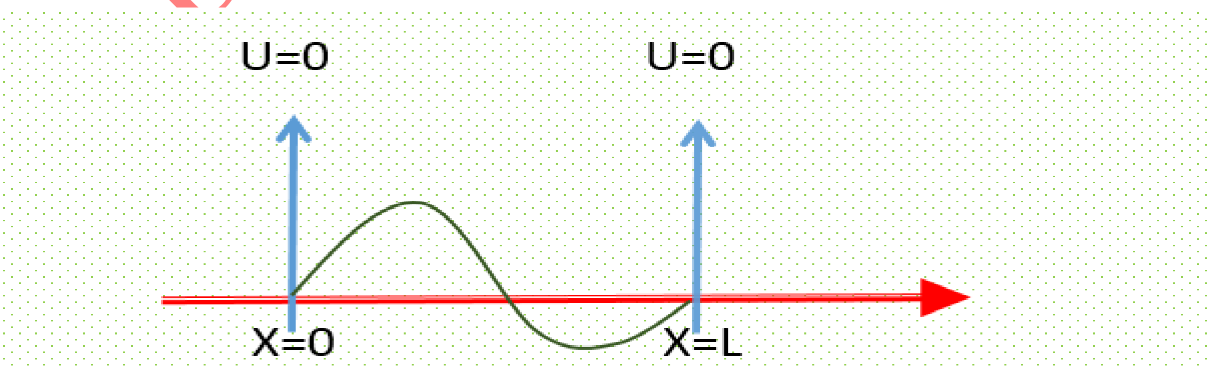


Figure: Boundary conditions of standing wave.

Consuming the wave capacity at x=0, by cancelling the Cos angle wave function. To be solvation:

$$\begin{pmatrix} U = Sin\omega t \,.\, Sin\frac{\omega x}{v} = 0 \\ U = Cos\omega t \,.\, Sin\frac{\omega x}{v} = 0 \end{pmatrix} \text{----17}$$

At the same thing U=0 at L=x, so that:

$$\begin{pmatrix} U = Sin\omega t \,.\, Sin\frac{\omega L}{v} = 0 \\ U = Cos\omega t \,.\, Sin\frac{\omega L}{v} = 0 \end{pmatrix} \text{----18}$$

Or

$$\text{Sin}\frac{\omega}{v}L = 0 \qquad \Rightarrow \qquad \text{Sin}0^{-1} = \frac{\omega}{v}L$$

Due to that $\text{Sin}0^{-1}$=nπ, since n is an integer number so that

$$n\pi = \frac{\omega}{v}L \qquad \Rightarrow \qquad \frac{n\pi}{L} = \frac{\omega}{v} \text{----19}$$

If they remember that Eq.19 is represented the wave equation at the condition of (n=2) and the frequency is equal to

$$v = \frac{\omega}{2\pi}\lambda$$

So that

$$\frac{\omega}{v} = \frac{2\pi}{\lambda} \text{ ---20;}$$

A simple condition of Eigenvalue can be achieved by substituting the value of ω /v from eq. 19 into equation 20 to get on:

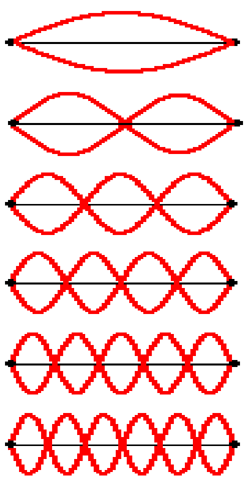
$$\frac{n\pi}{L} = \frac{2\pi}{\lambda} \quad ; \quad L=\frac{n\lambda}{2} \quad \rightarrow \quad \lambda=\frac{2L}{n} \text{ ----21}$$

All standing waves must be suited into eq.21, therefore can be written eq. 22 as follows:

$$\begin{pmatrix} U_n = Sin\omega t \, . \, Sin\frac{n\pi x}{L} = 0 \\ U_n = Cos\omega t \, . \, Sin\frac{n\pi x}{L} = 0 \end{pmatrix} \text{------22}$$

<u>The motion of standing is represented by oscillated motion and non-wave motion due to energy didn't distribute along the dimension of motion. The exchange of energy between kinetic energy and potential energy likes the system of the harmonic oscillator.</u>

The following figure represents some type of standing waves within L- length dimension. They concluded that's wave have points with a capacity value equal to zero (nodes), the nodes didn't vary within the time (since n=0, 1, 2, 3, …….). All allowed waves must be obeyed to **λ= 2L/n**.



Pattern	# of Loops	Length-Wavelength Relationship
	1	L = 1 / 2 • λ
	2	L = 2 / 2 • λ
	3	L = 3 / 2 • λ
	4	L = 4 / 2 • λ
	5	L = 5 / 2 • λ
	6	L = 6 / 2 • λ
--	n	L = n / 2 • λ