❖ Pictorial Representation of the Wave Equation of a Particle in One Dimensional Box and Its Influence on the Kinetic Energy of the Particle in Each Successive Quantum Level

The solution of the Schrodinger wave equation for a one-dimensional box gives the wave function as well as the energy of the system. The general form of wave-function representing various quantum mechanical states is given below.

$$\psi_n = \sqrt{\frac{2}{a}}\, Sin\frac{n\pi x}{a} \tag{497}$$

The energy of the system is given by equation (498) as:

$$E_n = \frac{n^2h^2}{8ma^2} \tag{498}$$

The general depiction of a particle trapped in a one-dimensional box with zero potential inside, along with the conditions outside, is shown below.

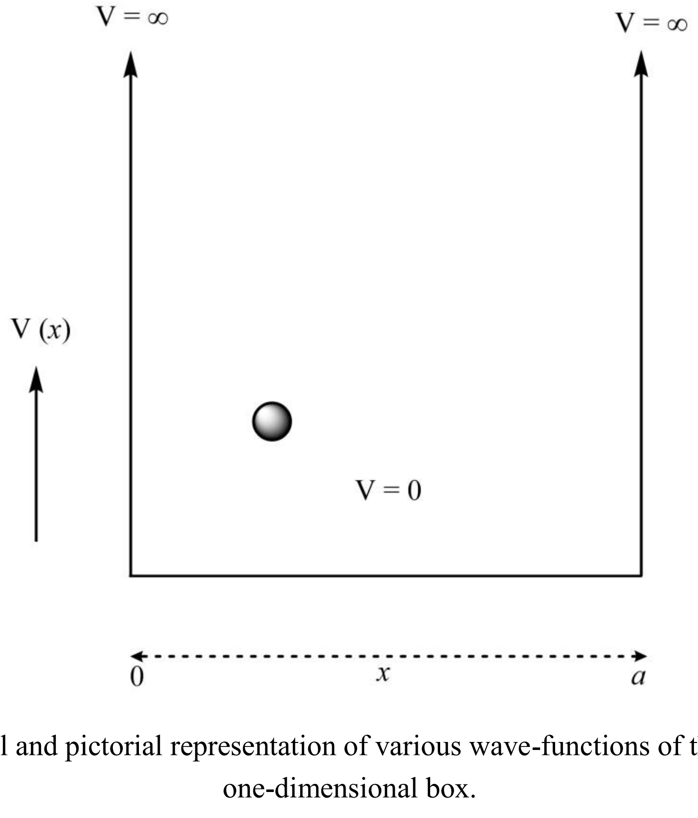

Figure 9. The graphical and pictorial representation of various wave-functions of the particle trapped in a one-dimensional box.

The pictorial representation of the wave-functions in different quantum mechanical states and the corresponding energies are shown below.

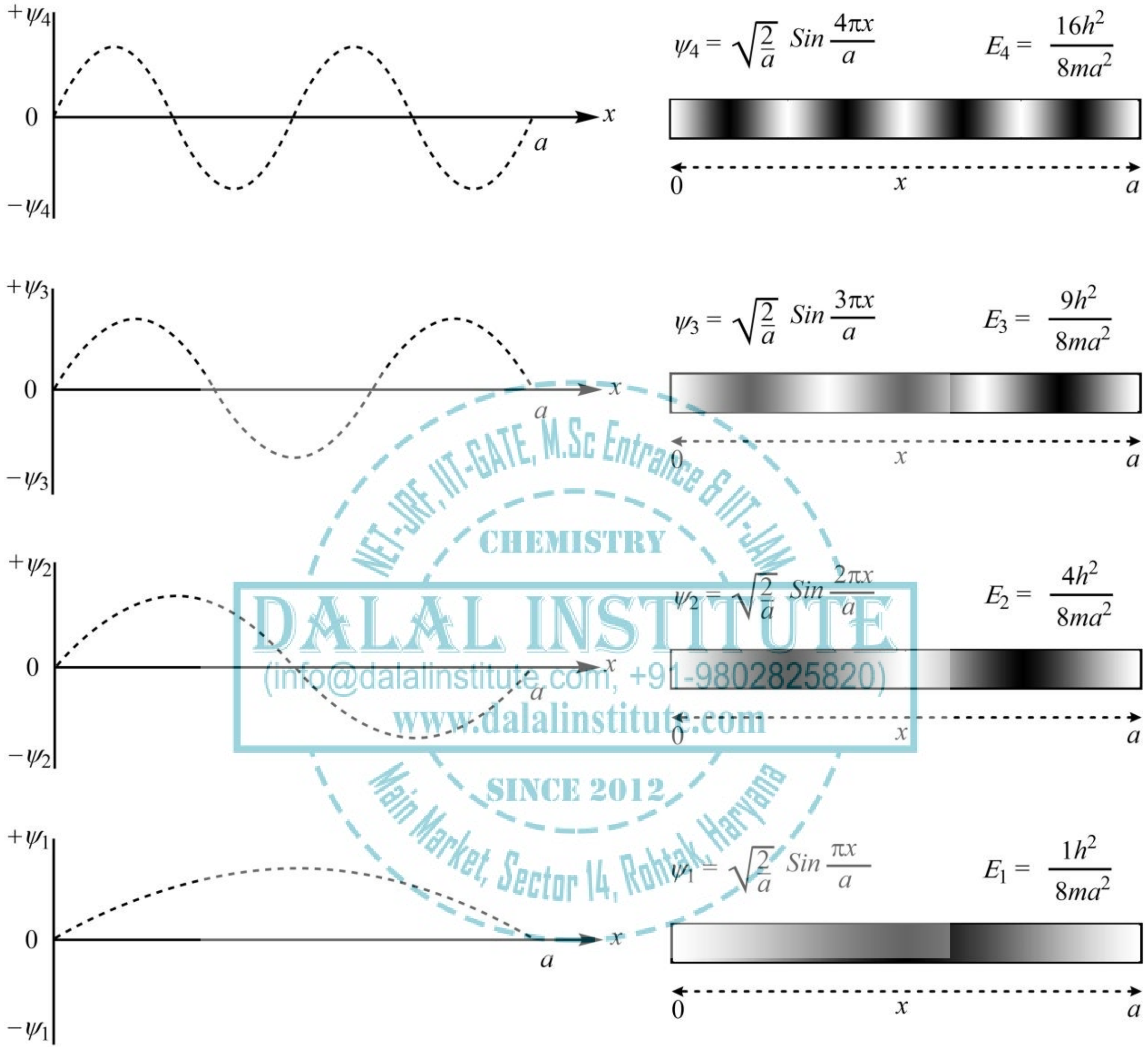

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Figure 10. The graphical and pictorial representation of various wave-functions of the particle trapped in a one-dimensional box.

It can be seen clearly from the figure given above that as the number of nodes in wave-function defining a particular quantum mechanical state increases, the energy of the state also increases.

Furthermore, we can also comment on the symmetry of different wave functions w.r.t the center of the box. The symmetry of different states can be classified mainly into two categories as given below.

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$$Symmetric \rightarrow Even\ function \rightarrow \psi_{odd}$$

and

$$Antisymmetric \rightarrow Odd\ function \rightarrow \psi_{even}$$

Hence, function like ψ_1, ψ_3, ψ_5 are symmetric while ψ_2, ψ_4, ψ_6 are antisymmetric. Some of the important results wavefunction and energy analysis for the particle in a one-dimensional box are listed below.

- ***Quantization of Energy***

Owing to the discrete domain of n i.e. 1, 2, 3 …. ∞; the kinetic energy associated with the particle, that is trapped in a one-dimensional box, can also have discrete or quantized values only. Therefore, the quantized variable is also popularly called as the “quantum number.

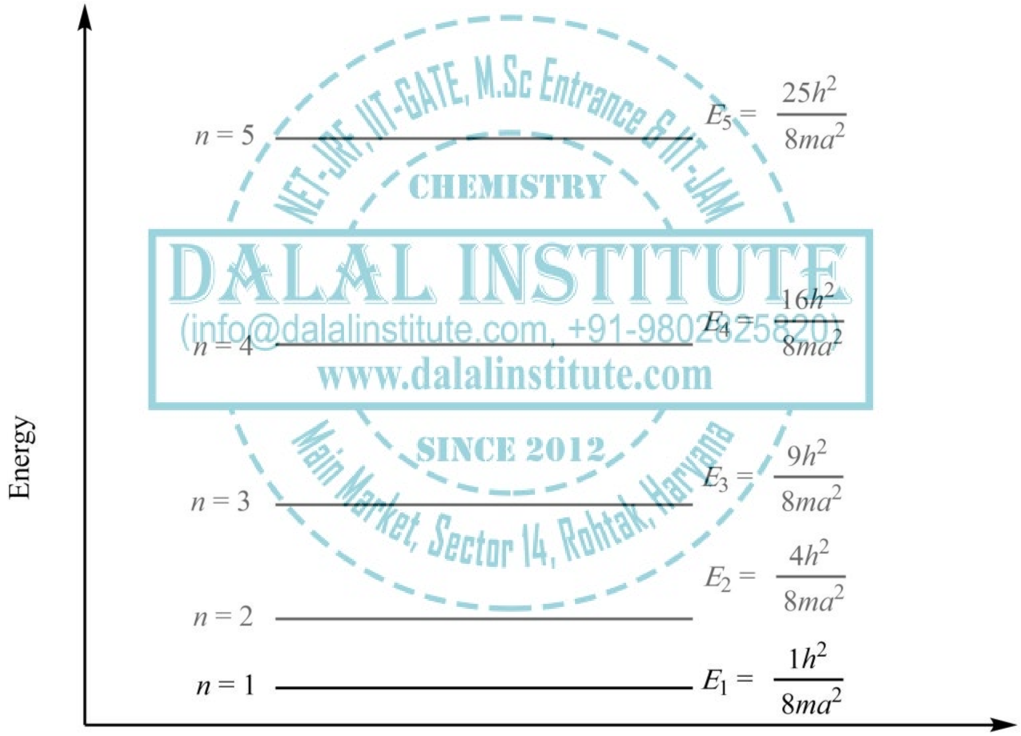

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Figure 11. The quantized or discrete energy levels a particle of mass m, confined in a one-dimensional box of length a.

It is also worthy to note that the energy gap between successive energy levels shows a linear divergence with the increasing value of the quantum number n. Moreover, the energy of particle also depends inversely upon the mass and the box length; which eventually means that the energy levels would become continuous if the mass or length of the box becomes very large, proving the Bohr’s correspondence principle.

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- ***Non-Quantization of the Energy of the Particle***

If the walls of the box are removed, the boundary conditions will no longer be applicable, and the particle would become free to move. In other words, the constant A, B and k can have any value; and therefore, states of the particle are not quantized anymore. The general expression for the energy of the particle is

$$E_n = \frac{n^2h^2}{8ma^2} \tag{498}$$

Hence, in such a case, a freely moving particle like an electron has restrictions and gives a continuous energy spectrum.

- ***Box length and the Wave Function at the Walls***

We have already studied that the magnitude of the wave function at the ends of the box must be equal to zero to maintain its continuity. This is possible only if the length of the box is an integral multiple of half of the wavelength. This can be proved as

$$E_n = \frac{n^2h^2}{8ma^2} \tag{499}$$

Also

$$E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m} \tag{500}$$

Using the de-Brogli relation ($\lambda = h/p$) in equation (500), we get

$$E = \frac{p^2}{2m} = \frac{(h/\lambda)^2}{2m} = \frac{h^2}{2m\lambda^2} \tag{501}$$

Now from equation (499) and (501), we conclude

$$\frac{n^2h^2}{8ma^2} = \frac{h^2}{2m\lambda^2} \tag{502}$$

or

$$\frac{n^2}{4a^2} = \frac{1}{\lambda^2} \tag{503}$$

or

$$a = n\left(\frac{\lambda}{2}\right) \tag{504}$$

This result of equation (504) also proves that the number of nodes in nth quantum mechanical state are n–1.

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➢ *The Probability Density*

The wave density of simply the probability density in the one-dimensional box is not the same at all the points. It is more noticeable when the quantum number defining the state is small. However, it becomes more and more uniform as *n* increases.

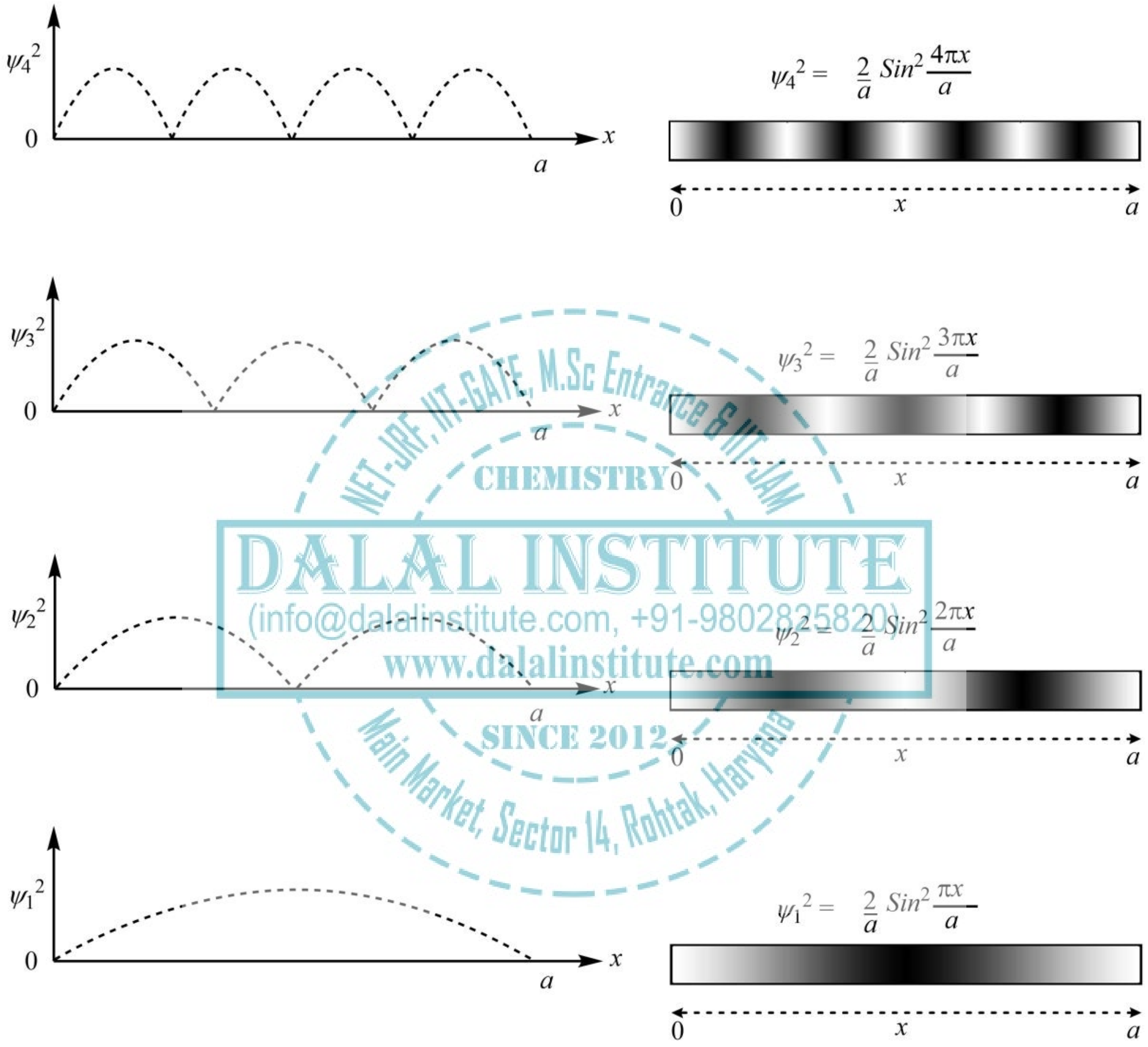

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Figure 12. The graphical and pictorial representation of the probability density of a particle with mass *m* and confined in a one-dimensional box of length *a*.

The increasing uniformity of with increasing value of *n* is in accordance with the Bohr's correspondence principle which states that the results of quantum mechanics approach classical values at very high quantum numbers.

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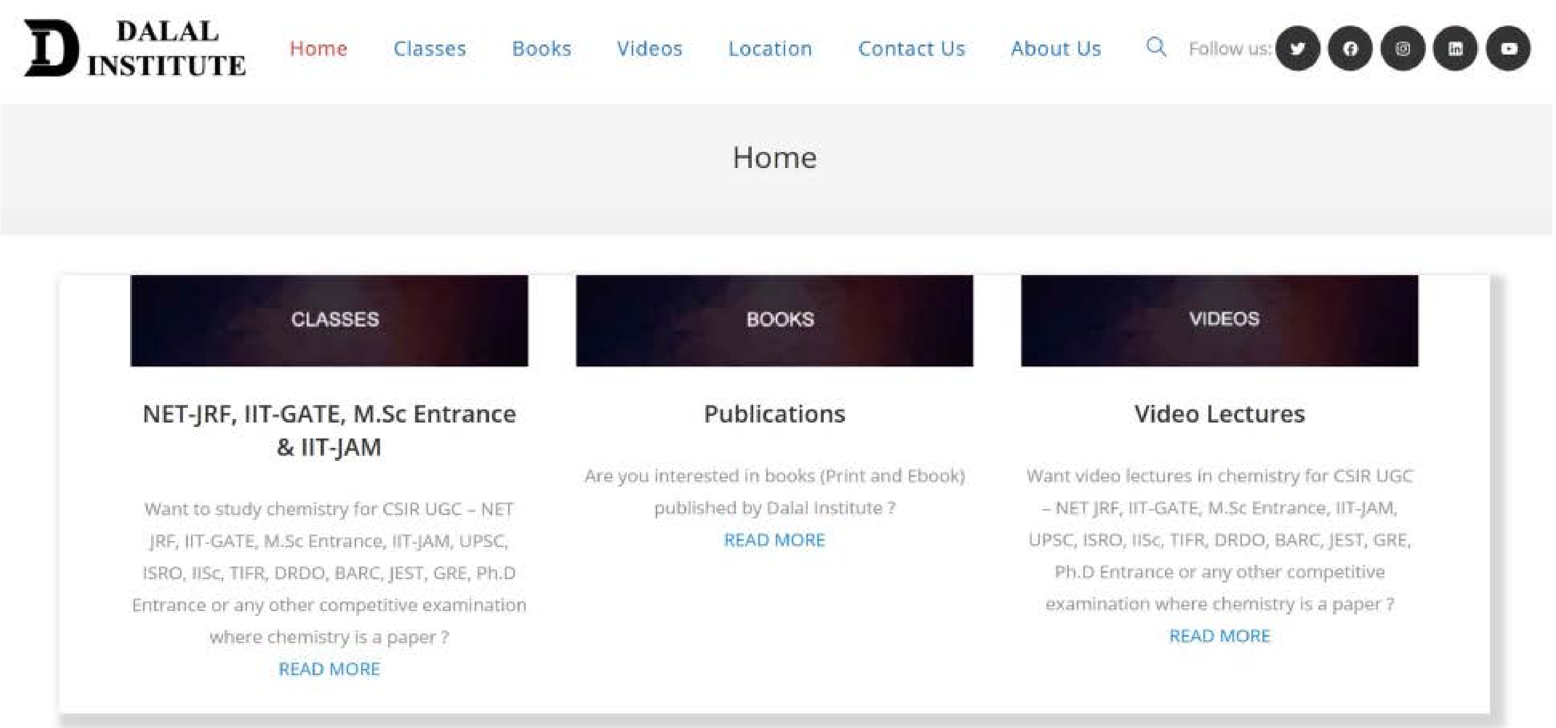

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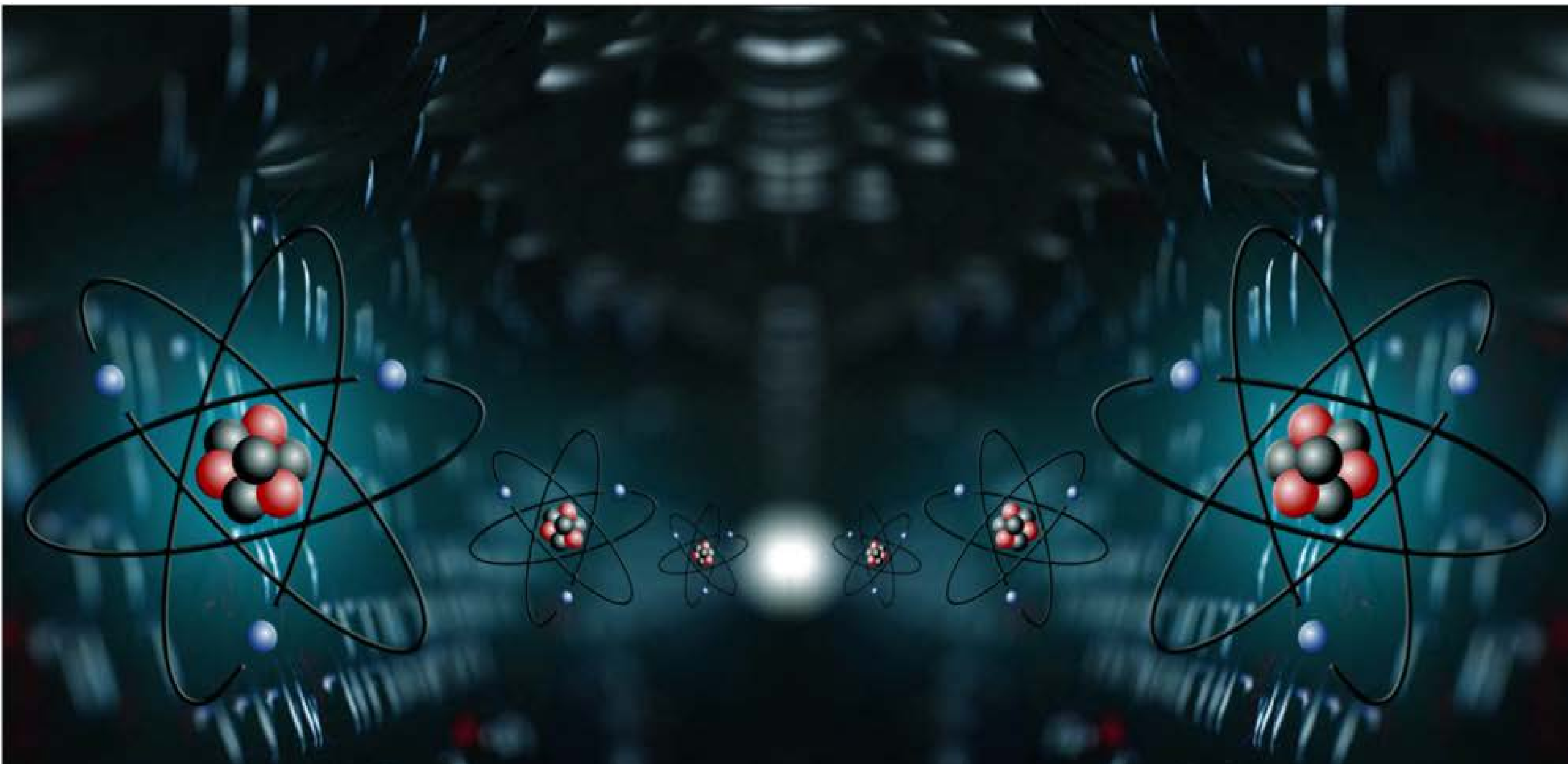

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