

❖ Hermitian Operators – Elementary Ideas, Quantum Mechanical Operator for Linear Momentum, Angular Momentum and Energy as Hermitian Operator

It is a quite well-known fact that all the physical properties are actually real quantities, and therefore are bound to have real values. It means that any operator which is used to represent a physical property must yield real values. In this section, we will discuss the elementary idea of Hermitian operators (named in honor of a great mathematician Charles Hermite), and will also prove that many important operators in quantum mechanics like linear momentum, angular momentum and Hamiltonian are Hermitian in nature.

➤ Elementary Idea of Hermitian Operator

Every physical property must have real eigen or expectation values, which therefore implies that the corresponding operators should have some special characteristics. One of the most important special characteristics includes a feature that the Hermitian conjugate of such an operator should be itself. In other words, if the Hermitian conjugate of an operator is itself, the operator is called as Hermitian; however, if the Hermitian conjugate of an operator is equal to its negative expression, the operator is called as anti-Hermitian or skew-Hermitian. Mathematically, we can say that

$$\text{if } A^\dagger = A; \quad A \text{ is Hermitian} \quad (316)$$

$$\text{if } A^\dagger = -A; \quad A \text{ is anti-Hermitian} \quad (317)$$

Where A is an operator whose Hermitian conjugate is represented by A^\dagger .

However, the obvious question regarding the aforementioned definition would be “what is a Hermitian conjugate and how is it obtained”. The answer is “the operator A^\dagger will be called as the Hermitian conjugate (or adjoint) of operator A if the operation of A^\dagger on the complex conjugate of function ψ gives the same result as when the A is operated over ψ ”. Mathematically, we can say that

$$\langle \psi | A | \psi \rangle = \int_{-\infty}^{+\infty} \psi^*(x) A \psi(x) dx = \langle \psi | A \psi \rangle = \langle A^\dagger \psi | \psi \rangle \quad (318)$$

or

$$\langle A^\dagger \phi | \psi \rangle = \langle \phi | A \psi \rangle \quad (319)$$

1. Hermitian conjugates of different operators: The Hermitian conjugates of different operators can be studied in three different categories.

i) Hermitian conjugates of quantum mechanical operators:

Let Q be any quantum mechanical operator, then by the definition of Hermitian conjugates operator, we have the following condition.

$$\langle \varphi | Q \psi \rangle = \langle Q^\dagger \varphi | \psi \rangle \tag{320}$$

If Q is the momentum operator, then we can proceed as discussed below.

$$\int \psi^* \hat{p}_x \psi dx = \int \psi \hat{p}_x \psi^* dx \tag{321}$$

$$\int \psi^* \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right) \psi dx = \int \psi \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right)^\dagger \psi^* dx \tag{322}$$

$$\int \psi \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right)^\dagger \psi^* dx = \int \psi \left(\frac{h}{2\pi i} \right)^\dagger \left(\frac{\partial}{\partial x} \right)^\dagger \psi^* dx \tag{323}$$

$$\int \psi \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right)^\dagger \psi^* dx = \int \psi \left(-\frac{h}{2\pi i} \right) \left(-\frac{\partial}{\partial x} \right) \psi^* dx \tag{324}$$

$$\int \psi \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right)^\dagger \psi^* dx = \int \psi \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right) \psi^* dx \tag{325}$$

Therefore, we can say that the Hermitian conjugate of the linear momentum operator is itself, and hence it is a Hermitian operator. Now from the most primitive definition of Hermitian operators, that all operators which correspond to observable quantities, we can say that the Hermitian conjugates of the following operator are themselves.

Operator	Hermitian conjugate
\hat{x}	\hat{x}
\hat{x}^2	\hat{x}^2
\hat{p}_x	\hat{p}_x
\hat{p}_x^2	\hat{p}_x^2
\hat{T}_x	\hat{T}_x
$\hat{V}(x)$	$\hat{V}(x)$
\hat{H}	\hat{H}

ii) Hermitian conjugates of a constant operator:

There are some operators which are complex numbers. The Hermitian conjugates of such operators are actually their complex conjugates. Let we have the operator A

$$\hat{A} = a + ib \tag{326}$$

and since the definition of Hermitian operator is

$$\langle \varphi | A \psi \rangle = \langle A^\dagger \varphi | \psi \rangle \quad (327)$$

gives the integer as

$$\langle \varphi | (a + ib) \psi \rangle = \langle (a - ib) \varphi | \psi \rangle = (a + ib) \langle \varphi | \psi \rangle \quad (328)$$

Hence, the Hermitian conjugates of constant operators are their complex conjugates. The Hermitian conjugates of some operators are given below.

Operator	Hermitian conjugate
$(a + ib)$	$(a + ib)^\dagger = (a - ib)$
$(+ib)$	$(+ib)^\dagger = (-ib)$
$\left(+\frac{i}{4}\right)$	$\left(+\frac{i}{4}\right)^\dagger = \left(-\frac{i}{4}\right)$

iii) Hermitian conjugates of a mathematical operator:

The Hermitian conjugates of mathematical operators can be obtained by obtaining their respective integrals as discussed below. Let we have a mathematical operator A

$$\hat{A} = \frac{d}{dx} \quad (326)$$

We use the following integral to derive the result

$$\left\langle \varphi \left| \frac{d}{dx} \psi \right. \right\rangle = \int_{-\infty}^{+\infty} \varphi^*(x) \frac{d\psi(x)}{dx} dx \quad (327)$$

Integrating the above equation by part, we get

$$\left\langle \varphi \left| \frac{d}{dx} \psi \right. \right\rangle = [\varphi^*(x)\psi(x)] - \int_{-\infty}^{+\infty} \frac{d\varphi^*(x)}{dx} \psi(x) dx \quad (328)$$

$$= 0 - \left\langle \frac{d}{dx} \varphi \left| \psi \right. \right\rangle \quad (329)$$

$$= - \left\langle \frac{d}{dx} \varphi \left| \psi \right. \right\rangle \quad (330)$$

Hence, the Hermitian conjugate of d/dx operator is $-d/dx$. Similarly, we can prove that the Hermitian conjugate of d^2/dx^2 is d^2/dx^2 .

2. Properties of Hermitian conjugates: From the definition and properties of scalar product, adjoints or Hermitian conjugate show the following properties.

i) Let C a constant and A as an operator.

$$(CA)^\dagger = C^* A^\dagger \quad (331)$$

For example

$$\left(\frac{i}{4} \frac{\partial}{\partial x}\right)^\dagger = \left(\frac{i}{4}\right)^\dagger \left(\frac{\partial}{\partial x}\right)^\dagger \quad (332)$$

$$\left(\frac{i}{4} \frac{\partial}{\partial x}\right)^\dagger = \left(-\frac{i}{4}\right) \left(-\frac{\partial}{\partial x}\right) \quad (333)$$

$$\left(\frac{i}{4} \frac{\partial}{\partial x}\right)^\dagger = \frac{i}{4} \frac{\partial}{\partial x} \quad (334)$$

ii) Let A and B as two operators.

$$(A+B)^\dagger = A^\dagger + B^\dagger \quad (335)$$

For example

$$\left(\frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2}\right)^\dagger = \left(\frac{\partial}{\partial x}\right)^\dagger + \left(\frac{\partial^2}{\partial x^2}\right)^\dagger \quad (336)$$

$$\left(\frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2}\right)^\dagger = \left(-\frac{\partial}{\partial x}\right) + \left(\frac{\partial^2}{\partial x^2}\right) \quad (337)$$

$$\left(\frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2}\right)^\dagger = \left(-\frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2}\right) \quad (338)$$

iii) Let A and B as two operators, then

$$(AB)^\dagger = A^\dagger B^\dagger \quad (339)$$

For example

$$\left(\frac{\partial}{\partial x} \frac{\partial^2}{\partial x^2}\right)^\dagger = \left(\frac{\partial}{\partial x}\right)^\dagger \left(\frac{\partial^2}{\partial x^2}\right)^\dagger \quad (340)$$

$$\left(\frac{\partial}{\partial x} \frac{\partial^2}{\partial x^2}\right)^\dagger = \left(-\frac{\partial}{\partial x}\right) \left(\frac{\partial^2}{\partial x^2}\right) \quad (341)$$

$$\left(\frac{\partial}{\partial x} \frac{\partial^2}{\partial x^2}\right)^\dagger = \left(-\frac{\partial^3}{\partial x^3}\right) \quad (342)$$

iv) Let A be the operators, then

$$(A^\dagger)^\dagger = A \quad (343)$$

For example

$$\left[\left(\frac{\partial}{\partial x}\right)^\dagger\right]^\dagger = \left(\frac{\partial}{\partial x}\right) \quad (344)$$

It should also be noted that the multiplication to an anti-hermitian operator by i makes it Hermitian, while the vice-versa is also equally true for adjoints.

v) For any operator A and its adjoint, the product (AA^\dagger) is Hermitian. For instance

$$\left(\frac{\partial}{\partial x}\right)\left(-\frac{\partial}{\partial x}\right) = -\frac{\partial^2}{\partial x^2} \quad (343)$$

vi) For any operator A and its adjoint, the sum $(A+A^\dagger)$ is Hermitian. For instance

$$(x + x^\dagger) = 2x \quad (343)$$

vii) For any operator A and its adjoint, then $AA^\dagger + A^\dagger A$ is Hermitian. For instance

$$(i3)(i3)^\dagger + (i3)^\dagger(i3) = (i3)(-i3) + (-i3)(i3) = 9 + 9 = 18 \quad (343)$$

3. Characterization of Hermitian operator: We know that the average value of any operator (say \hat{A}) in quantum mechanics is calculated by the equation given below.

$$\bar{A} = \int \psi^* \hat{A} \psi dx \quad (344)$$

Where ψ is the wave function representing any quantum mechanical state and ψ^* is its complex conjugate. Now because of the fact that the average value of any physical observable must be a real value, we can say that the operator used in equation (344) must follow the following condition.

$$\bar{A} = \bar{A}^* \quad (345)$$

$$\int \psi^* \hat{A} \psi dx = \left[\int \psi^* \hat{A} \psi dx \right]^* \quad (346)$$

$$\int \psi^* \hat{A} \psi dx = \int (\psi^*)^* (\hat{A} \psi)^* dx \quad (347)$$

$$\int \psi^* \hat{A} \psi dx = \int \psi (\hat{A} \psi)^* dx \quad (348)$$

Every linear operator that satisfies the equation (348) for all quantum-mechanically acceptable wave functions is called the Hermitian operator.

Besides the form given by equation (348), one more popular definition of a Hermitian operator is also given below.

$$\int f^* \hat{A} g dx = \int g (\hat{A} f)^* dx \quad (349)$$

From the equation, we can state that a Hermitian operator must fulfill the condition for the well-behaved functions f and g . It can be clearly seen that on the left side of the equation (349), \hat{A} is operated over the function g ; while on the right side, the \hat{A} is operated over the function f . However, if we put $f = g$, the equation (349) is also reduced to equation (348); indicating that both definitions are correct.

4. Properties of Hermitian operators: The important properties of Hermitian operators are discussed below.
i) *The eigenvalues of Hermitian operators are always real:*

Let \hat{A} be a Hermitian operator with a well-behaved wavefunction ψ representing a quantum mechanical state, then we can say that

$$\hat{A} \psi = a \psi \quad (350)$$

Each side of equation (350) can be expressed as an imaginary and a real part as well; with left-hand real part equal to the right-hand real part, while left side imaginary part equal to right imaginary one. After taking the complex conjugate of equation (350), the imaginary parts would reverse sign but still holding the condition of equivalence.

$$\hat{A}^* \psi^* = a^* \psi^* \quad (351)$$

Multiplying the equation (350) by ψ^* and integrating over the whole configurational space, we get

$$\int \psi^* \hat{A} \psi dx = a \int \psi^* \psi dx \quad (352)$$

Similarly, multiplying the equation (351) by ψ and integrating over the whole configurational space, we get

$$\int \psi \hat{A}^* \psi^* dx = a^* \int \psi \psi^* dx \quad (353)$$

Now because left-hand sides of equation (352) and (353) are equal to each other (owing to the Hermitian nature of the operator), the right-hand sides are also equivalent; therefore, we can say that

$$a^* \int \psi \psi^* dx = a \int \psi^* \psi dx \quad (354)$$

$$0 = (a - a^*) \int \psi^* \psi dx \quad (355)$$

Since the wave function is a square-integrable, the integral part of the equation (355) cannot be zero and left us with the only possibility given below.

$$(a - a^*) = 0 \quad (356)$$

$$a = a^* \quad (357)$$

The physical interpretation of the result given by equation (357) is that a must be real in order to yield zero from equation (356).

ii) Non-degenerate eigenfunctions of Hermitian operators are always orthogonal to each other:

Let ψ_m and ψ_n be two square-integrable eigenfunctions of a Hermitian operator \hat{A} ; therefore, we say

$$\hat{A}\psi_m = a_1\psi_m \quad (358)$$

also

$$\hat{A}^*\psi_n^* = a_2\psi_n^* \quad (359)$$

Multiplying the equation (358) by ψ_n^* and integrating over the whole configurational space, we get

$$\int \psi_n^* \hat{A}\psi_m dx = a_1 \int \psi_n^* \psi_m dx \quad (360)$$

Similarly, multiplying the equation (359) by ψ_m and integrating over the whole configurational space, we get

$$\int \psi_m \hat{A}^*\psi_n^* dx = a_2 \int \psi_m \psi_n^* dx \quad (361)$$

Now because left-hand sides of equation (360) and (361) are equal to each other (owing to the Hermitian nature of the operator), the right-hand sides are also equivalent; therefore, we can say that

$$a_1 \int \psi_n^* \psi_m dx = a_2 \int \psi_m \psi_n^* dx \quad (362)$$

$$(a_1 - a_2) \int \psi_m \psi_n^* dx = 0 \quad (363)$$

Since the wave functions used are non-degenerate i.e. $a_1 \neq a_2$; the only possibility we are left with for the equation to be true is given below.

$$\int \psi_m \psi_n^* dx = 0 \quad (364)$$

Hence, we can say that ψ_m and ψ_n are definitely orthogonal to each other.

iii) If two Hermitian operators commute, their product is also a Hermitian operator:

Let ψ_1 and ψ_2 be two well-behaved functions; while \hat{A} and \hat{B} as two Hermitian operators. Therefore, we can say that

$$\int \psi_1^* \hat{A} \hat{B} \psi_2 dx \quad (365)$$

Since \hat{A} is Hermitian, we can say that

$$\int \psi_1^* \hat{A} \hat{B} \psi_2 dx = \int \psi_1^* \hat{A} (\hat{B} \psi_2) dx \quad (366)$$

$$\int \hat{A}^* \psi_1^* \hat{B} \psi_2 dx = \int \psi_1^* \hat{A} (\hat{B} \psi_2) dx \quad (367)$$

Since \hat{B} is also Hermitian, therefore

$$\int (\hat{A}^* \psi_1^*) \hat{B} \psi_2 dx = \int \hat{B}^* \hat{A}^* \psi_1^* \psi_2 dx \quad (368)$$

From equation (366) and (368), we get

$$\int \psi_1^* \hat{A} \hat{B} \psi_2 dx = \int \hat{B}^* \hat{A}^* \psi_1^* \psi_2 dx \quad (369)$$

If the operator \hat{A} and \hat{B} commute with each other, we have

$$\hat{A} \hat{B} = \hat{B} \hat{A} \quad \text{or} \quad \hat{A}^* \hat{B}^* = \hat{B}^* \hat{A}^* \quad (370)$$

Therefore, equation (369) becomes

$$\int \psi_1^* \hat{A} \hat{B} \psi_2 dx = \int \hat{A}^* \hat{B}^* \psi_1^* \psi_2 dx \quad (371)$$

Which is the condition for the product operator to act as Hermitian.

iv) If two Hermitian operators do not commute, their commutator operator is anti-Hermitian in nature:

Let \hat{A} and \hat{B} as two Hermitian operators; therefore, we can say that their commutation must follow the following condition.

$$[\hat{A}, \hat{B}]^* = (\hat{A} \hat{B})^* - (\hat{B} \hat{A})^* \quad (372)$$

or

$$[\hat{A}, \hat{B}]^* = \hat{A}^* \hat{B}^* - \hat{B}^* \hat{A}^* = -(\hat{B}^* \hat{A}^* - \hat{A}^* \hat{B}^*) \quad (373)$$

or

$$[\hat{A}, \hat{B}]^* = -[\hat{B}, \hat{A}]^* \quad (374)$$

$$[\hat{A}, \hat{B}]^* = -[\hat{B}, \hat{A}]^* \quad (375)$$

For instance, consider the commutator of position and momentum operator

$$[\hat{x}, \hat{p}_x] = i \frac{h}{2\pi} \quad (376)$$

The commutator $i\hbar$ is antihermitian in nature.

➤ *The Linear Momentum Operator as Hermitian*

In order to prove the linear momentum operator as the Hermitian, we must find its Hermitian conjugate first. The general expression of linear momentum operator is

$$\hat{p}_x = \frac{h}{2\pi i} \frac{\partial}{\partial x} \quad (377)$$

Let \hat{p}_x^\dagger be the Hermitian conjugate which can be calculated as follows:

$$\hat{p}_x^\dagger = \left(\frac{h}{2\pi i}\right)^\dagger \left(\frac{\partial}{\partial x}\right)^\dagger \quad (378)$$

or

$$\hat{p}_x^\dagger = \left(-\frac{h}{2\pi i}\right) \left(-\frac{\partial}{\partial x}\right) \quad (379)$$

or

$$\hat{p}_x^\dagger = \left(\frac{h}{2\pi i}\right) \left(\frac{\partial}{\partial x}\right) \quad (380)$$

Comparing equation (377) and (380), we can see that the Hermitian conjugate of linear momentum operator is exactly equal to the linear momentum operator i.e. $\hat{p}_x^\dagger = \hat{p}_x$; proving that it is definitely a Hermitian operator.

➤ *The Angular Momentum Operator as Hermitian*

In order to prove the angular momentum operator as Hermitian, we must find its Hermitian conjugate first. The general expression of the angular momentum operator is

$$\hat{L} = \frac{h}{2\pi i} \left[\left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) + \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) + \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right] \quad (381)$$

Let \hat{L}_x^\dagger be the Hermitian conjugate which can be calculated as follows:

$$\begin{aligned}\hat{L}_x^\dagger &= \left[\frac{h}{2\pi i} \left[\left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) + \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) + \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right] \right]^\dagger \quad (382) \\ &= \left[\frac{h}{2\pi i} y \frac{\partial}{\partial z} - \frac{h}{2\pi i} z \frac{\partial}{\partial y} + \frac{h}{2\pi i} z \frac{\partial}{\partial x} - \frac{h}{2\pi i} x \frac{\partial}{\partial z} + \frac{h}{2\pi i} x \frac{\partial}{\partial y} - \frac{h}{2\pi i} y \frac{\partial}{\partial x} \right]^\dagger\end{aligned}$$

or

$$\begin{aligned}\hat{L}_x^\dagger &= \left(\frac{h}{2\pi i} \right)^\dagger (y)^\dagger \left(\frac{\partial}{\partial z} \right)^\dagger - \left(\frac{h}{2\pi i} \right)^\dagger (z)^\dagger \left(\frac{\partial}{\partial y} \right)^\dagger + \left(\frac{h}{2\pi i} \right)^\dagger (z)^\dagger \left(\frac{\partial}{\partial x} \right)^\dagger \quad (383) \\ &\quad - \left(\frac{h}{2\pi i} \right)^\dagger (x)^\dagger \left(\frac{\partial}{\partial z} \right)^\dagger + \left(\frac{h}{2\pi i} \right)^\dagger (x)^\dagger \left(\frac{\partial}{\partial y} \right)^\dagger - \left(\frac{h}{2\pi i} \right)^\dagger (y)^\dagger \left(\frac{\partial}{\partial x} \right)^\dagger\end{aligned}$$

or

$$\begin{aligned}\hat{L}_x^\dagger &= \left(-\frac{h}{2\pi i} \right) (y) \left(-\frac{\partial}{\partial z} \right) - \left(-\frac{h}{2\pi i} \right) (z) \left(-\frac{\partial}{\partial y} \right) + \left(-\frac{h}{2\pi i} \right) (z) \left(-\frac{\partial}{\partial x} \right) \quad (384) \\ &\quad - \left(-\frac{h}{2\pi i} \right) (x) \left(-\frac{\partial}{\partial z} \right) + \left(-\frac{h}{2\pi i} \right) (x) \left(-\frac{\partial}{\partial y} \right)\end{aligned}$$

or

$$\hat{L}_x^\dagger = \frac{h}{2\pi i} y \frac{\partial}{\partial z} - \frac{h}{2\pi i} z \frac{\partial}{\partial y} + \frac{h}{2\pi i} z \frac{\partial}{\partial x} - \frac{h}{2\pi i} x \frac{\partial}{\partial z} + \frac{h}{2\pi i} x \frac{\partial}{\partial y} - \frac{h}{2\pi i} y \frac{\partial}{\partial x} \quad (385)$$

$$\hat{L}_x^\dagger = \frac{h}{2\pi i} \left[\left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) + \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) + \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right] \quad (386)$$

Comparing equation (381) and (386), we can see that the Hermitian conjugate of the angular momentum operator is exactly equal to the angular momentum operator i.e. $\hat{L}_x^\dagger = \hat{L}_x$; proving that it is definitely a Hermitian operator.

➤ The Hamiltonian or Energy Operator as Hermitian

In order to prove the energy operator as Hermitian, we must find its Hermitian conjugate first. The general expression of the energy operator is

$$\hat{H} = \frac{-h^2}{8\pi^2 m} \frac{\partial^2}{\partial x^2} + V(x) \quad (387)$$

Let \hat{H}^\dagger be the Hermitian conjugate which can be calculated as follows:

$$\hat{H}^\dagger = \left[\frac{-h^2}{8\pi^2 m} \frac{\partial^2}{\partial x^2} + V(x) \right]^\dagger \quad (388)$$

or

$$\hat{H}^\dagger = \left[\frac{-h^2}{8\pi^2 m} \frac{\partial}{\partial x} \frac{\partial}{\partial x} + V(x) \right]^\dagger \quad (389)$$

$$\hat{H}^\dagger = \left(\frac{-h^2}{8\pi^2 m} \right)^\dagger \left(\frac{\partial}{\partial x} \right)^\dagger \left(\frac{\partial}{\partial x} \right)^\dagger + (V(x))^\dagger \quad (390)$$

or

$$\hat{H}^\dagger = \left(\frac{-h^2}{8\pi^2 m} \right) \left(-\frac{\partial}{\partial x} \right) \left(-\frac{\partial}{\partial x} \right) + (V(x)) \quad (391)$$

$$\hat{H}^\dagger = \frac{-h^2}{8\pi^2 m} \frac{\partial^2}{\partial x^2} + V(x) \quad (392)$$

Comparing equation (387) and (392), we can see that the Hermitian conjugate of energy operator is exactly equal to the energy operator i.e. $\hat{H}^\dagger = \hat{H}$; proving that it is defiantly a Hermitian operator.

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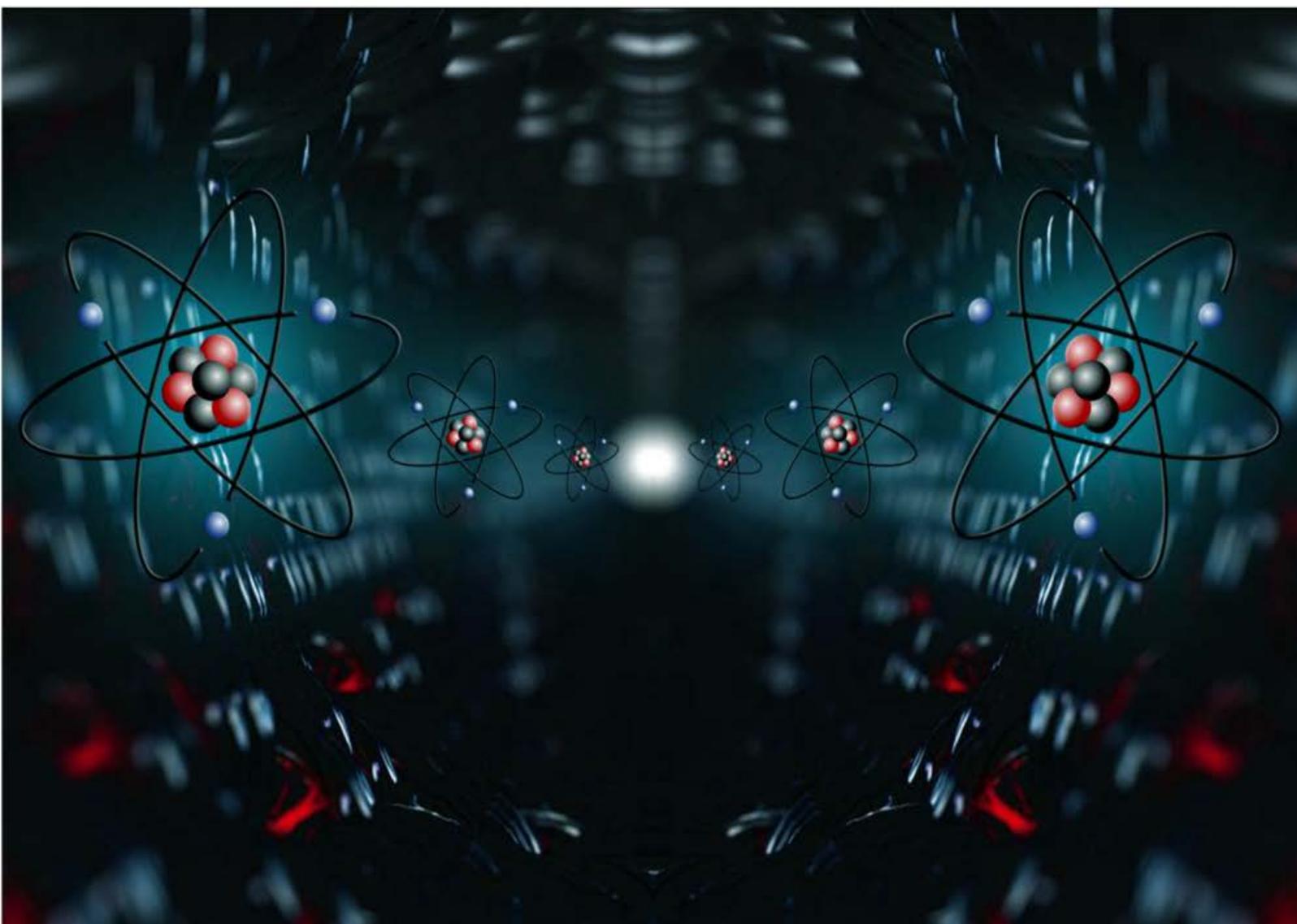
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