



**STUDY MATERIAL ON**  
**SYMMETRIES IN QUANTUM MECHANICS**  
(*MASTERS IN PHYSICS – SEMESTER II*)

VIVEKANANDA COLLEGE, THAKURPUKUR  
NAAC Accredited Grade - A

*By*

[Dr. Ambalika Biswas](#)

Assistant Professor, Department of Physics

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**Topic:** Irreducible spherical tensor operators, Wigner-Eckart theorem; Discrete symmetries parity and time reversal.

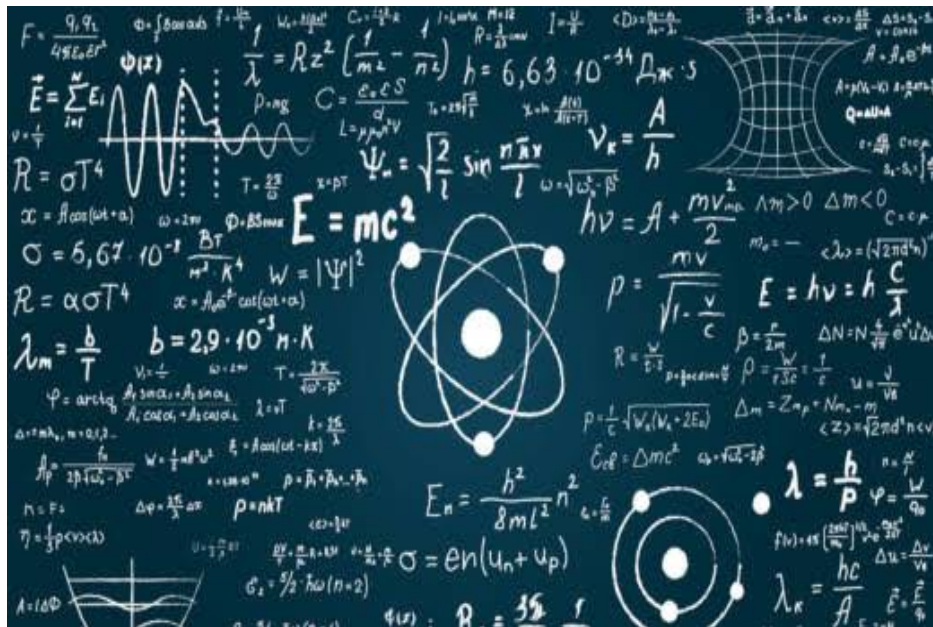
**Course Title:** Symmetries in Quantum Mechanics

**Paper:** Quantum Mechanics II

**Unit:** PHY 422

*If you are not completely confused by quantum mechanics, you do not understand it.*

JOHN WHEELER



## I. IRREDUCIBLE TENSOR OPERATORS

Rotationally symmetric ket  $|jm\rangle \implies [H, \mathbf{J}^2] = 0$ .

$|jm\rangle \xrightarrow{\text{Rotation}} |jm'\rangle$  given by rotation matrix  $D_{m'm}^j(R) = \langle jm' | e^{-i\mathbf{J}\cdot\phi/\hbar} | jm\rangle$ .

$D_{m'm}^j(R)$  is a  $(2j+1) \times (2j+1)$  dimensional matrix. We can write,

$$|jm\rangle \implies \mathcal{U}_R(\phi) |jm\rangle = \sum_{m'} |jm'\rangle \langle jm' | \mathcal{U}_R(\phi) |jm\rangle = \sum_{m'} D_{m'm}^j(R) |jm'\rangle$$

Rotation by an angle  $\alpha$  about  $y$ -axis of a spin-1/2 system,

$$D^{1/2}(\alpha) = \left\langle \frac{1}{2}, m' | e^{-i\sigma_y \alpha/2} | \frac{1}{2}, m \right\rangle = \begin{pmatrix} \cos \frac{\alpha}{2} & -\sin \frac{\alpha}{2} \\ \sin \frac{\alpha}{2} & \cos \frac{\alpha}{2} \end{pmatrix}$$

Well that was easy!!

What for integer values of  $j$ ? Spherical harmonics come to the rescue. Initial ket  $|z\rangle$  is along +ve  $z$ -axis. Final ket  $|n\rangle$  obtained by rotating around  $y$ -axis by  $\theta$  then along  $z$ -axis by  $\phi$ . So,

$$|n\rangle = \mathcal{U}_R(\phi, \theta) |z\rangle = \sum_l \sum_m \mathcal{U}_R(\phi, \theta) |lm\rangle \langle lm | z\rangle$$

Now the inner product with  $\langle lm' |$  gives,

$$\langle lm' | n\rangle = \sum_m D_{m'm}^l(\phi, \theta) \langle lm | z\rangle = \sum_m D_{m'm}^l(\phi, \theta) Y_{lm}^*(\theta, \phi)$$

where,

$$Y_{lm'}^*(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} D_{m'0}^l(\phi, \theta)$$

## II. IRREDUCIBLE SPHERICAL TENSORS

$\mathbf{V}$  is a vector i.e.  $V_i \rightarrow V'_i = R_{ij} V_j$ .

Under rotation  $|\alpha\rangle \rightarrow \mathcal{U}_R |\alpha\rangle$ .

$$\therefore \langle \alpha | V_i | \alpha \rangle \rightarrow \langle \alpha | \mathcal{U}_R^\dagger V_i \mathcal{U}_R | \alpha \rangle = R_{ij} \langle \alpha | V_j | \alpha \rangle$$

For any arbitrary ket,  $\mathcal{U}_R^\dagger V_i \mathcal{U}_R = R_{ij} V_j$ .

Rotation about  $z$ -axis means  $\mathcal{U}_R = 1 - i\epsilon J_z/\hbar$  and  $R(\epsilon) = \begin{pmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$$\therefore V_i + \frac{\epsilon}{i\hbar} [V_i, J_z] = R_{ij}(\epsilon) V_j$$

$$\text{yielding } V_x + \frac{\epsilon}{i\hbar} [V_x, J_z] = V_x - \epsilon V_y,$$

$$V_y + \frac{\epsilon}{i\hbar} [V_y, J_z] = V_y + \epsilon V_x,$$

$$V_z + \frac{\epsilon}{i\hbar} [V_z, J_z] = V_z.$$

$\therefore$  Definition of a tensor of rank 1 i.e., a vector is,

$$[V_i, J_j] = i\epsilon_{ijk} \hbar V_k$$

What about the transformation of higher rank tensors?

A 9-component cartesian tensor  $A_i B_j$  transforms as,

$$A_i B_j = \frac{1}{3} \mathbf{A} \cdot \mathbf{B} \delta_{ij} + \frac{A_i B_j - A_j B_i}{2} + \left( \frac{A_i B_j + A_j B_i}{2} - \frac{1}{3} \mathbf{A} \cdot \mathbf{B} \delta_{ij} \right) \text{ Complicated!!}$$

A spherical tensor of rank  $k$  transforms as,

$$\mathcal{U}_R^\dagger T_q^k \mathcal{U}_R = \sum_{q'=-k}^k D_{qq'}^k(R) T_{q'}^k$$

Well that's much more simplified!

Commutation relations:

$$[J_z, T_q^k] = q\hbar T_q^k,$$

$$[J_+, T_q^k] = \sqrt{k(k+1) - q(q+1)} \hbar T_{q+1}^k,$$

$$[J_-, T_q^k] = \sqrt{k(k+1) - q(q-1)} \hbar T_{q-1}^k.$$

### III. THE WIGNER-ECKART THEOREM

It states that the matrix elements of tensor operators with respect to angular momentum eigenstates satisfy,

$$\langle \alpha', j' m' | T_q^k | \alpha, j m \rangle = \langle j k; m q | j k; j' m' \rangle \frac{\langle \alpha', j' || T^k || \alpha, j \rangle}{\sqrt{2j+1}},$$

where the reduced matrix element is independent of  $m$ ,  $m'$  and  $q$ .

*Proof:* If  $\sum_j a_{ij} x_j = 0$  and  $\sum_j a_{ij} y_j = 0$  with  $i < j$  are two sets of linear homogeneous equations then  $x_j$  and  $y_j$  cannot be individually solved rather they are related  $\forall j$  by  $x_j = c y_j$  where  $c$  is a universal constant.

Now,

$$\begin{aligned} \langle \alpha', j' m' | \sqrt{k(k+1) - q(q+1)} \hbar T_{q+1}^k | \alpha, j m \rangle &= \langle \alpha', j' m' | [J_+, T_q^k] | \alpha, j m \rangle \\ \Rightarrow f_2(j', m') \hbar \langle \alpha', j' m' | T_q^k | \alpha, j m \rangle &= f_1(j, m) \hbar \langle \alpha', j' m' | T_q^k | \alpha, j m \rangle + f_1(k, q) \langle \alpha', j' m' | T_{q+1}^k | \alpha, j m \rangle \end{aligned}$$

Comparing the above with

$$f_2(j, m) \langle m_1, m_2 | j, m-1 \rangle = f_1(j_1, m_1) \langle m_1+1, m_2 | j, m \rangle + f_1(j_2, m_2) \langle m_1, m_2+1 | j, m \rangle$$

with some change in notation which is

$$\langle m_1, m_2+1 | j, m \rangle \rightarrow \langle \alpha', j' m' | T_{q+1}^k | \alpha, j m \rangle$$

we have,

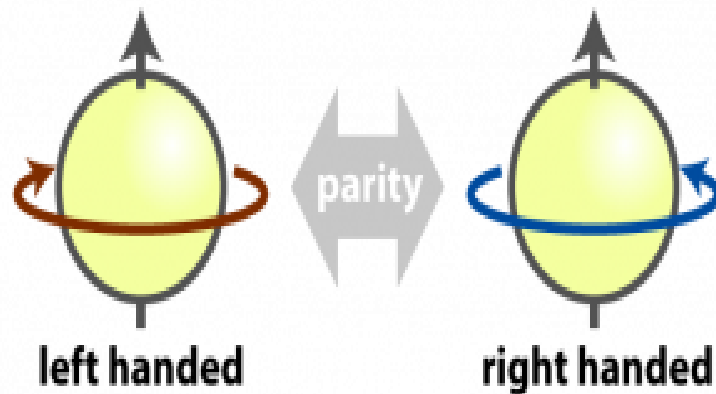
$$\langle \alpha', j' m' | T_{q+1}^k | \alpha, j m \rangle = C \langle m, q+1 | j', m' \rangle.$$

Here  $C$  is the universal proportionality constant independent of  $m$ ,  $m'$  and  $q$ . This constant carries the information about the dynamics of the system and is conventionally written as a double bar matrix element divided by  $\sqrt{2j+1}$ . This completes the proof.

### IV. DISCRETE SYMMETRY

#### A. Parity

- **Passive Viewpoint:** Parity changes a right-handed coordinate system into a left-handed one.



- **Active Viewpoint:** Under parity a ket  $|\alpha\rangle$  is transformed under parity as,  $|\alpha\rangle \rightarrow P|\alpha\rangle$  so that  $\langle\alpha|P^\dagger\mathbf{r}P|\alpha\rangle = -\langle\alpha|\mathbf{r}|\alpha\rangle$  which can be accomplished only if  $\mathbf{r}$  and  $P$  anticommute i.e.,  $\{\mathbf{r}, P\} = 0$ .

Hence, parity is also called space inversion since  $\mathbf{r}$  is the space coordinate.

Again,  $P^2|\mathbf{r}\rangle = |\mathbf{r}\rangle$  so that  $P^2$  has eigenvalue  $+1$ . Thus  $P^{-1} = P^\dagger = P$  has possible eigenvalues  $+1$  and  $-1$ .

*Physical quantities that are odd and even under Parity:*

- $\mathbf{r}$  odd under parity.
- $\mathbf{p}$  odd under parity.
- $\mathbf{L}=\mathbf{r}\times\mathbf{p}$  is even under parity.
- $\mathcal{U}_R$  is even under parity.
- $\mathbf{J}$  is even under parity.
- $\mathbf{S}$  is even under parity since  $\mathbf{J}=\mathbf{L}+\mathbf{S}$ .

1. *How do wave functions behave under parity?*

$\psi(\mathbf{r})$  is even or odd under parity depending on the parity of its state ket  $|\alpha\rangle$ . So,  $\psi(\mathbf{r}) = \psi(-\mathbf{r})$  if  $|\alpha\rangle$  is even under parity and odd otherwise.

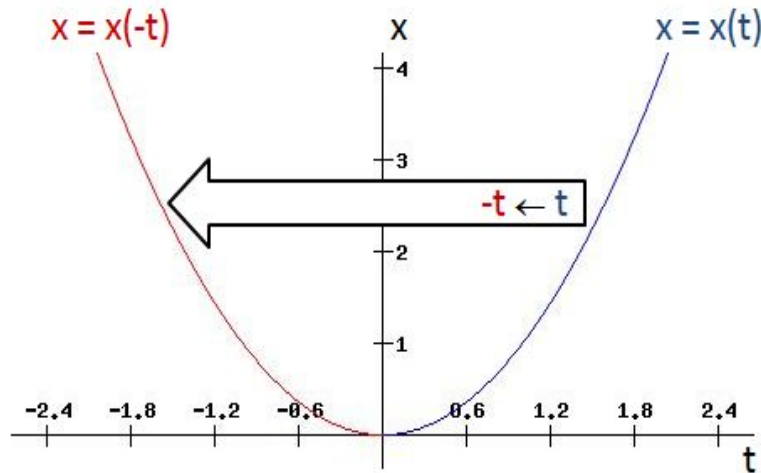
For orbital angular momentum eigenstates,  $\langle \mathbf{r} | \alpha, lm \rangle = R_\alpha(r) Y_{lm}(\theta, \phi)$  and under parity the spherical polar coordinates transform as,  $r \rightarrow r$ ,  $\theta \rightarrow \pi - \theta$  and  $\phi \rightarrow \pi + \phi$  and thus  $Y_{lm} \rightarrow (-1)^l Y_{lm}$ . Thus the orbital angular momentum wave function is even or odd depending on  $l$  being even or odd.

**One important theorem:**

If  $[H, P] = 0$  i.e., Hamiltonian is even under parity with a non-degenerate eigenket,  $|n\rangle$ , with energy  $E_n$  then  $|n\rangle$  is also a parity eigenket.

**Selection rule:** This rule states that parity- odd or even operators always connect states of opposite or same parity.

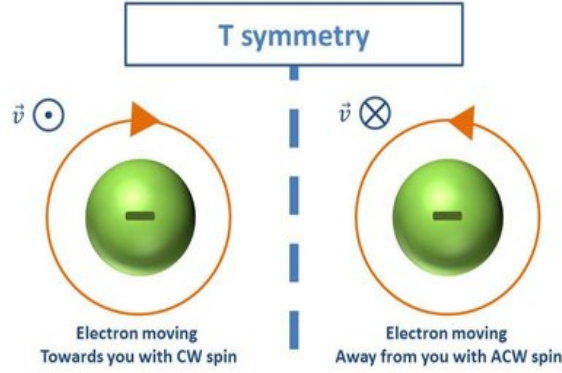
## B. Time reversal



**Time reversal** is nothing but **flashback!**

If the Hamiltonian is symmetric under time reversal that is if  $\mathbf{r}(t)$  is a solution of  $m\ddot{\mathbf{r}} + \nabla V(\mathbf{r})$  then  $\mathbf{r}(-t)$  is also a solution but the force should be conservative.

But the same is not applicable in QM for Schrödinger equation i.e., if  $\psi(\mathbf{r}, t)$  is a solution of the Schrödinger equation then  $\psi(\mathbf{r}, -t)$  is obviously not a solution since Schrödinger equation has first derivative in time. But the complex conjugate,  $\psi^*(\mathbf{r}, -t)$ , is a solution. The time reversed wave function corresponding to  $\psi(\mathbf{r}, t) = \langle \mathbf{r} | \alpha \rangle$  is  $\langle \mathbf{r} | \alpha \rangle^* = \langle \alpha | \mathbf{r} \rangle$ .



**Applying the T symmetry operation  
is like playing a movie in reverse**

For any symmetry operation like  $|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle$  and  $|\beta\rangle \rightarrow |\tilde{\beta}\rangle$  the inner product should be preserved i.e.,  $\langle \tilde{\alpha} | \tilde{\beta} \rangle = \langle \alpha | \beta \rangle$  for unitary operators. But since time reversal is not a unitary operator therefore we have to settle with a weaker condition:  $|\langle \tilde{\alpha} | \tilde{\beta} \rangle| = |\langle \alpha | \beta \rangle|$ . Thus for an antiunitary operator,  $\theta$ , for the transformations,  $|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = \theta |\alpha\rangle$  and  $|\beta\rangle \rightarrow |\tilde{\beta}\rangle = \theta |\beta\rangle$ , we must have,

$$\langle \tilde{\alpha} | \tilde{\beta} \rangle = \langle \alpha | \beta \rangle^* \text{ and } \theta(x |\alpha\rangle + y |\beta\rangle) = x^* \theta |\alpha\rangle + y^* \theta |\beta\rangle .$$

Any antiunitary operator may be defined as  $\theta = UK$ , where  $U$  is a unitary operator and  $K$  is the complex conjugation operator defined as,  $Kc |\beta\rangle = c^* K |\beta\rangle$ .

*Proof:*

Putting  $\theta = UK$  in  $\theta(x |\alpha\rangle + y |\beta\rangle)$  we have,

$$UK(x |\alpha\rangle + y |\beta\rangle) = x^* UK |\alpha\rangle + y^* UK |\beta\rangle = x^* \theta |\alpha\rangle + y^* \theta |\beta\rangle .$$

Thus we get the RHS of the equation  $\theta(x |\alpha\rangle + y |\beta\rangle) = x^* \theta |\alpha\rangle + y^* \theta |\beta\rangle$  which completes the proof.

*Proof of  $\langle \tilde{\alpha} | \tilde{\beta} \rangle = \langle \alpha | \beta \rangle^*$ :*

$|\alpha\rangle$  in terms of basis vectors  $|i\rangle$  is  $|\alpha\rangle = \sum_i |i\rangle \langle i | \alpha \rangle$  and so  $K |i\rangle = |i\rangle$  since  $|i\rangle$  is a column vector with one entry as 1 and rest 0. Thus,

$$|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = \sum_i \langle i | \alpha \rangle^* UK |i\rangle = \sum_i \langle \alpha | i \rangle U |i\rangle .$$

Similarly,  $|\tilde{\beta}\rangle = \sum_j \langle \beta | j \rangle U | j \rangle$  so that  $\langle \tilde{\beta} | = \sum_j \langle j | \beta \rangle \langle j | U^\dagger$ . Thus,

$$\langle \tilde{\beta} | \tilde{\alpha} \rangle = \sum_{i,j} \langle j | \beta \rangle \langle j | U^\dagger U | i \rangle \langle \alpha | i \rangle = \sum_i \langle \alpha | i \rangle \langle i | \beta \rangle = \langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^* .$$

*Physical quantities that are odd and even under Time reversal:*

- $\mathbf{E} \rightarrow \mathbf{E}$ .
- $\mathbf{B} \rightarrow -\mathbf{B}$ .
- $\rho \rightarrow \rho$ .
- $\mathbf{j} \rightarrow -\mathbf{j}$ .
- $\mathbf{v} \rightarrow -\mathbf{v}$ .
- $\mathbf{p} \rightarrow -\mathbf{p}$ .
- $\mathbf{J} \rightarrow -\mathbf{J}$ .
- $\mathbf{r} \rightarrow \mathbf{r}$ .

### 1. Time reversal operator

For antiunitary operators,  $HT = TH$  where  $H$  is the Hamiltonian. To see how operators change under  $T$  consider the transformations,  $|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = T|\alpha\rangle$  and  $|\beta\rangle \rightarrow |\tilde{\beta}\rangle = T|\beta\rangle$  and a linear operator  $O$  for which  $|\gamma\rangle \equiv O^\dagger|\beta\rangle$  so that  $\langle\gamma| = \langle\beta|O$ . Thus,

$$\langle\beta|O|\alpha\rangle = \langle\gamma|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\gamma}\rangle = \langle\tilde{\alpha}|TO^\dagger|\beta\rangle = \langle\tilde{\alpha}|TO^\dagger T^{-1}T|\beta\rangle = \langle\tilde{\alpha}|TO^\dagger T^{-1}|\tilde{\beta}\rangle .$$

For hermitian operator ( $O = O^\dagger$ ) to be even or odd under time reversal one should have  $TOT^{-1} = O$  and  $TOT^{-1} = -O$  respectively.

### 2. How do wave functions behave under time reversal?

For a spin zero single particle system in state  $|\alpha\rangle$  with wave function  $\langle\mathbf{r}|\alpha\rangle$  we have,

$$|\alpha\rangle = \int d^3r |\mathbf{r}\rangle \langle\mathbf{r}|\alpha\rangle .$$

Now on applying time reversal operator we have,

$$T | \alpha \rangle = \int d^3r T | \mathbf{r} \rangle \langle \mathbf{r} | \alpha \rangle^* = \int d^3r | \mathbf{r} \rangle \langle \mathbf{r} | \alpha \rangle^* .$$

Here,  $\mathbf{r}$  is unaffected by the time reversal operator. Thus  $\psi(\mathbf{r}) \xrightarrow{T} \psi^*(\mathbf{r})$ . Even the spherical harmonics  $Y_{lm}(\theta, \phi)$  gets complex conjugated which is nothing but multiplication by  $(-1)^m$  coming from  $e^{-im\phi}$ .

For a Hamiltonian being even under time reversal,  $HT = TH$  or  $HT | n \rangle = TH | n \rangle = E_n T | n \rangle$  where  $| n \rangle$  and  $E_n$  are the energy eigenket and energy eigenvalue. Thus  $T | n \rangle$  and  $| n \rangle$  are both energy eigenkets with eigenvalue  $E_n$  and hence degenerate. If we impose the condition of non-degeneracy then we land up on the conclusion that  $| n \rangle$  and  $T | n \rangle$  must represent the same state. The corresponding wave functions are  $\langle \mathbf{r} | n \rangle$  and  $\langle \mathbf{r} | n \rangle^*$  so that the wave functions are real apart from a position-independent phase factor.

### 3. *Kramers degeneracy*

Here comes spin to make our lives a bit more trickier! Spin behaves like angular momentum because of obvious reasons since spin is nothing but some angular momentum. Thus it is odd under time reversal. We now explore the possibility to construct the representation matrices of the spin generators in such a way that  $S_x$  and  $S_z$  are real while  $S_y$  is imaginary. For this we write  $T = UK$  where  $K$  has nothing to do with the real matrices such that  $\{S_x, U\} = 0$  and  $\{S_z, U\} = 0$ . Whereas for  $S_y$  we have  $[S_y, U] = 0$ . Thus in this particular representation we must have  $U = e^{-i\pi S_y/\hbar}$  giving  $T = e^{-i\pi S_y/\hbar} K$ . For spin-1/2 particles with  $S_y = \frac{1}{2}\hbar\sigma_y$ ,  $T = -i\sigma_y K$  giving  $T^2 = -1$  as  $K$  passing through two imaginary numbers gives a factor of  $(-1)^2$  and  $K^2 = 1$ . Lastly commenting for any general value of spin would be  $T^2 = e^{-2i\pi S_y/\hbar}$  with the general result  $T^2 = (-1)^{2j}$  which is in fact representation independent.

Now what is *Kramers degeneracy*? For this let us take a time reversal symmetric Hamiltonian where both  $| n \rangle$  and  $T | n \rangle$  have energy eigenvalue  $E_n$ . So, are these two states identical? If they are then  $T | n \rangle = e^{i\delta} | n \rangle$  where  $\delta$  is position independent phase factor. Thus,

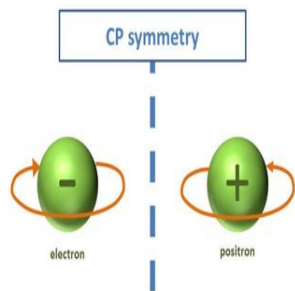
$$T^2 | n \rangle = T e^{i\delta} | n \rangle = e^{-i\delta} T | n \rangle = e^{-i\delta} e^{i\delta} | n \rangle = | n \rangle .$$

This is true for integer values of  $j$ . Thus if the total number of fermions be odd so that  $T^2 = -1$ , the states  $|n\rangle$  and  $T|n\rangle$  are bound to be different and the system must possess a twofold degeneracy irrespective of the form of the Hamiltonian. This is known as *Kramers degeneracy*! This degeneracy can be lifted if we apply any interaction that is odd under time reversal as for example magnetic field. With such  $T$ -odd interactions the degeneracy will get lifted and the two states will split.

Well a small note!

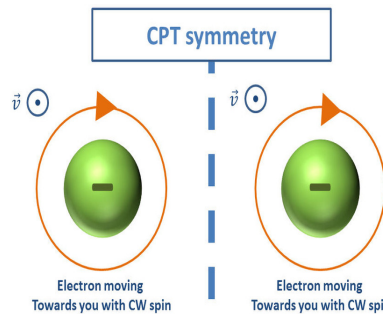
**Charge conjugation** is a transformation that switches all particles with their corresponding antiparticles, and thus changes the sign of all charges: not only electric charge but also the charges relevant to other forces.

Combining all three would give us the well known *CPT symmetry*. Charge, parity, and time reversal symmetry is a fundamental symmetry of physical laws under the simultaneous transformations of charge conjugation ( $C$ ), parity transformation ( $P$ ), and time reversal ( $T$ ). *CPT* is the only combination of  $C$ ,  $P$  and  $T$  that is observed to be an exact symmetry of nature at the fundamental level. The *CPT* theorem says that *CPT* symmetry holds for all physical phenomena, or more precisely, that any Lorentz invariant local quantum field theory with a Hermitian Hamiltonian must have *CPT* symmetry.



Applying the CP symmetry operation transforms matter into antimatter

(a)



The CPT symmetry operation is invariant

(b)