CHANGE OF QUANTUM STATES IN TIME

\[ i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi \]

**SCHRODINGER WAVE EQUATION**

*Hamiltonian*

If independent of time = Energy Operator

Its form is determined by the properties of the system in general:

\[ \hat{H} = \hat{T} + \hat{V} \]

\[ -\frac{\hbar^2}{2m} \hat{\Delta} \]

Potential Energy

Kinetic Energy

\[ \psi = \psi(x, t) \]

If \( \frac{\partial \hat{H}}{\partial t} = 0 \) (does not depend explicitly on the time)

The variables are separated

\[ \psi(x, t) = \psi(x) f(t) \]

\[ \frac{i\hbar}{f} \frac{\partial f}{\partial t} = \left( \frac{\hat{H} \psi(x)}{\psi(x)} \right) = E \] (constant)

**EIGENVALUE PROBLEM**

**STATIONARY STATES**

States with well-defined energy

\[ H \psi_E(x) = E \psi_E(x) \]

**WAVE FUNCTION OF A STATIONARY STATE**

\[ \psi(x, t) = \psi_E(x) e^{-iEt/\hbar} \]

Average value of physical quantity \( F \) (independent of time)

\[ \langle \hat{F} \rangle = \langle \psi(x) | \hat{F} | \psi(x) \rangle \]

Is constant in a stationary state

\( \hat{F} \) has well-defined value in state \( \psi \) if: [\( \hat{F}, \hat{H} \)] = 0
CHANGE IN TIME OF AVERAGE VALUES
OF PHYSICAL QUANTITIES

The average values of physical quantity are independent of the time in stationary states. How such average values change in arbitrary states?

\[ \langle \hat{F} \rangle = \int \psi^* \hat{F} \psi \, dx \equiv \langle \psi | \hat{F} | \psi \rangle = \langle \psi | \hat{F} | \psi \rangle \]

\[ \frac{d \langle \hat{F} \rangle}{dt} = \int \{ \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx + \frac{\partial \psi^*}{\partial t} \hat{F} \psi \, dx + \psi^* \frac{\partial \hat{F} \psi}{\partial t} \, dx \} \]

\[ \frac{\hbar}{i} \frac{\partial \psi}{\partial t} = i \hat{H} \psi \Rightarrow \quad \frac{\partial \psi^*}{\partial t} = \frac{1}{i\hbar} (\hat{H} \psi^*) , \quad \frac{\partial ^* \psi}{\partial t} = -\frac{1}{i\hbar} (\hat{H}^* \psi^*) \]

\[ \frac{d \langle \hat{F} \rangle}{dt} = \int \{ \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx - \frac{1}{i\hbar} (\hat{H} \psi^*) \hat{F} \psi \, dx + \frac{1}{i\hbar} \psi^* \hat{F} (\hat{H} \psi) \, dx \} \]

\[ = \int \{ \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx + \frac{1}{i\hbar} \left( -\hat{H} \psi^* \hat{F} \psi + \psi^* \hat{F} (\hat{H} \psi) \right) \, dx \} \]

\[ (\hat{F}, \hat{A}_q) = (q, \hat{A}_q^*) \]

\[ (\hat{H} \psi, \psi) = (\hat{F} \psi, \psi)^* = (\psi, \hat{H}^* \psi)^* = (\psi, \hat{F} \psi) = \hat{F} \quad \hat{A}_q \]

\[ \int \psi^* \hat{H}^* \psi \, dx , \quad \hat{H}^* = \hat{H} \]

\[ \frac{d \langle \hat{F} \rangle}{dt} = \int \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx + \frac{1}{i\hbar} \int \left( (\psi^*) \hat{H} \psi - (\hat{H} \psi^*) \hat{F} \psi \right) \, dx \]

\[ = \int \{ \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx + \frac{1}{i\hbar} \psi^* [\hat{F}, \hat{H}] \psi \, dx \} \]

\[ \frac{d \hat{F}}{dt} = \int \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx + \frac{1}{i\hbar} \left[ \hat{F}, \hat{H} \right] \psi \, dx \]

**DEF.**

\[ \frac{d \hat{F}}{dt} = \int \psi^* \frac{\partial \hat{F}}{\partial t} \psi \, dx \]

**DERIVATIVE OF OPERATOR IN THE SENSE OF ITS AVERAGE VALUE**

\[ \frac{d \hat{F}}{dt} = \frac{\partial \hat{F}}{\partial t} + \frac{1}{i\hbar} \left[ \hat{F}, \hat{H} \right] \]

"SYMMETRY OF PHYSICS" OPERATOR EQUATION
\[
\frac{dF}{dt} = \frac{df}{dt} + \frac{1}{i\hbar} [F, H] \\
\text{and} \quad \text{if} \quad F = 0 \quad (\text{does not explicitly depend on the time})
\]

**THEN:**

\[
\frac{dF}{dt} = 0 \quad \text{QUANTUM MECHANICAL INTEGRAL OF MOTION}
\]

**DOES NOT CHANGE IN TIME FOR ANY STATE**

### Integrals of Motion and Symmetry

Knowing integrals of motion we can formulate corresponding conservation laws to understand physical properties of a system.

**Integrals of Motion**

\[ \Downarrow \]

**Conservation Laws**

\[ \text{Closely connected with the symmetry of quantum mechanical systems} \]

\[ (= \text{invariance of the Hamiltonian under certain coordinate transformations}) \]

### Unitary Transformations

\[
SS^+ = S^+S = 1 \quad \text{\[S^{-1}\]} \quad \Rightarrow \quad S^+ = S^{-1}
\]

\[ \phi = S \psi \]

**New Function**

**Scalar Product (Hermitian, Inner) is not changed**

\[
(\phi, \phi) = (S\psi, S\psi) = (\psi, S^+S\psi)^* = (\psi, \psi)^* = (\psi, \psi) \quad \text{(Normalization!)}
\]

**How the operators are changed under S?**

\[
S \psi = F_\psi \psi
\]

\[
S \psi' = SF_\psi S^{-1} S \psi
\]

\[ \phi' = \frac{\phi}{\phi} \]

\[ \phi' = F_\phi \phi \quad \text{IF} \quad F_\phi = SF_\psi S^{-1} \]

**Rule of transformation of all operators**
Each physical quantity may be represented by many (\( \infty \)) operators that differ from each other by unitary transformation, however — the properties of such physical quantity must be independent of any transformation.

The following properties have to be conserved:

1. Linearity and hermicity
2. Commutation relations
   \[ \{A, B\} = i \mathcal{C} \]
   \[ S A S^{-1} S B S^{-1} = S B S^{-1} S A S^{-1} \]
   \[ A' \cdot B' = B' \cdot A' = i \mathcal{C}' \]
   \[ \{A', B'\} = i \mathcal{C}' \]
3. Spectrum of eigenvalues is not changed
4. Algebraic relations between operators are not changed
5. Matrix elements are not changed

\[ \langle \psi | F | \phi \rangle = \int \psi^* S F S \psi \phi \, d\xi = \int \psi^* \phi \, d\xi = \langle \psi' | F' | \phi' \rangle \]

The invariance of Hamiltonian under certain transformation \( F \) means

\[ F(H\psi) = H(F\psi) \]

Action of \( F \) on \( H\psi \)  
Action of \( H \) on function \( F\psi \)

\[ \downarrow \text{reduced to the condition} \]

\[ FH = HF \Rightarrow \{F, H\} = 0 \]

- Common eigenfunctions
- Simultaneously measurable observables (if \( F^{ \dagger } = F \), and obviously \( H = H^{\dagger} \))

**Symmetry of Quantum Mechanical System**
LIE'S THEORY OF CONTINUOUS GROUPS
(SOME CONCEPTS) PRESENTATION DUE TO G. RACAH

\[ x^i = f^i(x_0^1, x_0^2, \ldots, x_0^n; a^1, a^2, \ldots, a^n) \]
\[ i = 1, 2, \ldots, n \]

THESE EQUATIONS CARRY
\[ x_0 = (x_0^1, x_0^2, \ldots, x_0^n) \rightarrow x = (x^1, x^2, \ldots, x^n), \text{ both points are in } n\text{-dimensional space} \]

IT IS POSTULATED THAT THE SET OF PARAMETERS
\( (a^1, a^2, \ldots, a^n) = \alpha \) DEFINES THE TRANSFORMATION COMPLETELY AND UNIQUELY

WHEN \( \alpha = 0 \), THE POINT \( x_0 \) IS TRANSFORMED IN ITSELF \( x = f(x, 0) \)

THESE TRANSFORMATIONS FOR VARIOUS \( \alpha \) FORM CONTINUOUS GROUP \( \text{IF:} \)

1. THE RESULT OF PERFORMING IN SUCCESSION TWO TRANSFORMATIONS
\[ x = f(x_0, \alpha), \quad x' = f(x, \beta) \]
\[ x' = f(x_0, \gamma) \]
\[ \gamma = (\varphi \gamma) (a, b) \]
\[ \text{BY SINGLE TRANSFORMATION} \]
\[ \text{REPRODUCED} \]
\[ \text{SUCH PARAMETERS CAN BE FOUND} \]

2. TO EVERY TRANSFORMATION OF THE SET THERE CORRESPONDS A UNIQUE INVERSE TRANSFORMATION THAT ALSO BELONGS TO THE SET

GENERAL TRANSFORMATION
\[ x = f(x_0, \alpha) \]
\[ \text{WHEN } \alpha \text{ ARE CHANGED BY INFINITESIMAL AMOUNTS} \]

THE INCREMENTS IN THE COORDINATES ARE DETERMINED BY THE EQUATION:
\[ dx^i = \frac{\partial f^i(x_0, \alpha)}{\partial a^\sigma} da^\sigma \]  \( \text{(SUM OVER } \sigma \text{ IMPLIED)} \)

BUT
\[ x = f(x_1, \alpha) \Rightarrow dx^i = u^i \delta a^\sigma \]
\[ \text{PARAMETERS OF INFINITESIMAL SIZE} \]
\[ \text{WHERE} \]
\[ u^i = \left( \frac{\partial f^i(x_1, \alpha)}{\partial a^\sigma} \right)_{a=0} \]
The infinitesimal transformation $x \xrightarrow{f} x + dx$ induces in a function $F(x)$ transformation $F(x) \xrightarrow{dF(x)} F(x) + dF(x)$.

Where
\[
\frac{dF(x)}{dx} = \frac{\partial F}{\partial x_i} dx_i
\]

\[
\begin{aligned}
&dx_i = u_i^a \partial \alpha^a \\
&u_i^a = \left( \frac{\partial f_i(x, \alpha)}{\partial \alpha^a} \right)_{\alpha = 0}
\end{aligned}
\]

\[
dF(x) = u_i^a \delta \alpha^a \frac{\partial F}{\partial x_i}
\]

The operator responsible for this infinitesimally close to identity

\[
S_\alpha = 1 + \delta \alpha^a \dot{x}_a
\]

\[
\dot{x}_a = u_i^a (x) \frac{\partial F}{\partial x_i}
\]

Infinite number of infinitesimal transformations $\Rightarrow$ finite transformation

\[
a_j = m \delta a_j \Rightarrow \delta a_j = \frac{a_j}{m} \quad m \to \infty \quad \delta a_j \to 0
\]

\[
U(\delta a_1, \delta a_2, \ldots, \delta a_r) = I + \sum_{k=1}^{r} \delta a_k \dot{x}_k
\]

\[
U(a_1, a_2, \ldots, a_r) = \lim_{m \to \infty} \left[ U\left( \frac{a_1}{m}, \frac{a_2}{m}, \ldots, \frac{a_r}{m} \right) \right]^m = \exp\left( \sum_{k=1}^{r} a_k \dot{x}_k \right)
\]

Group of transformations $U(a_1, a_2, \ldots, a_r)$ determines the symmetry of a system if

\[
[U, \dot{\hat{H}}] = 0 \quad \text{(symmetrical groups)}
\]

Unitary operators $U = U^{-1}$ imply $U^* = U^{-1}$ and $U^2 = I \Rightarrow U = U^{-1} = U^{-1} = U^+$ and $U = U^+$ for observables.
INTEGRALS OF MOTION CONNECTED
WITH THE PROPERTIES OF SPACE AND TIME

\[ \frac{d\hat{F}}{dt} = \frac{\partial \hat{F}}{\partial t} + \frac{1}{i\hbar} [\hat{F}, \hat{H}] \]

PHYSICAL SYSTEM IS DEFINED IF HAMILTONIAN IS GIVEN

IF \[ [\hat{F}, \hat{H}] = 0 \Rightarrow \text{SYMMETRIC GROUP} \]

\[ + \frac{\partial \hat{F}}{\partial t} = 0 \] (INDEPENDENT OF TIME)

\[ \frac{d\hat{F}}{dt} = 0 \Rightarrow \text{CONSERVATION LAW} \]

1. DISPLACEMENT IN TIME - UNIFORMITY OF TIME
TIME DISPLACEMENT OPERATOR (CHANGE OF QUANTUM STATE IN TIME)

\[ S(t-t_0) = e^{-i\frac{\hbar}{\Delta t} \hat{H}(t-t_0)} \]

TRANSFORMATION \( t_0 \rightarrow t \) THROUGH THE INTERVAL \( \Delta t = t-t_0 \)

INFINITESIMAL TRANSFORMATION OF DISPLACEMENT IN TIME BY \( \Delta t \):

\[ U(\Delta t) = I - \frac{i}{\hbar} \Delta t \hat{H} \] INFINITESIMALLY CLOSE TO UNITY \( (\text{IDENTITY}) \)

GENERATOR

SINCE TIME IS UNIFORM THE HAMILTONIAN OF ANY CLOSED SYSTEM (NO EXTERNAL FORCES OR CONSTANT EXTERNAL FORCES) DOES NOT DEPEND EXPlicitly ON THE TIME

\[ \frac{\partial \hat{H}}{\partial t} = 0 \Rightarrow \frac{d\hat{H}}{dt} = \frac{1}{i\hbar} [\hat{H}, \hat{H}] = 0 \]

FROM THE DEF.

\[ \frac{d\langle F \rangle}{dt} = \langle \psi | \frac{d\hat{F}}{dt} | \psi \rangle \Rightarrow \frac{d\langle E \rangle}{dt} = 0 \]

UNIFORMITY OF TIME ENERGY CONSERVATION LAW
UNIFORMITY OF SPACE: PROPERTIES OF A CLOSED SYSTEM DO NOT CHANGE UNDER ANY PARALLEL DISPLACEMENT OF THE SYSTEM AS A WHOLE

HAMILTONIAN OF A SYSTEM MUST BE INVARIANT

INFINITESIMAL DISPLACEMENT $\delta x$

$$D(\delta x) = I - \frac{i}{\hbar} \delta x \hat{d}_x$$

EXAMPLE: DISPLACEMENT IN ONE DIMENSION (DIRECTION)

* $D(\delta x) = I - \frac{i}{\hbar} \delta x \hat{d}_x$, $\delta y = \delta z = 0$

AS A RESULT OF $D$, ANY OPERATOR $\hat{S}$ BECOMES:

$$\hat{S}_D = D \hat{S} D^{-1} = (I - \frac{i}{\hbar} \delta x \hat{d}_x) \hat{S} (I + \frac{i}{\hbar} \delta x \hat{d}_x) = D^{-1} = D^+(UNITARY)$$

$$= (\hat{S} - \frac{i}{\hbar} \delta x \hat{d}_x \hat{S})(I + \frac{i}{\hbar} \delta x \hat{d}_x)$$

$\delta x$ is of infinitesimal size! KEEPING THE FIRST ORDER TERMS

$$\hat{S}_D = \hat{S} - \frac{i}{\hbar} [\hat{d}_x, \hat{S}] \delta x$$

FOR A PARTICULAR OPERATOR: $\hat{S} = \hat{x}, \hat{y}, \hat{z}$ (POSITION OPERATOR)

FROM *

$$\hat{S}_D = x - \delta x, y, z$$

$$x - \delta x = x - \frac{i}{\hbar} \delta x [\hat{d}_x, x]$$

$$\frac{-i\hbar}{\hbar}$$

$$\frac{0}{\hbar}$$

$$[\hat{d}_x, x] = -i\hbar$$

$$[\hat{d}_x, y] = 0$$

$$[\hat{d}_x, z] = 0$$

$$\hat{d}_x = \hat{p}_x$$

GENERATOR OF PARALLEL SPATIAL DISPLACEMENT OF A SYSTEM

MOMENTUM OF A FREE PARTICLE
IN GENERAL

\[ D(\delta \tau) = I - \frac{i}{\hbar} \delta \tau \mathbf{p} , \quad \mathbf{p}(p_x, p_y, p_z) \]

FINITE SPATIAL DISPLACEMENT

\[ D(\tau) = e^{-i\frac{\hbar}{\mathbf{p}} \cdot \mathbf{r}} = e^{-i\frac{\hbar}{\mathbf{p}} x p_x} e^{-i\frac{\hbar}{\mathbf{p}} y p_y} e^{-i\frac{\hbar}{\mathbf{p}} z p_z} \]

The components of momentum \( \mathbf{p} \) commute with each other.

EQUATION OF MOTION

\[ \frac{d\mathbf{p}}{dt} = \frac{\partial \mathbf{p}}{\partial t} + \frac{1}{i\hbar} [\mathbf{p}, H] \Rightarrow \frac{d\mathbf{p}}{dt} = 0 \]

Momentum of a free particle is an integral of motion as a result of uniformity of space.

IN THE CASE OF A SYSTEM OF PARTICLES THE GENERATORS ARE SUM-OPERATOR OF THE MOMENTA OF ALL PARTICLES AND IN variance with respect to spatial displacements

\[ \Rightarrow \text{Law of conservation of the total momentum of a system} \]

3. ISOTROPY OF SPACE = THE EQUIVALENCE OF ALL DIRECTIONS LEADS TO THE INVARIANCE OF THE PROPERTIES OF CLOSED SYSTEMS UNDER ARBITRARY ROTATIONS VAlID ALSO FOR SYSTEMS IN CENTRALLY SYMMETRICAL FIELDS (ATOMS)

ROTATION IN SPACE OF A PHYSICAL SYSTEM IN A STATE REPRESENTED BY KET \( |\alpha\rangle \) OF WAVE FUNCTION \( \psi_\alpha(\tau) \)

\[ \hat{R} = \text{Represented} \begin{bmatrix} R_{xx} & R_{xy} & R_{xz} \\ R_{yx} & R_{yy} & R_{yz} \\ R_{zx} & R_{zy} & R_{zz} \end{bmatrix} \]

\[ \{ R_{ij} = R_{ij}^* \text{ (REAL)} \}
\[ \text{ORTHONORMAL (IN ROWS AND (UNITARY) Columns) } \]
\[ \text{det} |R| = \pm 1 \]

\[ \text{det} |R| = 1 : \text{Proper Rotations} \]
\{ R \} - MATRIX REPRESENTATION OF ROTATIONS
FOR ALL ROTATIONS

9 ELEMENTS - 6 CONDITIONS = 3 PARAMETERS
\( R_{ij} \) (ORTHONORMAL)

\{ R \} FORM THREE-PARAMETER GROUP \( O(3) \) LIE GROUP
THE ORTHOGONAL GROUP
IN THREE DIMENSIONS

- CONTINUOUS: ITS ELEMENTS CAN BE LABELED BY ONE OR MORE
CONTINUOUSLY VARYING PARAMETERS

- COMPACT: EVERY INFINITE SEQUENCE OF ELEMENTS OF THE GROUP
HAS A LIMIT ELEMENT THAT ALSO IS IN THE GROUP

INFINITESIMAL ROTATION

\[ R(\delta \phi) = I - \frac{i}{\hbar} \delta \phi \hat{X} \]

GENERATORS OF INFINITESIMAL
ROTATIONS ABOUT THREE COORDINATE
3 PARAMETERS AXES THROUGH THE ANGLES
\( \delta \phi_x, \delta \phi_y, \delta \phi_z \)

GENERATORS SATISFY THE SAME COMMUTATION
RELATIONS AS
ANGULAR MOMENTUM OPERATORS

\[ R(\delta \phi) = I - \frac{i}{\hbar} \sum_k \delta \phi_k \hat{J}_k \]

FINITE TRANSFORMATION

\[ R(\phi) = e^{-i \phi \hat{J}_z} \]

\[ [\hat{J}_i, \hat{J}_j] = i \hbar \delta_{ij} \]

EQUATION OF MOTION:

\[ \frac{d\hat{J}}{dt} = \frac{\partial \hat{J}}{\partial t} + \frac{i}{\hbar} [\hat{J}, \hat{H}] \]

\( \text{ANGULAR MOMENTUM IS INTEGRAL} \)
OF MOTION IF

\[ [\hat{J}, \hat{H}] = 0 \]

AND ROTATIONS ARE SYMMETRY OPERATIONS
= ISOPTROPY OF SPACE

GOOD QUANT. NUMBERS
MULTIPLE CONSECUTIVE APPLICATIONS OF INFINITESIMAL TRANSFORMATIONS ⇒

CONTINUOUS TRANSFORMATIONS

TRANSLATIONS (SPACE, TIME)

ROTATIONS

INvariance of Hamiltonian ⇒

Conservation Laws

Angular Momentum

Linear Momentum

Energy

These laws correspond to the conservation laws of classical mechanics

Symmetry conditions (quantum mechanics)

Continuous Transform.

Discrete Transform.

- Cannot be reduced to infinitesimal transformations
- Invariance under such transformation does not lead to conservation laws in classical mechanics

In quantum mechanics there is no difference between continuous and discrete transf.

↓

Conservation Laws

Inversion (space, time)

Permutation
4. **Spatial Inversion**: Simultaneous change in sign of all spatial coordinates

\[ x \rightarrow -x, \ y \rightarrow -y, \ z \rightarrow -z \]

Right-handed system \( \rightarrow \) Left-handed system

**Classical Sens:**

- \( \mathbf{r} \rightarrow -\mathbf{r} \)
- \( \mathbf{p} \rightarrow -\mathbf{p} \)
- \( \mathbf{F} \rightarrow -\mathbf{F} \)
- \( \mathbf{t} \rightarrow t \)
- \( E \rightarrow E \) (energy)
- \( m \rightarrow m \)
- \( e \rightarrow e \)

**Classical Equations of Motion and Maxwell Equations are Invariant**; only in Quantum Mechanics it is seen that this invariance leads to a new property.

\[ \hat{\mathbf{p}} \rightarrow -\hat{\mathbf{p}} \]

**Operator**: \( \hat{\mathbf{p}} \psi(\mathbf{r}) = \psi(-\mathbf{r}) \)

(with nuclear & electromagnetic forces)

**The Hamiltonian of a Closed System Is Invariant under an Inversion** (Symmetry between left-handed and right-handed systems of coordinates)

\[ \hat{\mathbf{H}} \hat{\mathbf{p}} = \hat{\mathbf{p}} \hat{\mathbf{H}} \]

**Eigenvalue Problem**:

\[ \hat{\mathbf{p}} \psi(\mathbf{r}) = p \psi(\mathbf{r}) \]

\[ \hat{\mathbf{p}}^2 = \hat{\mathbf{I}} \]

\[ \psi(\mathbf{r}) = p^2 \psi(\mathbf{r}) \Rightarrow p = \pm 1 \]

\[ \hat{\mathbf{p}} \psi(\mathbf{r}) = \pm \psi(\mathbf{r}) \]

**Two Classes of Wave Functions**:

- \( \hat{\mathbf{p}} \psi(\mathbf{r}) = \psi(\mathbf{r}) \Rightarrow \psi_+ (\mathbf{r}) \) Even States
- \( \hat{\mathbf{p}} \psi(\mathbf{r}) = -\psi(\mathbf{r}) \Rightarrow \psi_- (\mathbf{r}) \) Odd States

\[ [\hat{\mathbf{H}}, \hat{\mathbf{p}}] = 0 \]

The Parity of State is an Integral of Motion

**Law**: Conservation of Parity
Not the generators but operators of inversion represent observables

\[ \hat{p}^2 = \hat{I} \]
\[ p^{-1} \hat{p} = \hat{p}^{-1} \quad \text{but} \quad \hat{p}^+ = \hat{p}^{-1} \]
\[ p = p^+ \]

**Parity** - purely quantum mechanical property of a state

**Is it important property?** How far is it from nature?

5. **Time Reversal:** Opposite sense of progression of time

\[ t \rightarrow -t \]

Two classes:

- \( \bar{\psi} \rightarrow \bar{\psi} \)
- \( e \rightarrow e \)
- \( m \rightarrow m \)
- \( \bar{\psi} (=m\bar{\psi}) \rightarrow \bar{\psi} \)
- \( \bar{t} \rightarrow -\bar{t} \)
- \( \bar{p} \rightarrow -\bar{p} \)
- \( \bar{l} \rightarrow -\bar{l} \)

\( \hat{\mathcal{J}} \) - symmetry operator for closed isolated physical systems

If \( \psi_k \) is an eigenstate of Hamiltonian (independent of time) with energy eigenvalue \( E_k \), then \( \hat{\mathcal{J}} \psi_k \) is also the eigenstate with the same eigenvalue

\[ [\hat{\mathcal{J}}, \hat{A}] = 0 \]
\[ \hat{\mathcal{J}} = \hat{\mathcal{O}} \hat{\mathcal{K}} \]

**Complex Conjugation Operator**

**Antiunitary Operator**

\[ \hat{\mathcal{K}} : \hat{\mathcal{K}} \psi_k = \psi_k^* \]

\[ \hat{\mathcal{K}} (c_1 \psi_1 + c_2 \psi_2) = c_1^* \hat{\mathcal{K}} \psi_1 + c_2^* \hat{\mathcal{K}} \psi_2 \]

\[ \hat{\mathcal{K}}^2 = \hat{1} \]

**How to find operator \( \hat{\mathcal{O}} \)?**

**Its form depends on Hamiltonian**

1. **Hamiltonian for particles without spin** (without external electromagnetic field)
   
   \[ \hat{H} = \hat{H} \text{ (real)} \]
   
   \[ \hat{H}^* = \hat{H} \]
   
   \[ \hat{O} = \hat{1} \]
   
   \[ \hat{\mathcal{J}} = \hat{\mathcal{K}} \]
2. HAMILTONIAN WITH SPIN-DEPENDENT OPERATORS (SPIN \(1/2\))

\[ \hat{\mathbf{\sigma}} \]

**Operator Equation**

\[ \hat{\sigma}_x \hat{\sigma}^*_x = -\hat{\sigma}_x \hat{\sigma}_x \]

If the representation of \(\hat{\sigma}\) is the following:

\[ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

Then

\[ \sigma_x = i \sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

\[ \hat{\mathbf{\sigma}} = i \sigma_y \hat{\mathbf{\mathbf{\chi}}} \]

For the system of \(N\) particles with spin \(1/2\) (electrons)

\[ \hat{\mathbf{J}}_N = i^N \sigma_{_1} \sigma_{_2} \ldots \sigma_{_N} \hat{\mathbf{\chi}} \]

\[ \hat{\mathbf{J}}_N^2 = (-1)^N \]

**Conclusions:**

\[ H \Psi = E \Psi \]

\[ [H, \sigma_j] = 0 \quad \sigma_j H \psi = H \sigma_j \psi \]

\[ H \sigma_j \psi = E \sigma_j \psi \quad \Rightarrow \quad \sigma_j \psi = \alpha \psi \quad |\alpha|^2 = 1 \]

**Eigenvalue Problem**

\[ \begin{cases} \sigma_j \psi = \alpha \psi \\ \sigma_j^2 \psi = \sigma_j (\sigma_j \psi) = \alpha \sigma_j \psi \end{cases} \]

\[ (-1)^N \psi \]

**Only if** \(N = \text{even}\)!

What happens if \(N\) is odd?

The assumption \(\psi\) is not correct!

\(\sigma_j \psi \} \quad \text{TWO DIFFERENT FUNCTIONS} \quad \text{KRAMERS DOUBLETS}\)
6. PERMUTATIONS - IF ALL PARTICLES IN A SYSTEM ARE THE SAME (IDENTICAL), THE HAMILTONIAN IS INVARIANT UNDER INTERCHANGE OF POSITION OF ANY TWO PARTICLES

\[ \hat{P}_{kl} : \text{OPERATOR OF PERMUTATION OF PARTICLES } k \text{ AND } l \]

\[ \hat{P}_{kl} H = H \hat{P}_{kl} \]

INTEGRAL OF MOTION

SYMMETRY CONDITIONS

EXAMPLE: TWO PARTICLES

\[ \hat{P}_{12} \psi(1,2) = \lambda \psi(1,2) \]

REAL EIGENVALUE

\[ P_{12}^2 \psi(1,2) = \lambda^2 \psi(1,2) \]

\[ \psi(1,2) = \lambda^2 \psi(1,2) \Rightarrow \lambda^2 = \pm 1 \]

\[ \hat{P}_{12} \psi_s(1,2) = \psi_s(1,2) \]

SYMmetric FUNCTION

\[ \hat{P}_{12} \psi_a(1,2) = -\psi_a(1,2) \]

ANTISYMMETRIC FUNCTION

FOR ARBITRARY NUMBER OF IDENTICAL PARTICLES: THE WAVEFUNCTION HAS TO BE OF THE SAME SYMMETRY WITH RESPECT TO THE INTERCHANGE OF ANY PAIR OF PARTICLES; THE SYMMETRY OF THE WAVEFUNCTION CANNOT BE CHANGED BY AN EXTERNAL PERTURBATION

NORMALIZED

SYMmetric FUNCTION

\[ \frac{1}{N!} \sum_{\pi} \hat{P}\psi = \gamma_s \]

Fermions

(INTEGRAL SPIN)

\[ 0, \frac{\hbar}{2}, 2\frac{\hbar}{2}, ... \]

CONCLUSION:

BASIC POSTULATE:

INDISTINGUISHABILITY OF IDENTICAL PARTICLES
ANTISYMMETRIC FUNCTION (IDENTICAL FERMIONS)

\[ \Psi_A^{(1\ldots N)} = \frac{1}{\sqrt{N!}} \sum_{\pi} (-1)^{\pi} \Gamma^\pi \Psi^{(1\ldots N)} \]

SINGLE-PARTICLE APPROXIMATION (SINGLE-ELECTRON APP.)

\[ \Psi^{(1\ldots N)} = \Phi_1(1)\Phi_2(2)\ldots\Phi_N(N) \]

\[ \pm \Phi_1(3)\Phi_2(2)\ldots\Phi_N(N) \]

\[ \pm \Phi_1(5)\Phi_2(1)\ldots\Phi_N(N) \]

\[ \vdots \]

\[ N! \text{ POSSESSIONS} \]

\[ N=2 \]

\[ \Psi_A^{(1,2)} = \frac{1}{\sqrt{2}} \left( \Phi_1(1)\Phi_2(2) - \Phi_1(2)\Phi_2(1) \right) = \frac{1}{\sqrt{2}} \begin{vmatrix} \Phi_1(1) & \Phi_1(2) \\ \Phi_2(1) & \Phi_2(2) \end{vmatrix} \]

SLATER DETERMINANT

IN GENERAL

\[ \Psi_A^{(1\ldots N)} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Phi_1(1) & \Phi_1(2) & \ldots & \Phi_1(N) \\ \Phi_2(1) & \Phi_2(2) & \ldots & \Phi_2(N) \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_N(1) & \Phi_N(2) & \ldots & \Phi_N(N) \end{vmatrix} \]

ALL POSSIBILITIES (N!) TAKEN INTO ACCOUNT

PAULI PRINCIPLE INCLUDED!