CHANGE OF QUANTUM STATES IN TIME

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

SCHRÖDINGER WAVE EQUATION

HAMILTONIAN

IF INDEPENDENT OF TIME = ENERGY OPERATOR

ITS FORM IS DETERMINED BY THE PROPERIES OF THE SYSTEM

IN GENERAL:

$$\hat{H} = \underbrace{\hat{T}}_{-\frac{\hbar^2}{2m}\Delta} + \hat{V}$$

POTENTIAL ENERGY

KINETIC ENERGY

$$\Psi \equiv \Psi(x,t)$$

IF $\frac{\partial H}{\partial t} = 0$ (DOES NOT DEPEND EXPLICITLY ON THE TIME)

THE VARIABLES ARE SEPARATED $\Psi(x,t) = \Psi(x) f(t)$

$$\frac{i\hbar}{f}\frac{\partial f}{\partial t} = \underbrace{\frac{H\Psi(x)}{\Psi(x)} = E}$$ (CONSTANT)

$$H\Psi_E(x) = E\,\Psi_E(x)$$ EIGENVALUE PROBLEM

STATIONARY STATES

STATES WITH WELL-DEFINED ENERGY

$$\Downarrow$$

$$f(t) = e^{-iEt/\hbar}$$

WAVE FUNCTION OF A STATIONARY STATE

$$\Psi(x,t) = \Psi_E(x)\, e^{-iEt/\hbar}$$

AVERAGE VALUE OF PHYSICAL QUANTITY F (INDEP. 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 Ψ IF: $[\hat{F}, H] = 0$)

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?

$$\langle\hat{F}\rangle = \int \psi^* \hat{F} \psi \, dx \equiv (\psi, \hat{F}\psi) \equiv \langle\psi|\hat{F}|\psi\rangle$$

$$\frac{d\langle F\rangle}{dt} = \int \left\{ \psi^* \frac{\partial F}{\partial t} \psi \, dx + \frac{\partial \psi^*}{\partial t} F \psi \, dx + \psi^* F \frac{\partial \psi}{\partial t} dx \right\}$$

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

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

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

$$(f, Ag) = (g, A^+ f)^*$$

$$(H\psi, F\psi) = (\underbrace{F\psi}_{f}, \underbrace{H}_{A}\underbrace{\psi}_{g})^* = (\psi, H^+ F\psi)^{**} = (\psi, H^+ F \psi) =$$

$$\int \psi^* H^+ F \psi \, dx, \quad H^+ = H$$

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

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

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

DEF. $\frac{d\langle\hat{F}\rangle}{dt} = \int \psi^* \frac{d\hat{F}}{dt} \psi \, dx$ DERIVATIVE OF OPERATOR IN THE SENSE OF ITS AVERAGE VALUE

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

OPERATOR EQUATION

" SYMMETRY OF PHYSICS "

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

IF: $\frac{\partial F}{\partial t} = 0$ (DOES NOT EXPLICITLY DEPEND ON THE TIME) and IF: $[F,H] = 0$ (COMMUTES WITH HAMILTONIAN)

THEN:

$$\frac{dF}{dt} = 0$$

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 } CLOSELY CONNECTED WITH THE SYMMETRY OF QUATUM MECHANICAL SYSTEMS (= INVARIANCE OF THE HAMILT. UNDER CERTAIN COORDINATE TRANSFORMAT.)

UNITARY TRANSFORMATIONS

$$SS^+ = S^+S = 1\!\!1 \quad / S^{-1} \quad \Rightarrow \quad S^+ = S^{-1}$$

$$\phi = S\,\Psi$$

NEW FUNCTION

SCALAR PRODUCT (HERMITEAN, INNERT –) IS NOT CHANGED

$$(\phi,\phi) = (S\Psi, S\Psi) = (\Psi, S^+S\Psi)^* = (\Psi,\Psi)^* = \langle\Psi,\Psi\rangle$$ (NORMALIZATION!)

HOW THE OPERATORS ARE CHANGED UNDER S?

$$S \backslash \quad \Psi' = F_\Psi \Psi$$

$$\underbrace{S\Psi'}_{\phi'} = S F_\Psi S^{-1} \underbrace{S\Psi}_{\phi}$$

$$\phi' = F_\phi \phi \quad \text{IF} \quad F_\phi = S F_\Psi S^{-1}$$

RULE OF TRANSFORMATION OF ALL OPERATORS

EACH PHYSICAL QUANTITY MAY BE REPRESENTED BY MANY (∞) 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

$$ {}_S\backslash [A,B]=iC /_{S^{-1}} $$

$$ SAS^{-1}SBS^{-1} - SBS^{-1}SAS^{-1} = iSCS^{-1} $$

$$ A' \quad B' \quad - \quad B' \quad A' \quad = iC' \qquad [A',B']=iC' $$

3. SPECTRUM OF EIGENVALUES IS NOT CHANGED
4. ALGEBRAIC RELATIONS BETWEEN OPERATORS ARE NOT CHANGED
5. MATRIX ELEMENTS ARE NOT CHANGED

$$ \langle\psi|F|\phi\rangle = \int \psi^* F \phi \, d\tau = \int \underbrace{\psi^* S^{-1}}_{\psi'} \underbrace{SFS^{-1}}_{F'} \underbrace{S\phi}_{\phi'} d\tau = \langle\psi'|F'|\phi'\rangle $$

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 $F\psi$

$\Downarrow$ REDUCED TO THE CONDITION

$$ FH = HF \Rightarrow [F,H]=0 $$

$\Downarrow$

– COMMON EIGENFUNCTIONS
– SIMULTANEOUSLY MEASURABLE OBSERVABLES (IF $F^+=F$, AND OBVIOUSLY $H=H^+$)

SYMMETRY OF QUANTUM MECHANICAL SYSTEM

LIE'S THEORY OF CONTINUOUS GROUPS

(SOME CONCEPTS) PRESENTATION DUE TO G. RACAH

$$x^i = f^i(x_0^1, x_0^2, \dots x_0^n; a^1, a^2, \dots a^r)$$

$i = 1, 2, \dots n$ THESE EQUATIONS CARRY

$x_0 = (x_0^1, x_0^2, \cdots x_0^n) \Longrightarrow x = (x^1, x^2, \dots x^n)$, BOTH POINTS ARE IN n- DIMENSIONAL SPACE

IT IS POSTULATED THAT THE SET OF PARAMETERS

$(a^1, a^2, \dots a^r) = a$ DEFINES THE TRANSFORMATION COMPLETELY AND UNIQUELY

WHEN $a = 0$, THE POINT x_0 IS TRANSFORMED IN ITSELF $x = f(x, 0)$

THESE TRANSFORMATIONS FOR VARIOUS a FORM CONTINUOUS GROUP IF:

1. THE RESULT OF PERFORMING IN SUCCESSION TWO TRANSFORMATIONS

   $x = f(x_0, a)$, $x' = f(x, b)$ $\underline{\underline{\text{REPRODUCED}}}$ BY SINGLE TRANSFORMATION

   $$x' = f(x_0, c)$$

   SUCH PARAMETERS CAN BE FOUND $c^\sigma = \varphi^\sigma(a, b)$

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

GENERAL TRANSFORMATION

$x = f(x_0, a)$ WHEN a ARE CHANGED BY INFINITESIMAL AMOUNTS

THE INCREMENTS IN THE COORDINATES ARE DETEMINED BY THE EQUATION:

$$dx^i = \frac{\partial f^i(x_0, a)}{\partial a^\sigma} da^\sigma \qquad \text{(SUM OVER } \sigma \text{ IMPLIED)}$$

BUT SINCE $x = f(x, 0) \Rightarrow$

$$dx^i = u_\sigma^i \, \delta a^\sigma$$

← PARAMETERS OF INFINITESIMAL SIZE

WHERE $u_\sigma^i = \left(\dfrac{\partial f^i(x, a)}{\partial a^\sigma}\right)_{a=0}$

THE INFINITESIMAL TRANSFORMATION

$x \xrightarrow{f} x + dx$ INDUCES IN A FUNCTION $F(x)$ TRANSFORMATION

$$F(x) \longrightarrow F(x) + dF(x)$$

WHERE

$$dF(x) = \frac{\partial F}{\partial x^i} dx^i$$

$$\begin{cases} dx^i = u^i_\sigma \delta a^\sigma \\ u^i_\sigma = \left(\dfrac{\partial f^i(x,a)}{\partial a^\sigma} \right)_{a=0} \end{cases}$$

$$dF(x) = u^i_\sigma \delta a^\sigma \frac{\partial F}{\partial x^i}$$

THE OPERATOR RESPONSIBLE FOR THIS

$$S_a = 1 + \delta a^\sigma \hat{X}_\sigma$$

INFINITESIMALLY CLOSE TO IDENTITY

$$\hat{X}_\sigma = u^i_\sigma (x) \frac{\partial}{\partial x^i}$$

INFINITESIMAL OPERATORS OF THE GROUP

X_σ – GENERATORS, THEY SATISFY EQUATION:

$$[\hat{X}_\sigma, \hat{X}_\varsigma] = C^\tau_{\sigma\varsigma} \hat{X}_\tau$$

STRUCTURE CONSTANTS

THIS EQUATION DEFINES THE STRUCTURE OF THE GROUP

WHEN PERFORMING IN SUCCESSION INFINITE NUMBER OF INFINITESIMAL TRANSFORMATIONS $\Rightarrow$ FINITE TRANSFORMATION

$$a_j = n\delta a_j \Rightarrow \delta a_j = \frac{a_j}{n} \; : \; \begin{array}{l} n \to \infty \\ \delta a_j \to 0 \end{array}$$

$$U(\delta a_1, \delta a_2, \ldots \delta a_r) = I + \sum_{k=1}^{r} \delta a_k X_k$$

$$U(a_1, a_2, \ldots a_r) = \lim_{n\to\infty} \left[U\left(\frac{a_1}{n}, \frac{a_2}{n}, \ldots \frac{a_r}{n}\right) \right]^n =$$

$$= \lim_{n\to\infty} \left(I + \sum_{k=1}^{r} \frac{a_k}{n} X_k \right)^n = \exp\left(\sum_{k=1}^{r} a_k \hat{X}_k \right)$$

GROUP OF TRANSFORMATIONS $U(a_1, a_2, \ldots a_r)$ DETERMINES THE SYMMETRY OF A SYSTEM IF

$$[\hat{U}, \hat{H}] = 0$$

(SYMMETRICAL GROUPS)

$U^+ = U^{-1}$ (UNITARY OPERATORS)

IF IN PARTICULAR

$U^2 = I \Rightarrow U = U^{-1} \Rightarrow U^{-1} = U^+$ AND $\boxed{U = U^+}$ } **OBSERVABLES** (THE SAME PROPERTIES ARE VALID FOR GENERATORS)

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

$+ \frac{\partial F}{\partial t} = 0$ (INDEPENDENT OF TIME)

$\frac{dF}{dt} = 0$ $\Rightarrow$ CONSERVATION LAW

1. DISPLACEMENT IN TIME - UNIFORMITY OF TIME

TIME DISPLACEMENT OPERATOR (CHANGE OF QUANTUM STATE IN TIME)

$$S(t-t_0) = e^{-i/\hbar \hat{H}(t-t_0)}$$

TRANSFORMATION $t_0 \xrightarrow{S} t$ THROUGH THE INTERVAL $\Delta t = t - t_0$

INFINITESIMAL TRANSFORMATION OF DISPLACEMENT IN TIME BY δt:

$$U(\delta t) = \hat{I} - \frac{i}{\hbar}\delta t \hat{H}$$

INFINITESIMALLY CLOSE TO UNITY (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

$$\frac{\partial H}{\partial t} = 0 \quad \Rightarrow \quad \frac{dH}{dt} = \frac{1}{i\hbar}[H, H] = 0$$

HAMILTONIAN IS INVARIANT

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

$\Downarrow$

ENERGY CONSERVATION LAW

2. UNIFORMITY OF SPACE: PROPERTIES OF A CLOSED SYSTEM DO NOT CHANGE UNDER ANY PARALLEL DISPLACEMENT OF THE SYSTEM AS A WHOLE

$\Downarrow$

HAMILTONIAN OF A SYSTEM MUST BE INVARIANT

INFINITESIMAL DISPLACEMENT $\delta\vec{r}$

$$D(\delta\vec{r}) = I - \frac{i}{\hbar}\,\delta\vec{r}\,\hat{\vec{d}}$$

GENERATORS

$$\delta\vec{r} = \delta x\,\delta y\,\delta z$$

EXAMPLE: DISPLACEMENT IN ONE DIMENSION (DIRECTION)

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

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

$$\Omega_D = D\Omega D^{-1} = \left(I - \frac{i}{\hbar}\delta x\,\hat{d}_x\right)\Omega\left(I + \frac{i}{\hbar}\delta x\,\hat{d}_x\right) =$$

$D^{-1} = D^{+}$ (UNITARY)

$$= \left(\Omega - \frac{i}{\hbar}\delta x\,\hat{d}_x\Omega\right)\left(I + \frac{i}{\hbar}\delta x\,\hat{d}_x\right) =$$

$$= \Omega + \frac{i}{\hbar}\Omega\,\delta x\,\hat{d}_x - \frac{i}{\hbar}\delta x\,\hat{d}_x\Omega + \cancel{\frac{1}{\hbar^2}\delta x^2 \hat{d}_x\Omega\hat{d}_x}$$

δx is of infinitesimal size! KEEPING THE FIRST ORDER TERMS

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

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

FROM $*$

$$\Omega_D = x - \delta x \quad , \quad y \quad , \quad z$$

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

$$y = y - \frac{i}{\hbar}\underbrace{[\hat{d}_x, y]}_{0}\,\delta x$$

$$z = z - \frac{i}{\hbar}\underbrace{[\hat{d}_x, z]}_{0}\,\delta x$$

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

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

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

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

MOMENTUM OF A FREE PARTICL

GENERATOR OF PARALLEL SPATIAL DISPLACEMENT OF A SYSTEM

IN GENERAL

$$D(\delta\bar{r}) = I - \frac{i}{\hbar}\delta\bar{r}\,\bar{p}\ , \qquad \bar{p}(p_x, p_y, p_z)$$

FINITE SPATIAL DISPLACEMENT

$$D(\bar{r}) = e^{-i/\hbar\,\bar{r}\bar{p}} = e^{-i/\hbar\, x p_x}\, e^{-i/\hbar\, y p_y}\, e^{-i/\hbar\, z p_z}$$

THE COMPONENTS OF MOMENTUM $\hat{\bar{p}}$ COMMUTE WITH EACH OTHER

EQUATION OF MOTION

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

IF POTENTIAL IS CONSTANT
HAMILTONIAN IS INVARIANT

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

INVARIANCE WITH RESPECT TO SPATIAL DISPLACEMENTS

$\Rightarrow$ **LAW OF CONSERVATION OF THE TOTAL MOMENTUM OF A SYSTEM**

3. ISOTROPY OF SPACE $\equiv$ THE EQUIVALECE 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 $\psi_\alpha(\bar{r})$

$$\hat{R} \underset{\text{REPRESENTED}}{=} \begin{bmatrix} R_{xx} & R_{xy} & R_{xz} \\ R_{yx} & R_{yy} & R_{yz} \\ R_{zx} & R_{zy} & R_{zz} \end{bmatrix}$$

ROTATION OPERATOR

$R_{ij} = R_{ij}^*$ (REAL)

ORTHONORMAL (IN ROWS AND COLUMNS)

(UNITARY)

$\det|R| = \pm 1$

$\det|R| = 1$: PROPER ROTATIONS

$\{R\}$ – MATRIX REPRESENTATION OF ROTATIONS
FOR ALL ROTATIONS

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

$\{R\}$ 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

$$R(\delta\bar{\varphi}) = I - \frac{i}{\hbar}\,\delta\bar{\varphi}\,\hat{X}$$

3 PARAMETERS

GENERATORS OF INFINITESIMAL ROTATIONS ABOUT THREE COORDINATE AXES THROUGH THE ANGLES $\delta\varphi_x, \delta\varphi_y, \delta\varphi_z$

GENERATORS SATISFY THE SAME COMMUTATION RELATIONS AS ANGULAR MOMENTUM OPERATORS

$$R(\delta\bar{\varphi}) = I - \frac{i}{\hbar}\sum_{k}^{3}\delta\varphi_k\,\hat{J}_k$$

WHICH ANGULAR MOMENTUM?

ORBITAL ℓ, L, SPIN S, s
TOTAL J, INTERMEDIATE...

THE CHOICE DEPENDS ON HAMILTONIAN

FINITE TRANSFORMATION

$$R(\varphi) = e^{-i/\hbar\,\bar{\varphi}\bar{J}}$$

$[J_i, J_k] = i\hbar J_l$

EQUATION OF MOTION:

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

$$\frac{\partial\hat{J}}{\partial t} = 0$$

ANGULAR MOMENTUM IS INTEGRAL OF MOTION IF

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

AND ROTATIONS ARE SYMMETRY OPERATIONS = ISOTROPY OF SPACE

$Af_A = \alpha f_A$, $[A,B]=0$

$B \backslash$ $BAf_A = ABf_A = \alpha Bf_A$

$Bf_A = \beta f_A$

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 TRANSFOR.

- 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

$x \to -x, \quad y \to -y, \quad z \to -z$

RIGHT-HANDED SYSTEM $\Rightarrow$ LEFT-HANDED SYSTEM

CLASSICAL SENS:

$\bar{r} \to -\bar{r}$

$\bar{p} \to -\bar{p}$

$\bar{v} \to -\bar{v}$

$\bar{F} \to -\bar{F}$

ALL POLAR VECTORS

$\bar{L} = \bar{r} \times \bar{p} \to \bar{L}$ (AXIAL VECTOR = PSEUDOVECTOR)

$t \to t$

$E \to E$ (energy)

$m \to m$

$e \to e$

CLASSICAL EQUATIONS OF MOTION AND MAXWELL EQUATIONS ARE INVARIANT; ONLY IN QUANTUM MECHANICS IT IS SEEN THAT THIS INVARIANCE LEADS TO A NEW PROPERTY.

$\hat{P}$ - OPERATOR : $\hat{P}\,\psi(\bar{r}) = \psi(-\bar{r})$

THE HAMILTONIAN OF A CLOSED SYSTEM (WITH NUCLEAR & ELECTROMAGNETIC FORCES) IS INVARIANT UNDER AN INVERSION (≡ SYMMETRY BETWEEN LEFT-HANDED AND RIGHT-HANDED SYSTEMS OF COORDINATES)

$$\hat{H}\hat{P} = \hat{P}\hat{H}$$

(THE CASE OF WEAK INTERACTIONS THAT DETERMINE β-DECAY OF ATOMIC NUCLEI AND DECAY OF MUONS, PIONS AND HYPERONES IS EXCLUDED)

$$\psi(-\bar{r}) = p\,\psi(\bar{r})$$

EIGENVALUE PROBLEM:

$$\hat{P}\,\psi(\bar{r}) = p\,\psi(\bar{r}) \quad \Big/ \hat{P}$$

$\hat{P}^2 = \hat{I}$

$$\psi(\bar{r}) = p^2\,\psi(\bar{r}) \Rightarrow p = \pm 1$$

$$\hat{P}\,\psi(\bar{r}) = \pm\,\psi(\bar{r})$$

TWO CLASSES OF WAVE FUNCTIONS:

$\hat{P}\,\psi(\bar{r}) = \psi(\bar{r}) \Rightarrow \psi_+(\bar{r})$ EVEN STATES

$\hat{P}\,\psi(\bar{r}) = -\psi(\bar{r}) \Rightarrow \psi_-(\bar{r})$ ODD STATES

SINCE $[\hat{H}, \hat{P}] = 0$ THE PARITY OF STATE IS AN INTEGRAL OF MOTION

LAW: CONSERVATION OF PARITY

NOT THE GENERATORS BUT OPERATORS OF INVERSION REPRESENT OBSERVABLES

$$P^{-1} \backslash \hat{P}^2 = \hat{I}$$

$$\hat{P} = \hat{P}^{-1} \quad \text{BUT} \quad \hat{P}^+ = \hat{P}^{-1}$$

$$P = P^+$$

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

$$t \to -t$$

TWO CLASSES:

$\bar{r} \to \bar{r}$	$t \to -t$
$e \to e$	$\bar{v} \to -\bar{v}$
$m \to m$	$\bar{p} \to -\bar{p}$
$\bar{F}(=m\ddot{\bar{r}}) \Rightarrow \bar{F}$	$\bar{l} \to -\bar{l}$

$\hat{J}$ – SYMMETRY OPERATOR FOR CLOSED ISOLATED PHYSICAL SYSTEMS

IF $\Psi_{\bar{k}}$ IS AN EIGENSTATE OF HAMILTONIAN (INDEPENDENT OF TIME) WITH ENERGY EIGENVALUE $E_{\bar{k}}$, THEN $J\Psi_{\bar{k}}$ IS ALSO THE EIGENSTATE WITH THE SAME EIGENVALUE

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

Ψ_a: $\quad i\hbar \frac{\partial \Psi_a}{\partial t} = H\Psi_a$ SCHRÖDINGER EQUATION

$\downarrow \hat{\mathcal{T}}$

Ψ_{-a} $\quad -i\hbar \frac{\partial \Psi_{-a}}{\partial t} = H\Psi_{-a}$ H IS INVARIANT

$t \to -t$

COMPLEX CONJUGATE $\quad -i\hbar \frac{\partial \Psi_a^*}{\partial t} = H^*\Psi_a^*$ VERY SIMILAR!

$\hat{O}$

ASSUMPTION:

$\forall \hat{O}$: $\quad \hat{O}^+ = \hat{O}^{-1}$, $\quad \hat{O}\hat{H}^* = \hat{H}\hat{O}$ OPERATOR EQUATION

$$-i\hbar \frac{\partial O\Psi_a^*}{\partial t} = OH^*\Psi_a^*$$

$$-i\hbar \frac{\partial O\Psi_a^*}{\partial t} = HO\Psi_a^*$$

$\Psi_{-a} = \hat{\mathcal{T}}\Psi_a$: $\quad \Psi_{-a} = O\Psi_a^* = O\mathcal{K}\Psi_a$

$$\boxed{\hat{\mathcal{T}} = \hat{O}\hat{\mathcal{K}}}$$

COMPLEX CONJUGATION OPERATOR

ANTIUNITARY OPERATOR

$\hat{\mathcal{K}}$: $\quad \hat{\mathcal{K}}\Psi_k = \Psi_k^*$ ANTILINEAR OPERATOR { DOES NOT REPRESEN ANY OF OBSERVABLES

$\hat{\mathcal{K}}(c_1\Psi_1 + c_2\Psi_2) = c_1^*\mathcal{K}\Psi_1 + c_2^*\mathcal{K}\Psi_2$

$\hat{\mathcal{K}}^2 = \hat{I}$

HOW TO FIND OPERATOR $\hat{O}$? **ITS FORM DEPENDS ON HAMILTONIAN**

1. HAMILTONIAN FOR PARTICLES WITHOUT SPIN $(S=0)$ (WITHOUT EXTERNAL ELECTROMAGNETIC FIELD)

$\hat{H}^* = \hat{H}$ (REAL)

$$OH^* = HO = OH \Rightarrow \hat{O} = \hat{1}$$

$$\hat{\mathcal{T}} = \hat{\mathcal{K}}$$

2. HAMILTONIAN WITH SPIN-DEPENDENT OPERATORS (SPIN 1/2)

$\hat{O} \equiv \hat{O}_\sigma$

OPERATOR EQUATION $\quad \hat{O}_\sigma \bar{\sigma}^* = -\bar{\sigma}\, \hat{O}_\sigma$

IF THE REPRESENTATION OF $\bar{\sigma}$ IS THE FOLLOWING:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

THEN

$$O_\sigma = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\hat{\mathcal{T}} = i\sigma_y \hat{\mathcal{K}}$$

FOR THE SYSTEM OF N PARTICLES WITH SPIN 1/2 (ELECTRONS)

$$\mathcal{T}_N = i^N \sigma_{1y} \sigma_{2y} \ldots \sigma_{Ny} \hat{\mathcal{K}}$$

$\hat{\mathcal{T}}_N \hat{\mathcal{T}}_N \equiv \hat{\mathcal{T}}_N^2 = (-1)^N \qquad$ N - NUMBER OF PARTICLES

CONCLUSIONS:

$$H\Psi = E\Psi$$

$(*)$ THESE FUNCTIONS HAVE TO BE LINEARLY DEPENDENT!

$[H, \mathcal{T}_n] = 0 \qquad \mathcal{T}_n H \Psi = \mathcal{T}_n E \Psi$

$$H(\mathcal{T}_n\Psi) = E(\mathcal{T}_n\Psi) \Rightarrow \mathcal{T}_n \Psi = a\Psi \ , \ |a|^2 = 1$$

EIGENVALUE PROBLEM

$$\mathcal{T}_n \Psi = a\Psi$$

$$\mathcal{T}_n^2 \Psi = \mathcal{T}_n (a\Psi) = a^* \mathcal{T}_n \Psi = a^* a\, \Psi = \Psi$$

$$\mathcal{T}_n^2 \Psi = (-1)^N \Psi$$

ONLY IF N = EVEN!

WHAT HAPPENS IF N IS ODD?

THE ASSUMPTION $(*)$ **IS NOT CORRECT!**

$\left.\begin{matrix} \mathcal{T}_n \Psi \\ \Psi \end{matrix}\right\}$ TWO DIFFERENT FUNCTIONS

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

$\hat{P}_{kl}$: OPERATOR OF PERMUTATION OF PARTICLES K. 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

$P^2 = \mathbb{1}$, $P^+ = P^{-1}$

P^{-1}

$P = P^{-1}$ $P = P^+$

$\hat{P}_{12}$

$$P_{12}^2 \Psi(1,2) = \lambda^2 \Psi(1,2)$$

$$\Psi(1,2) = \lambda^2 \Psi(1,2) \Rightarrow \lambda^2 = \pm 1$$

$$\hat{P}_{12} \Psi_s(1,2) = \Psi_s(1,2)$$ SYMMETRIC FUNCTION

$$\hat{P}_{12} \Psi_a(1,2) = -\Psi_a(1,2)$$ ANTISYMMETRIC FUNCTION

FOR ARBITRARY NUMBER OF IDENTCAL 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

$$\frac{1}{\sqrt{N!}} \sum_P \hat{P} |\Psi\rangle = |\Psi_s\rangle$$

NUMBER OF PERMUT.

BOSONS

(INTEGRAL SPIN)
$0, \hbar, 2\hbar, \ldots$

ANTISYMMETRIC FUNCTION

$$\frac{1}{\sqrt{N!}} \sum_P (-1)^{\varepsilon(P)} \hat{P} |\Psi\rangle = |\Psi_A\rangle$$

FERMIONS

(HALF-ODD-INTEGRAL SPIN)
$1/2\hbar, 3/2\hbar, 5/2\hbar \ldots$
ELECTRONS, PROTONS, NEUTRONS

CONCLUSION:

BASIC POSTULATE:

INDISTINGUISHABILITY OF IDENTICAL PARTICLES

ANTISYMMETRIC FUNCTION (IDENTICAL FERMIONS)

$$\Psi_A(1\ldots N) = \frac{1}{\sqrt{N!}} \sum_{\hat{P}} (-1)^{\varepsilon(\hat{P})} \hat{P}\, \Psi(1\ldots N)$$

SINGLE-PARTICLE APPROXIMATION (SINGLE-ELECTRON APP.)

$$\Psi(1,\ldots N) = \varphi_1(1)\varphi_2(2)\ldots\varphi_N(N)$$

$$?\pm \varphi_1(3)\varphi_2(2)\ldots\varphi_N(N)$$

$$?\pm \varphi_1(5)\varphi_2(1)\ldots\varphi_N(N)$$

$$\vdots$$

$\varphi_i(i)$ – SINGLE PARTICLE STATES

$N!$ POSSIBILITIES

$N=2$

$$\Psi_A(1,2) = \frac{1}{\sqrt{2}}\big(\varphi_1(1)\varphi_2(2) - \overset{\varepsilon(P)=1}{\varphi_1(2)\varphi_2(1)}\big) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_1(1) & \varphi_1(2) \\ \varphi_2(1) & \varphi_2(2) \end{vmatrix}$$

SLATER DETERMINANT

IN GENERAL

$$\Psi_A(1\ldots N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_1(1) & \varphi_1(2) & \ldots & \varphi_1(N) \\ \varphi_2(1) & \varphi_2(2) & \ldots & \varphi_2(N) \\ \vdots & \vdots & & \vdots \\ \varphi_N(1) & \varphi_N(2) & \ldots & \varphi_N(N) \end{vmatrix}$$

ALL POSSIBILITIES ($N!$) TAKEN INTO ACCOUNT

PAULI PRINCIPLE INCLUDED!