# Advanced Quantum Mechanics

Winter term 2019/20

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## Chapter 1 : Recapitulation : structure of the quantum theory

### 1.1 State space

* classical mechanics : maximal information = values $\{q_i, p_i\} \in$ phase space (coordinates $q_i$, momenta $p_i$)

* quantum mechanics : state vector $|\psi\rangle$ in a typically $\infty$-dimensional state space $\mathcal{H}$ known as Hilbert space (axioms: see books, Nolting / Weinberg)

Dirac's "bra-ket" notation : $|\psi\rangle \in \mathcal{H}$ ("ket")

Norm $\| |\psi\rangle \|^2 = (|\psi\rangle, |\psi\rangle)$

Scalar product : $(|\varphi\rangle, |\psi\rangle) \in \mathbb{C}$

Properties : linearity $(|\chi\rangle, [\alpha|\psi\rangle + \beta|\varphi\rangle]) = \alpha(|\chi\rangle, |\psi\rangle) + \beta(|\chi\rangle, |\varphi\rangle)$

symmetry $(|\varphi\rangle, |\psi\rangle)^* = (|\psi\rangle, |\varphi\rangle)$

positivity $(|\psi\rangle, |\psi\rangle) > 0$ for $|\psi\rangle \neq \underset{\text{zero vector}}{\underbrace{0}}$

Special case:

$\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3)$ square-integrable functions on $\mathbb{R}^3$

$$(|\varphi\rangle, |\psi\rangle) = \int d^3x \; \varphi^*(\vec{x}) \, \psi(\vec{x})$$

Describe one non-relativistic particle.

Remark: $|\psi\rangle$ and $\lambda|\psi\rangle$ $(\lambda \neq 0, \lambda \in \mathbb{C})$ describe the same state.

Physical state is a one-dimensional complex subspace of $\mathcal{H}$ (equivalence class, projective geometry)

Convention: take representative

$\| |\psi\rangle \| = 1$ → still $\{e^{i\alpha}|\psi\rangle \mid \alpha \in \mathbb{R}\}$ one state

* Dual space

$\mathcal{H}^*$ is the space of linear functionals $\mathcal{H} \longrightarrow \mathbb{C}$

For each "ket" $|\varphi\rangle$ there is a "bra" $\langle\varphi|$ such that

$$\langle\varphi|\psi\rangle = (\langle\varphi|, \langle\psi|)$$

This defines a mapping

$$\mathcal{H} \longrightarrow \mathcal{H}^*$$
$$|\varphi\rangle \longmapsto \langle\varphi|$$

It is anti-linear: $(\lambda|\varphi\rangle) \longmapsto \lambda^*\langle\varphi|$

Proof: $(\lambda|\varphi\rangle, |\psi\rangle) = (|\psi\rangle, \lambda|\varphi\rangle)^* = \lambda^*(|\varphi\rangle, |\psi\rangle)$ ∎

* Continuum states

states of the type $\langle p|p'\rangle = \delta(p-p')$, $p, p' \in \mathbb{R}$

$\Rightarrow \langle p|p\rangle = \delta(0) = \infty$

not a physical state (distributions)

Superposition of continuum states can form a physical state

Example: plane waves $e^{i\vec{p}\cdot\vec{x}}$ enlarge the space $\mathcal{L}^2(\mathbb{R}^3)$

Continuum states also have "bra-ket" mapping

* In the following we write the scalar product in the "bra-ket" notation:

$$\langle \chi | \psi \rangle \equiv \left( |\chi\rangle , |\psi\rangle \right) .$$

## 1.2 Observable

Consider an operator

$$\begin{aligned} A : \mathcal{H} &\longrightarrow \mathcal{H} \\ |\psi\rangle &\longmapsto A|\psi\rangle \end{aligned}$$

A is linear if $A\left(|\psi\rangle + |\varphi\rangle\right) = A|\psi\rangle + A|\varphi\rangle$ , $A(\lambda|\psi\rangle) = \lambda A|\psi\rangle$

The adjoint $A^+$ of any operator A (linear or not) is defined through:

$$\begin{tikzcd}
\mathcal{H} : \; |\psi\rangle \arrow[r, mapsto] \arrow[d, mapsto] & A^+|\psi\rangle =: |\chi\rangle \arrow[d, mapsto] \\
\mathcal{H}^* : \; \langle\psi| \arrow[r, mapsto] & \langle\psi| A = \langle\chi|
\end{tikzcd}$$

$$\Longleftrightarrow \quad \langle \varphi | A^+ | \psi \rangle = \langle \psi | A | \varphi \rangle^*$$

Proof: define $|\chi\rangle = A^+|\psi\rangle$, so $\langle\chi| = \langle\psi|A$ :

$$\langle\varphi|A^+|\psi\rangle = \langle\varphi|\chi\rangle \underset{\substack{\uparrow \\ \text{property of scalar product}}}{=} \langle\chi|\varphi\rangle^* = \langle\psi|A|\varphi\rangle^* \qquad \blacksquare$$

It follows: $(\lambda A)^+ = \lambda^* A^+$ .

Basis $\{|i\rangle\}$ of $\mathcal{H}$ : any $|\psi\rangle = \sum_i c_i |i\rangle$ . A is linear

$$(A^+)_{ij} = \langle i|A^+|j\rangle = \langle j|A|i\rangle^* = (A_{ji})^*$$

$\Longleftrightarrow$ matrices, adjoint = transposed complex conjugate

A is Hermitian or self-adjoint if A is linear and $A = A^+$.

Physical measurable quantities are represented by Hermitian operators.

Expectation value:

$$\langle A\rangle_{|\psi\rangle} = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle} = \langle\psi|A|\psi\rangle \quad \text{if} \quad \langle\psi|\psi\rangle = 1$$

$$A = A^{+} \Rightarrow \langle A\rangle_{|\psi\rangle} \text{ is real.}$$

### 1.2.1 Discrete spectrum

A Hermitian with discrete eigenvectors

$$A|i\rangle = a_i|i\rangle \quad , \; i\in\mathbb{N} \quad , \; \langle i|i\rangle = 1 \; .$$

- $a_i \in \mathbb{R}$

  Proof: $a_i = \langle i|a_i|i\rangle = \langle i|A|i\rangle \underset{\overset{\uparrow}{A=A^{+}}}{=} \langle i|A|i\rangle^{*} = a_i^{*}$ ☒

- Eigenvectors are orthogonal.

  Proof: $\langle i|A|j\rangle = a_j\langle i|j\rangle = \langle j|A^{+}|i\rangle^{*} = a_i\langle i|j\rangle$

  If $a_i \neq a_j \Rightarrow \langle i|j\rangle = 0$.

  If eigenvalue $a_i = a_j$ is degenerate one can choose multiple eigenvectors to the same $a_i$ such that $\langle i|j\rangle = \delta_{ij}$ (Gram-Schmidt). ☒

- Completeness (Proof is non-trivial):

$$\sum_i \underbrace{|i\rangle\langle i|}_{\text{projector onto } |i\rangle} = \underbrace{\mathbb{1}}_{\text{identity operator}}$$

$\{|i\rangle\}$ form a complete orthonormal set (CON)

$$\Rightarrow |\psi\rangle = \underbrace{\sum_i |i\rangle\langle i|}_{\mathbb{1}}\psi\rangle = \sum_i \underbrace{\langle i|\psi\rangle}_{\text{component w.r.t. CON}} |i\rangle$$

$$A|\psi\rangle = \sum_i A|i\rangle\langle i|\psi\rangle = \sum_i a_i |i\rangle\langle i|\psi\rangle$$

$$\Rightarrow \quad A = \sum_i a_i |i\rangle\langle i| \quad \text{spectral decomposition}$$

$$A^2 = \sum_{i,j} a_i a_j |i\rangle \underbrace{\langle i|j\rangle}_{=\delta_{ij}} \langle j| = \sum_i a_i^2 |i\rangle\langle i|$$

Definition: $f(A) := \sum_i f(a_i) |i\rangle\langle i|$ function of operator A

* Physical interpretation:

$\{a_i\}$ are the possible quantized measurement values of A

$$\langle A\rangle_{|\psi\rangle} = \sum_i a_i \langle\psi|i\rangle\langle i|\psi\rangle = \sum_i a_i |\langle i|\psi\rangle|^2 \qquad (\langle\psi|\psi\rangle = 1)$$

$$= \sum_i a_i p_i$$

$p_i = |\langle i|\psi\rangle|^2$ = probability to measure value $a_i$ for state $|\psi\rangle$

$$1 = \langle\psi|\psi\rangle = \sum_i p_i \ , \quad p_i \geq 0$$

* Complete set of observables:

A and B form a complete set of observables if:

1. $[A, B] = AB - BA = 0$
2. for a pair of eigenvalues $a_i$ of A and $b_i$ of B there exists only one eigenvector $|i\rangle$ (no further degeneracy)

Property 1. implies that there exists a basis of simultaneous eigenvectors $A|i\rangle = a_i|i\rangle$ , $B|i\rangle = b_i|i\rangle$.

The definition can be generalized for more than two observables

Example: hydrogen atom

Hamilton operator H, angular momentum $\vec{L}^2$ and its component $L_3$ form a complete set.

* Preparation of a quantum system in a definite state:

$$|\psi\rangle \xrightarrow[\substack{\text{a complete set} \\ A, B, \dots, M}]{\text{measurement of}} \text{filters values } (a_i, b_i, \dots, m_i)$$

⇒ The systems is afterwards in the prepared state $|a_i\, b_i \cdots m_i\rangle$

⇒ collapse of the wave function $|\psi\rangle$.

## 1.2.2. Position and momentum

Examples of observables with a continuum spectrum (range of values)

For a non-relativistic particle there are position operators

$$\vec{\hat{x}} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$$

and associated continuum eigenstates $|\vec{y}\rangle$ with

$$\vec{\hat{x}}\,|\vec{y}\rangle = \vec{y}\,|\vec{y}\rangle \quad , \quad \hat{x}_j\,|\vec{y}\rangle = y_j\,|\vec{y}\rangle \ , j \in 1,2,3 \ , \ y_j \in \mathbb{R} .$$

Spectrum of $\hat{x}_j = \mathbb{R}$.

$\hat{x}_j^+ = \hat{x}_j$, Hermitian.

* $\hat{x}_1, \hat{x}_2, \hat{x}_3$ are simultaneously diagonal in the basis $|\vec{y}\rangle$

⇒ $[\hat{x}_i, \hat{x}_j] = 0$

* 3 components can be measured simultaneously

* eigenvectors are indexed by the eigenvalue $(\vec{y})$

$\{\hat{x}_1, \hat{x}_2, \hat{x}_3\}$ is a complete set

* continuum states: $\langle \vec{y} | \vec{z} \rangle = \delta^{(3)}(\vec{y} - \vec{z}) = \prod_{i=1}^{3} \delta(y_i - z_i)$

* completeness: $\int d^3y\, |\vec{y}\rangle \langle \vec{y}| = \mathbb{1}$

$$|\psi\rangle = \int d^3y \; |\vec{y}\rangle \, \langle \vec{y}|\psi\rangle$$

$\langle \vec{y}|\psi\rangle =: \psi(\vec{y})$ : wave function, Schrödinger representation

* isomorphism $\mathcal{H} \cong \mathcal{L}^2(\mathbb{R}^3)$ :

$$\langle \varphi|\psi\rangle = \langle \varphi| \underbrace{\int d^3y \; |\vec{y}\rangle\langle \vec{y}|}_{\mathbb{1}} \psi\rangle = \int d^3y \; \varphi^*(\vec{y})\,\psi(\vec{y})$$

$$\langle \psi|\psi\rangle < \infty \iff \int d^3y \; |\psi(\vec{y})|^2 < \infty$$

* action of the position operator in the Schrödinger representation:

$$|\psi\rangle \longmapsto \hat{x}_j \, |\psi\rangle$$

$$\psi(\vec{y}) = \langle \vec{y}|\psi\rangle \longmapsto \langle \vec{y}|\,\hat{x}_j|\psi\rangle = y_j \langle \vec{y}|\psi\rangle = y_i \, \psi(\vec{y})$$

multiplication operator. Interpretation:

$$\langle \psi|\vec{\hat{x}}\,|\psi\rangle = \int d^3y \; \langle \psi|\vec{y}\rangle\langle \vec{y}|\vec{\hat{x}}|\psi\rangle = \int d^3y \; \vec{y} \; |\langle \vec{y}|\psi\rangle|^2$$

$$\rho(\vec{y}) = |\langle \vec{y}|\psi\rangle|^2$$

$\rho(\vec{y})\, d^3y$ = probability that the particle is in a small volume $d^3y$ centered at $\vec{y}$

$$\int d^3y \; \rho(\vec{y}) = \langle \psi|\psi\rangle = 1$$

Observable: $P_{\Delta V} = \int_{\Delta V} d^3x \; |\vec{x}\rangle\langle \vec{x}|$

$\langle \psi|\, P_{\Delta V}\, |\psi\rangle = \int_{\Delta V} d^3x \; \rho(\vec{x})$ probability to find the particle in a volume $\Delta V$

$\cong \rho(\vec{x}) \underbrace{|\Delta V|}_{\text{volume}}$ if $|\Delta V|$ small and $\rho$ smooth

Preparation of a state: localize a particle in $\Delta V$ through measurement $\Rightarrow$ collapse of $|\psi\rangle$ to $P_{\Delta V}|\psi\rangle$ = state after the measurement

Momentum operator $\vec{\hat{p}}$:

$$\langle\vec{x}|\hat{p}_j|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x_j}\langle\vec{x}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x_j}\psi(\vec{x})$$

$\hbar = \frac{h}{2\pi}$, $h$ = Planck's constant = $6.6262 \times 10^{-34}$ J·s

$\hat{p}_j$ is Hermitian:

$$\langle\vec{x}|\hat{p}_j^\dagger|\psi\rangle = \langle\psi|\hat{p}_j|\vec{x}\rangle^* = \left[\int d^3y\, \langle\psi|\vec{y}\rangle \frac{\hbar}{i}\frac{\partial}{\partial y_j}\langle\vec{y}|\vec{x}\rangle\right]^* \overset{\leftarrow \text{partial integration}}{=}$$

$$= \left[\int d^3y \left(-\frac{\hbar}{i}\frac{\partial}{\partial y_j}\langle\psi|\vec{y}\rangle\right)\langle\vec{y}|\vec{x}\rangle\right]^*$$

$$= \int d^3y\, \langle\vec{x}|\vec{y}\rangle \frac{\hbar}{i}\frac{\partial}{\partial y_j}\langle\vec{y}|\psi\rangle = \langle\vec{x}|\hat{p}_j|\psi\rangle$$

Definition of $\hat{p}_j$ implies $[\hat{p}_j, \hat{x}_k] = \frac{\hbar}{i}\delta_{jk}$:

$$\langle\vec{y}|\hat{p}_j\hat{x}_k|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial y_j}\langle\vec{y}|\hat{x}_k|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial y_j} y_k\langle\vec{y}|\psi\rangle$$

$$= \frac{\hbar}{i}\delta_{jk}\langle\vec{y}|\psi\rangle + y_k\frac{\hbar}{i}\frac{\partial}{\partial y_j}\langle\vec{y}|\psi\rangle$$

$$= \langle\vec{y}|\frac{\hbar}{i}\delta_{jk} + \hat{x}_k\hat{p}_j|\psi\rangle$$

- operator identity
- $\hat{p}_1, \hat{x}_1$ cannot be simultaneously measured

Eigenstates of $\vec{\hat{p}}$: $\hat{p}_j|\vec{q}\rangle = q_j|\vec{q}\rangle$:

$$\langle\vec{x}|\hat{p}_j|\vec{q}\rangle = q_j\langle\vec{x}|\vec{q}\rangle \Leftrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x_j}\langle\vec{x}|\vec{q}\rangle = q_j\langle\vec{x}|\vec{q}\rangle$$

$$\Rightarrow \langle\vec{x}|\vec{q}\rangle = N\cdot e^{\frac{i}{\hbar}\vec{q}\cdot\vec{x}}$$

$$\langle \vec q\,|\,\vec q\,'\rangle = \int d^3x\,\langle \vec q\,|\,\vec x\rangle\langle \vec x\,|\,\vec q\,'\rangle = |N|^2 \int d^3x\; e^{\frac{i}{\hbar}(\vec q\,'-\vec q)\cdot\vec x}$$

$$= \delta^{(3)}(\vec q-\vec q\,') \quad \text{if} \quad N = (2\pi\hbar)^{-\frac{3}{2}}$$

$$\rightsquigarrow \quad \langle \vec x\,|\,\vec q\,'\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{\frac{i}{\hbar}\vec q\,'\cdot\vec x}$$

$$\left.\begin{array}{l} \langle \vec x\,|\,\psi\rangle = \psi(\vec x) \\[1em] \langle \vec q\,|\,\psi\rangle =: \tilde\psi(\vec q) \end{array}\right\} \quad \psi \text{ and } \tilde\psi \text{ are related by Fourier transformation}$$

$$\tilde\psi(\vec q) = \int d^3x\,\langle \vec q\,|\,\vec x\rangle\langle \vec x\,|\,\psi\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3x\;\psi(\vec x)\,e^{-\frac{i}{\hbar}\vec q\cdot\vec x}$$

### 1.2.3 Heisenberg Uncertainty Principle

discrete spectrum ; $\langle\psi|\psi\rangle = 1$ :

$p_i = |\langle i|\psi\rangle|^2$ = probability to measure the value $a_i$ for the observable $A = \sum_i a_i\,|i\rangle\langle i|$

Remark: in case of degenerate orthonormal states $|i,k\rangle$ with the same eigenvalue $a_i$: $p_i = \sum_k |\langle i,k|\psi\rangle|^2$

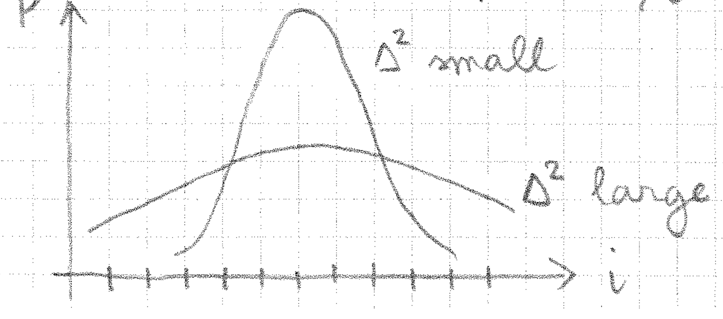
Mean value ("expectation value"): $\bar a = \sum_i p_i a_i = \langle\psi|A\psi\rangle = \langle A\rangle_{|\psi\rangle}$

Uncertainty, defined as the root mean square deviation:

$$\Delta^2_{A,|\psi\rangle} = \sum_i p_i\,(a_i-\bar a)^2 \geq 0$$

$$\Delta^2_{A,|\psi\rangle} = 0 \quad \Rightarrow \quad p_i\,(a_i-\bar a)^2 = 0 \quad \forall i$$

$$\Rightarrow \quad p_i = \delta_{i,i_0} \quad \Rightarrow \quad |\psi\rangle = (\text{phase})\cdot|i_0\rangle$$



$$\Delta^2_{A,|\psi\rangle} = \sum_i p_i \, (a_i - \bar{a})^2 = \sum_i |\langle i|\psi\rangle|^2 (a_i - \bar{a})^2$$

$$= \langle\psi| \left[ \sum_i |i\rangle\langle i| \, (a_i - \bar{a})^2 \right] |\psi\rangle$$

$$= \langle\psi| \, (A - \bar{a})^2 |\psi\rangle$$

$$= \| (A - \bar{a})|\psi\rangle \|^2 = \text{norm squared of } (A - \bar{a})|\psi\rangle$$

$$= \langle\psi| \, A^2 - 2\bar{a}A + \bar{a}^2 |\psi\rangle$$

$$= \langle\psi| \, A^2 |\psi\rangle - (\langle\psi|A|\psi\rangle)^2$$

Generalized version of the Heisenberg uncertainty principle: when $[A,B] = iC$ $(\Rightarrow C = C^+)$ for observables $A, B$, then the following holds for any normed state $|\psi\rangle$, $\langle\psi|\psi\rangle = 1$:

$$\Delta^2_{A,|\psi\rangle} \cdot \Delta^2_{B,|\psi\rangle} \geq \frac{1}{4} \left( \langle\psi|C|\psi\rangle \right)^2 .$$

Proof: see exercises.

Define $a = A - \bar{a}$, $a = a^+$; $b = B - \bar{b}$, $b = b^+$

Schwarz inequality: for any two states $|\chi\rangle$ and $|\chi'\rangle$

$$|\langle\chi'|\chi\rangle|^2 \leq \langle\chi'|\chi'\rangle \langle\chi|\chi\rangle$$

Let $|\chi\rangle = b|\psi\rangle$, $|\chi'\rangle = a|\psi\rangle$ :

$$|\langle\psi|ab|\psi\rangle|^2 \leq \langle\psi|a^2|\psi\rangle \langle\psi|b^2|\psi\rangle = \Delta^2_{A,|\psi\rangle} \cdot \Delta^2_{B,|\psi\rangle}$$

$$|\langle\psi|ab|\psi\rangle|^2 = \langle\psi|ab|\psi\rangle \cdot \langle\psi|ab|\psi\rangle^* = \langle\psi|ab|\psi\rangle \cdot \langle\psi|\underbrace{ba}_{=(ab)^+}|\psi\rangle$$

$$ab = \frac{1}{2}\{a,b\} + \frac{1}{2}[a,b] \qquad (\{a,b\} = ab + ba \text{ anti-commutator})$$

$$ba = \frac{1}{2}\{a,b\} - \frac{1}{2}[a,b]$$

$$|\langle\psi|ab|\psi\rangle|^2 = \langle\psi| \tfrac{1}{2}\{a,b\} + \tfrac{1}{2}[a,b] |\psi\rangle \cdot \langle\psi| \tfrac{1}{2}\{a,b\} - \tfrac{1}{2}[a,b] |\psi\rangle$$

$$= \left( \langle\psi| \tfrac{1}{2}\{a,b\} |\psi\rangle \right)^2 - \left( \langle\psi| \tfrac{1}{2}[a,b] |\psi\rangle \right)^2$$

$$|\langle\psi|ab|\psi\rangle|^2 = \frac{1}{4}\underbrace{\left(\langle\psi|\{a,b\}|\psi\rangle\right)^2}_{\text{real}\,,\,\geq 0} + \frac{1}{4}\underbrace{\left(\langle\psi|\,i[a,b]\,|\psi\rangle\right)^2}_{\text{real}\,,\,\geq 0}$$

since $\{a,b\}$ and $i[a,b]$ are Hermitian.

$$i[a,b] = i\left[(A-\bar{a}),(B-\bar{b})\right] = i[A,B] = -C$$

$$\Rightarrow \quad \Delta^2_{A,|\psi\rangle}\cdot\Delta^2_{B,|\psi\rangle} \geq |\langle\psi|ab|\psi\rangle|^2 \geq \frac{1}{4}\left(\langle\psi|C|\psi\rangle\right)^2$$

$\boxed{\text{k}}$

Special case: $A = \hat{x}_k$, $B = \hat{p}_k$, $[\hat{x}_k, \hat{p}_k] = i\hbar$ $\quad (C = \hbar\cdot\mathbb{1})$

$$\Rightarrow \Delta^2_{\hat{x}_k,|\psi\rangle}\cdot\Delta^2_{\hat{p}_k,|\psi\rangle} \geq \frac{\hbar^2}{4}$$

* $\hat{x}_k$, $\hat{p}_k$ cannot be simultaneously measure with arbitrary precision

* $\hat{x}_k$ - eigenstate $\Rightarrow$ $\hat{p}_k$ completely undetermined and vice-versa

## 1.3 Dynamics (time evolution)

Hamilton operator $H = H^+$ determines the time evolution through Schrödinger's equation:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H\,|\psi(t)\rangle$$

* initial condition $|\psi(t_0)\rangle$ through preparation

* $|\psi(t)\rangle$ unique solution

Time evolution of the expectation value of an observable A:

$$\langle A\rangle_{|\psi(t)\rangle} = \frac{\langle\psi(t)|A|\psi(t)\rangle}{\langle\psi(t)|\psi(t)\rangle}$$

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle \longmapsto \langle\psi(t)|\frac{i}{\hbar}H^+ = \langle\psi(t)|\frac{i}{\hbar}H$$

$$\Rightarrow \frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \frac{i}{\hbar}\langle\psi(t)|H|\psi(t)\rangle - \frac{i}{\hbar}\langle\psi(t)|H|\psi(t)\rangle = 0$$

$$\frac{d}{dt}\langle\psi(t)|A|\psi(t)\rangle = \frac{i}{\hbar}\langle\psi(t)|HA|\psi(t)\rangle - \frac{i}{\hbar}\langle\psi(t)|AH|\psi(t)\rangle$$

$$+ \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle$$

$$= -\frac{i}{\hbar}\langle\psi(t)|[A,H]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle$$

Choosing $\langle\psi(t_0)|\psi(t_0)\rangle = 1 \Rightarrow \langle\psi(t)|\psi(t)\rangle = 1 \quad \forall t \Rightarrow$

$$\frac{d}{dt}\langle A\rangle_{|\psi(t)\rangle} = -\frac{i}{\hbar}\langle\psi(t)|[A,H]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle$$

If $[A,H]=0$ and $\frac{\partial A}{\partial t}=0$ then $\langle A\rangle_{|\psi(t)\rangle}$ is constant and A is called a conserved quantity.

Stationary states

If $\frac{\partial H}{\partial t} = 0$ : $H = \sum_n E_n |n\rangle\langle n|$ (discrete spectrum)

$E_n$ : allowed energy values

( can be generalized to continuum or mixed spectrum

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \overset{\frac{\partial H}{\partial t}=0}{\Longrightarrow} |\psi(t)\rangle = e^{-\frac{i}{\hbar}H(t-t_0)}|\psi(t_0)\rangle$$

$$|\psi(t)\rangle = \sum_n \underbrace{e^{-\frac{i}{\hbar}E_n(t-t_0)}}_{\text{phases}}|n\rangle\langle n|\psi(t_0)\rangle$$

Determination of $\{|n\rangle, E_n\} \Leftrightarrow$ solution of dynamics

If $|\psi(t_0)\rangle = |m\rangle$ (energy eigenstate), then

$|\psi(t)\rangle = e^{-\frac{i}{\hbar}E_m(t-t_0)}|m\rangle$ stationary state

(constant physical state)

If $\frac{\partial H}{\partial t}=0$, $\frac{\partial A}{\partial t}=0$ and $[H,A]=0$ there exists a basis of simultaneous eigenvectors

$$A|n\rangle = a_n|n\rangle \quad \text{and} \quad H|n\rangle = E_n|n\rangle .$$

If $|\psi(t_0)\rangle = |m\rangle$ then $|\psi(t)\rangle$ remains eigenstate of $A$ and $H$ with eigenvalues $(a_m, E_m)$. $a_n$ are called "good quantum numbers"

Schrödinger's equation in the Schrödinger representation for a non-relativistic particle:

$$H = \frac{\vec{P}^2}{2m} + V(\vec{x}) \qquad (\text{correspondence principle})$$

$$\psi(\vec{x},t) = \langle \vec{x} | \psi(t)\rangle$$

$$i\hbar \langle \vec{x}| \frac{d}{dt} |\psi(t)\rangle = \langle \vec{x}| \left[ \frac{\vec{P}^2}{2m} + V(\vec{x}) \right] |\psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x},t) = \left[ -\frac{\hbar^2}{2m} \Delta + V(\vec{x}) \right] \psi(\vec{x},t)$$

$$\Delta = \vec{\nabla}^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \quad \text{Laplace operator}$$

So far:

a) Schrödinger picture : - states are time-dependent
- observables are time-independent (operators)

Also possible:

b) Heisenberg picture : - states time-independent
- observables time-dependent
- same time-dependence of expectation values

c) Dirac or interaction picture :

$$H = \underbrace{H_0}_{\text{time-indep.}} + \underbrace{H_1(t)}_{\text{(time-dep.) perturbation}} \quad (\text{"interaction"})$$

Mixed form: time-dependence of

- states determined from $H_1$
- observables determined from $H_0$

## 1.4 Classic problems

Exactly solvable potentials $V(\vec{x}) \propto \vec{x}^2, \frac{1}{|\vec{x}|}$.

### 14.1 The Harmonic Oscillator

$\vec{x} \to x$, one-dimensional:

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$\langle x|n\rangle = d_n H_n(\xi) e^{-\frac{1}{2}\xi^2}, \quad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x$$

normalization ↗ ↖ Hermite polynomial

- solution of differential equation + boundary conditions (normed states ! $\Leftrightarrow$ exponentially falling solution)

or

- algebraic method:

$$H = \hbar\omega\left(a^+ a + \frac{1}{2}\right)$$

$$a = \frac{i}{\sqrt{2m\omega\hbar}}\hat{p} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}, \quad a^+ = \frac{-i}{\sqrt{2m\omega\hbar}}\hat{p} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}$$

$[a, a^+] = 1$ commutation relation

$a|0\rangle = 0$, $E_0 = \frac{1}{2}\hbar\omega$ ground state

$$\left.\begin{array}{l} |n\rangle \propto \underset{\nwarrow \text{creation operator}}{a^+}|n-1\rangle \propto (a^+)^n|0\rangle \\ \\ |n-1\rangle \propto \underset{\nwarrow \text{annihilation operator}}{a}|n\rangle \end{array}\right\} \text{lowering } (a) \text{ and raising } (a^+) \text{ operators}$$

$|n\rangle$ : state with n quanta,

$$\text{energy} = E_n = n \cdot \hbar\omega + \underbrace{\frac{1}{2}\hbar\omega}_{\text{zero point, ground state energy}}$$

Remark: in three dimension the harmonic oscillator is

$$H = \frac{\hat{\vec{p}}^2}{2m} + \frac{1}{2} m\omega^2 \hat{\vec{x}}^2$$

$$= \sum_{i=1}^{3} \left[ \frac{\hat{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}_i^2 \right]$$ sum of three one-dimensional oscillators

$$\Rightarrow E_n = E_{n_1} + E_{n_2} + E_{n_3} = \left( n_1 + n_2 + n_3 + \frac{3}{2} \right) \hbar\omega$$

$$\psi_n(\vec{x}) = \psi_{n_1}(x_1) \cdot \psi_{n_2}(x_2) \cdot \psi_{n_3}(x_3)$$ (separable solution)

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## 1.4.2 The Hydrogen Atom

$$H = \frac{\hat{\vec{p}}^2}{2m} - \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\hat{\vec{x}}|}$$

$e = 1.60219 \cdot 10^{-19}$ C

$\varepsilon_0 = 8.85419 \cdot 10^{-12} \frac{C}{V \cdot m}$

reduced mass $m = m_e \left(1 + \frac{m_e}{m_p}\right)^{-1} \approx m_e$

since $\frac{m_p}{m_e} = 1836.11$

Schrödinger's equation for stationary states $\psi(\vec{x}) e^{-iEt}$:

$$\left( -\frac{\hbar^2}{2m} \Delta - \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\vec{x}|} \right) \psi(\vec{x}) = E \psi(\vec{x})$$

Polar coordinates $\psi(\vec{x}) \rightarrow \psi(r, \theta, \varphi)$:

$$\Delta = \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \underbrace{\frac{\vec{L}^2}{r^2 \hbar^2}}_{\text{centrifugal term}}$$

$\vec{L} = \hat{\vec{x}} \times \vec{p}$ angular momentum, in polar coordinates:

$$-\frac{1}{\hbar^2} \vec{L}^2 = \frac{1}{\sin^2\theta} \left[ \sin\theta \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{\partial^2}{\partial\varphi^2} \right]$$

$$L_3 = \frac{\hbar}{i} \frac{\partial}{\partial\varphi}$$

$\{H, L_3, \vec{L}^2\}$ form a complete set of observables:

$$\psi_{n\ell m}(r,\theta,\varphi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi) \qquad n > \ell$$

$$\vec{L}^2 \cdot Y_{\ell m} = \ell(\ell+1)\hbar^2 Y_{\ell m}$$

$$L_3 Y_{\ell m} = m\hbar\, Y_{\ell m} \qquad m = -\ell, -\ell+1, \dots, \ell-1, \ell$$

$Y_{\ell m}(\theta,\varphi)$ : spherical harmonics

complete orthonormal set on the unit sphere $(\theta,\varphi)$ :

$$(f,g) = \int d\Omega\, f^* g \quad , \int d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta$$

$$(Y_{\ell m}, Y_{\ell' m'}) = \delta_{\ell\ell'}\delta_{mm'}$$

$$Y_{\ell m} = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\; \underbrace{P_\ell^m(\cos\theta)} e^{im\varphi}$$

associated Legendre polynomials,

polynomials of degree $\ell$ in $\sin\theta$ and $\cos\theta$

- radial function for bound states :

$E < 0$ , discrete spectrum

$$R_{n\ell} = \underbrace{d_{n\ell}}_{\text{normalization}}\; e^{-\frac{r}{na_B}} \left(\frac{2r}{na_B}\right)^{\ell} \underbrace{L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_B}\right)}$$

associated Laguerre polynomials

degree $n-\ell-1 \geq 0$

$$a_B = \frac{4\pi\varepsilon_0}{e^2}\frac{\hbar^2}{m} = 0.529\ \text{Å} \quad (1\ \text{Å} = 10^{-10}\ \text{m}) \quad \text{Bohr radius}$$

$$H\psi_{n\ell m} = E_n \psi_{n\ell m}$$

$$E_n = \frac{-E_R}{n^2}$$ Balmer formula

$n = 1, 2, 3, \dots$ principal quantum number

degeneracy $= n^2$

$$E_R = \frac{\hbar^2}{2m a_B^2} = 13.605\ \text{eV} \quad \text{Rydberg energy}$$

Transitions $n \rightarrow m$: $\hbar \underbrace{\nu_{nm}}_{\text{frequency of the emitted photon = quantum of light}} = -E_R\left(\frac{1}{n^2}-\frac{1}{m^2}\right)$ $\quad n > m$

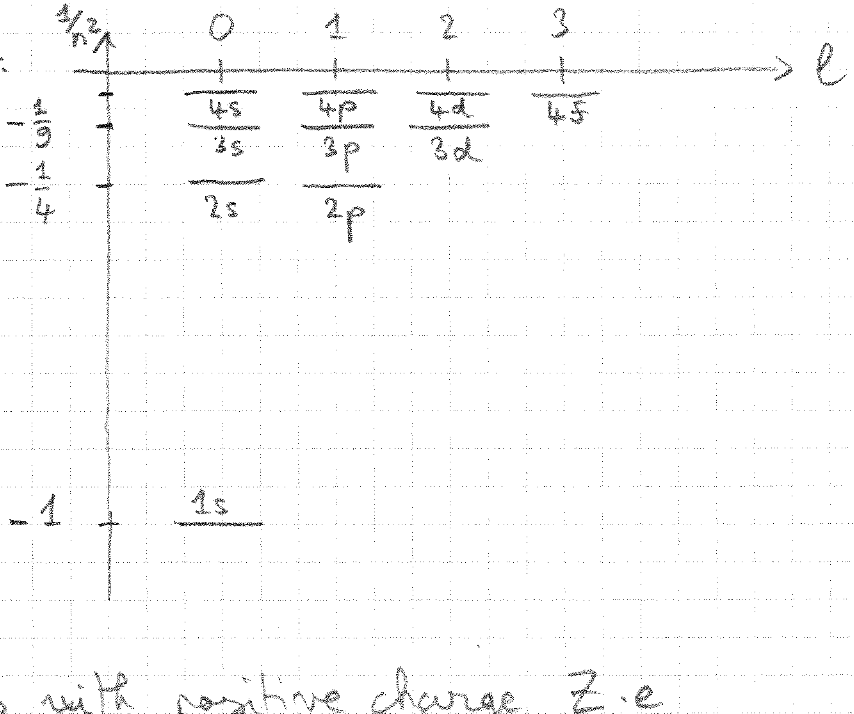
This formula explains the observed spectral lines.

- scattering states for $E > 0$

Remarks:

- symmetry of the $\frac{1}{r}$ potential is actually $SO(4)$ not only $SO(3)$
  Conservation of the Runge-Lenz-Pauli vector $\vec{A}$,
  explains $n^2$ degeneracy of $E_n$
- nomenclature:
  $n \leftrightarrow$ electron shell: $n=1$ ("K shell"), $n=2$ ("L shell"),
  $n=3$ ("M shell"), ...
  $\ell = (0,1,2,3,\ldots) \leftrightarrow (s,p,d,f,\ldots)$ - orbitals

  term diagram:



- atomic nucleus with positive charge $Z \cdot e$
  $\Rightarrow$ replace the argument $r$ of $R_{n\ell}(r)$ by $Z \cdot r$

## 1.5 Composite systems

State spaces $\mathcal{H}_1$ and $\mathcal{H}_2$

$$\mathcal{H} = \underbrace{\mathcal{H}_1 \otimes \mathcal{H}_2}_{\text{direct product space}} \quad , \qquad |\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}$$

$\left.\begin{array}{l} \{|i\rangle\} \text{ CON on } \mathcal{H}_1 \\ \{|\alpha\rangle\} \text{ CON on } \mathcal{H}_2 \end{array}\right. \Rightarrow \{|i\rangle \otimes |\alpha\rangle\}$ CON on $\mathcal{H}$

$|\psi\rangle \in \mathcal{H}$ : $|\psi\rangle = \sum_{i,\alpha} C_{i\alpha} \, |i\rangle \otimes |\alpha\rangle$

$\dim(\mathcal{H}) = \dim(\mathcal{H}_1) \cdot \dim(\mathcal{H}_2)$

Operators : $A_i : \mathcal{H}_i \longrightarrow \mathcal{H}_i$

$$\left.\begin{array}{l} A_1 \longrightarrow A_1 \otimes \mathbb{1} \\ A_2 \longrightarrow \mathbb{1} \otimes A_2 \end{array}\right\} \begin{array}{l}\text{operators on } \mathcal{H} \text{, for example} \\ \text{observables of the composite system}\end{array}$$

$$(A \otimes B)\,|\psi\rangle = \sum_{i,\alpha} C_{i\alpha} \left(A|i\rangle\right) \otimes \left(B|\alpha\rangle\right)$$

Example : 2 particles :

basis $\{|\vec{x}_1\rangle \otimes |\vec{x}_2\rangle = |\vec{x}_1 \vec{x}_2\rangle\}$

$\psi(\vec{x}_1, \vec{x}_2) = \langle \vec{x}_1 \vec{x}_2 | \psi\rangle$

$$H = \frac{\hat{\vec{p}}_1^{\,2} \otimes \mathbb{1}}{2m_1} + \frac{\mathbb{1} \otimes \hat{\vec{p}}_2^{\,2}}{2m_2} + V\left(\hat{\vec{x}}_1 \otimes \mathbb{1} - \mathbb{1} \otimes \hat{\vec{x}}_2\right)$$

$$\hat{=} \frac{\hat{\vec{p}}_1^{\,2}}{2m_1} + \frac{\hat{\vec{p}}_2^{\,2}}{2m_2} + V\left(\hat{\vec{x}}_1 - \hat{\vec{x}}_2\right)$$

Example : particle with spin

$\mathcal{H}_1 \cong \mathcal{L}^2(\mathbb{R}^3) \quad , \quad \mathcal{H}_2 = \mathbb{C}^2$

basis $\{|\vec{x}\rangle \otimes |\alpha\rangle = |\vec{x}\,\alpha\rangle\}$ , $\alpha = \pm$

$\psi_\alpha(\vec{x}) = \langle \vec{x}\,\alpha | \psi\rangle$

Hamilton operator for a particle with spin → see Chapter 3 (Pauli equation)

# 2. The Quantum Theory of the Angular Momentum

## 2.1 Symmetry and Conserved Observable

Consider an active transformation $\mathcal{T}$ of the system :

$$|\psi\rangle \xrightarrow{\quad\mathcal{T}\quad} |\psi'\rangle$$

active $\Leftrightarrow$ $\mathcal{T}$ transforms the system but not the system of coordinates

$|\psi\rangle \leftrightarrow$ ray $\{e^{i\alpha}|\psi\rangle,\ \alpha \in \mathbb{R}\}$ , $\langle\psi|\psi\rangle = 1$

To represent a symmetry, $\mathcal{T}$ must preserve probabilities:

if $|\psi\rangle \xrightarrow{\mathcal{T}} |\psi'\rangle$ and $|\varphi\rangle \xrightarrow{\mathcal{T}} |\varphi'\rangle$ then

$$|\langle\varphi'|\psi'\rangle|^2 = |\langle\varphi|\psi\rangle|^2$$

This is a condition on rays.

A transformation $\mathcal{T}$ is a symmetry of the dynamics if

$$\begin{tikzcd}
|\psi(t_0)\rangle \arrow[r, "\mathcal{T}"] \arrow[d] & |\psi'(t_0)\rangle \arrow[d] \\
|\psi(t)\rangle \arrow[r, dashed, "\mathcal{T}", "\uparrow \text{ yields the same result}"'] & |\psi'(t)\rangle
\end{tikzcd}$$

$\downarrow$ : solve $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$

Theorem of Wigner about the representation of symmetries:
there are just two ways to represent such a transformation $\mathcal{T}$:

a) by a linear unitary operator :

$$\langle\varphi'|\psi'\rangle = \langle\varphi|\psi\rangle$$

$$|\psi'\rangle = \mathcal{U}|\psi\rangle , \quad |\varphi'\rangle = \mathcal{U}|\varphi\rangle , \quad \mathcal{U}^\dagger\mathcal{U} = \mathbb{1} = \mathcal{U}\mathcal{U}^\dagger$$

$$\mathcal{U}(\alpha|\psi\rangle + \beta|\chi\rangle) = \alpha\,\mathcal{U}|\psi\rangle + \beta\,\mathcal{U}|\chi\rangle , \quad \alpha,\beta \in \mathbb{C}$$

b) by an antilinear antiunitary operator:

$$\langle\varphi'|\psi'\rangle = \langle\varphi|\psi\rangle^*$$

antilinear: $\mathcal{U}\left(\alpha|\psi\rangle + \beta|\chi\rangle\right) = \alpha^*\,\mathcal{U}|\psi\rangle + \beta^*\,\mathcal{U}|\chi\rangle$

For antiunitary operator the definition of adjoint is changed to

$$\left(\mathcal{U}^\dagger|\varphi\rangle, |\psi\rangle\right) = \left(|\varphi\rangle, \mathcal{U}|\psi\rangle\right)^* \Rightarrow \mathcal{U}^\dagger\mathcal{U} = \mathbb{1}$$

Symmetries represented by antiunitary operators all involve a change in the direction of time' flow (time reversal)

In the following: unitary transformations

$\mathcal{U}: \mathcal{H} \longrightarrow \mathcal{H}, \quad |\psi\rangle \xrightarrow{\mathcal{U}} |\psi'\rangle = \mathcal{U}|\psi\rangle$

If $\mathcal{U}(\alpha)$ depends on $\alpha \in \mathbb{R}$ with $\mathcal{U}(0) = \mathbb{1}$ (for example $\alpha$ = rotation angle) then:

$$|\psi'(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi'(0)\rangle = e^{-\frac{i}{\hbar}Ht}\,\mathcal{U}(\alpha)|\psi(0)\rangle \quad \longrightarrow \ \downarrow$$

$$= \mathcal{U}(\alpha)\,e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle \quad \downarrow \ \longrightarrow$$

same result $\Leftrightarrow \left[\mathcal{U}(\alpha), H\right] = 0 \quad \forall\alpha$

If $\alpha$ is infinitesimally small:

$$\mathcal{U}(\alpha) = \mathbb{1} + \alpha\cdot T + \mathcal{O}(\alpha^2) \quad ; \quad T = \left.\frac{d\mathcal{U}}{d\alpha}\right|_{\alpha=0}$$

$$\mathcal{U}\mathcal{U}^\dagger = (\mathbb{1} + \alpha\cdot T)(\mathbb{1} + \alpha\cdot T^\dagger) + \mathcal{O}(\alpha^2)$$

$$= \mathbb{1} + \alpha(T + T^\dagger) + \mathcal{O}(\alpha^2)$$

$$\mathcal{U}\mathcal{U}^\dagger = \mathbb{1} \Rightarrow T = -T^\dagger$$

We define $A = iT$, $A = A^\dagger$. A is known as the generator of the symmetr

Symmetry of the dynamics $\Leftrightarrow [A, H] = 0 \quad \left(\Leftarrow \frac{d}{d\alpha}\left[\mathcal{U}(\alpha), H\right] = 0\right)$

$\Rightarrow$ A is a conserved observable

Many if not all of the operators representing observables in quantum mechanics are the generators of symmetries. Measurement apparatus for A is still to be found!

Compare to Noether theorem of classical mechanics:

$[A, H] = 0 \longrightarrow \{A, H\} = 0$ Poisson bracket

$\frac{dH}{d\alpha} = \{A, H\}$ : A is generator of the symmetry transformation

$\frac{dA}{dt} = \{H, A\}$ : Hamilton function H is generator of time evolution

$$\{H, A\} = \sum_i \frac{\partial H}{\partial p_i}\frac{\partial A}{\partial q_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i}$$

## 2.1.1 Translations

Example: n particles, $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_n$

Basis $|\vec{x}_1 \vec{x}_2 \dots \vec{x}_n\rangle$

Potential $V = V(\vec{x}_i - \vec{x}_j)$ only depends on difference of coordinates

$\Rightarrow$ invariance under translation $\vec{x}_i \to \vec{x}_i + \vec{a} \quad \forall i$

Define $$\underset{\displaystyle \psi_{\vec{a}}(\vec{x}_1, \dots, \vec{x}_n)}{\underset{\shortparallel}{\langle \vec{x}_1 \dots \vec{x}_n | \psi_{\vec{a}} \rangle}} := \underset{\displaystyle \psi(\vec{x}_1 - \vec{a}, \dots, \vec{x}_n - \vec{a})}{\underset{\shortparallel}{\langle \vec{x}_1 - \vec{a} \dots \vec{x}_n - \vec{a} | \psi \rangle}}$$

$$|\psi_{\vec{a}}\rangle =: \mathcal{U}(\vec{a})\,|\psi\rangle$$

Remarks:

1) sign: if $|\psi\rangle$ has a peak at $\vec{x}_j = 0$ then $|\psi_{\vec{a}}\rangle$ is peaked at $\vec{x}_j = \vec{a}$

2) unitarity: $\langle \varphi | \mathcal{U}^\dagger(\vec{a}) \mathcal{U}(\vec{a}) | \psi \rangle = \int d^3x_1 \dots d^3x_n \langle \varphi | \mathcal{U}^\dagger(\vec{a}) | \vec{x}_1 \dots \vec{x}_n \rangle \langle \vec{x}_1 \dots \vec{x}_n | \mathcal{U}(\vec{a}) | \psi$

$$= \int d^3x_1 \dots d^3x_n \langle \varphi_{\vec{a}} | \vec{x}_1 \dots \vec{x}_n \rangle \langle \vec{x}_1 \dots \vec{x}_n | \psi_{\vec{a}} \rangle$$

$$= \int d^3x_1 \dots d^3x_n \langle \varphi | \vec{x}_1 - \vec{a} \dots \vec{x}_n - \vec{a} \rangle \langle \vec{x}_1 - \vec{a} \dots \vec{x}_n - \vec{a} | \psi \rangle = \langle \varphi | \psi \rangle$$

by change of variables $\vec{x}_j' = \vec{x}_j - \vec{a}$, $d^3x_j' = d^3x_j$

holds for all $|\varphi\rangle, |\psi\rangle \Rightarrow U^\dagger(\vec{a})\,U(\vec{a}) = \mathbb{1}$

analogously $U(\vec{a})\,U(\vec{a})^\dagger = \mathbb{1}$ :

$$|\psi_{\vec{a}}\rangle = U(\vec{a})\,|\psi\rangle \underset{U^\dagger U = \mathbb{1}}{\Rightarrow} |\psi\rangle = U^\dagger(\vec{a})\,|\psi_{\vec{a}}\rangle \Rightarrow U^\dagger(\vec{a}) = U(-\vec{a})$$

Generator, $\vec{a} = \vec{\varepsilon}$ infinitesimal :

$$\langle \vec{x}_1 \dots \vec{x}_n | \psi_{\vec{\varepsilon}} \rangle = \psi(\vec{x}_1 - \vec{\varepsilon}, \dots, \vec{x}_n - \vec{\varepsilon}) \underset{\substack{\uparrow \\ \text{Taylor expansion}}}{\simeq} \left(1 - \vec{\varepsilon} \cdot \sum_{k=1}^{n} \vec{\nabla}_{x_k}\right) \psi(\vec{x}_1, \dots, \vec{x}_n)$$

$$= \langle \vec{x}_1 \dots \vec{x}_n | \left(\mathbb{1} - \frac{i}{\hbar}\, \vec{\varepsilon} \cdot \sum_{k=1}^{n} \underset{\substack{\uparrow \\ (\mathbb{1} \otimes \dots \otimes \vec{p} \otimes \dots \otimes \mathbb{1}) \\ \text{kth particle}}}{\vec{p}_k}\right) |\psi\rangle$$

$$U(\vec{\varepsilon}) \simeq \mathbb{1} - \frac{i}{\hbar}\, \vec{\varepsilon} \cdot \vec{P}$$

$\vec{P} = \sum_{k=1}^{n} \vec{p}_k$ is the total momentum

If the potential $V$ is invariant under translations : $V = V(\vec{x}_i - \vec{x}_j)$

$\Rightarrow [H, \vec{P}] = 0$ (please verify)

Finite translation :

$$U(\vec{a}) = \lim_{N \to \infty} \underbrace{U\left(\frac{\vec{a}}{N}\right)^N}_{\text{N times translation by } \frac{\vec{a}}{N}} = \lim_{N \to \infty} \left(\mathbb{1} - \frac{i}{\hbar} \frac{\vec{a}}{N} \cdot \vec{P}\right)^N = e^{-\frac{i}{\hbar}\vec{a} \cdot \vec{P}}$$

compare $e^{a\frac{d}{dx}} f(x) = f(x) + a f'(x) + \frac{1}{2} a^2 f''(x) + \dots = f(x+a)$.

Example : $n = 2$, $V(\vec{x}_1 - \vec{x}_2)$

$$\psi(\vec{x}_1, \vec{x}_2) = e^{i\vec{K}\,\frac{m_1 \vec{x}_1 + m_2 \vec{x}_2}{m_1 + m_2}}\, \varphi(\vec{x}_1 - \vec{x}_2)$$

$$P_j \psi = \left[(\hat{p}_1)_j + (\hat{p}_2)_j\right] \psi = \frac{\hbar}{i}\left(\frac{\partial}{\partial (x_1)_j} + \frac{\partial}{\partial (x_2)_j}\right) \psi \underset{\substack{\uparrow \\ P_j \varphi = 0}}{=} \hbar K_j \psi$$

$P_1, P_2, P_3, H, \ldots$ diagonal $\Rightarrow$ center-of-mass motion is described by a plane wave

Translation eigenstate: $\mathcal{U}(\vec{a})\,|\psi\rangle = e^{-i\vec{a}\cdot\vec{K}}\,|\psi\rangle$

Time translation:

it is a symmetry if $\frac{\partial H}{\partial t} = 0$ ; H itself is the generator:

$$\begin{tikzcd}
{|\psi(t_0)\rangle} \arrow[r] \arrow[d] & {|\psi(t_0+\tau)\rangle = \underbrace{e^{-\frac{i}{\hbar}\tau H}}_{\mathcal{U}(\tau)}\,|\psi(t_0)\rangle} \arrow[d] \\
{|\psi(t)\rangle} \arrow[r, dashed] & {|\psi(t+\tau)\rangle}
\end{tikzcd}$$

Schrödinger equation for $\frac{\partial H}{\partial t} = 0 \Rightarrow |\psi(t)\rangle = e^{-\frac{i}{\hbar}(t-t_0)H}\,|\psi(t_0)\rangle$

$H \Leftrightarrow$ energy, generator of time translation $= \mathcal{U}(\underbrace{t-t_0}_{\text{time translation}})\,|\psi(t_0)\rangle$

## 2.1.2 Rotations

$\vec{x} \longmapsto R\vec{x}$ , $x_j \longmapsto \sum_{k=1}^{3} R_{jk}\,x_k \equiv R_{jk}\,x_k$

$RR^T = \mathbb{1}$ , $\det(R) = +1$ (Einstein's summation convention)

$R \in SO(3)$ = special orthogonal group in 3 dimensions

Infinitesimal rotations:

$\vec{x} \longmapsto \vec{x} + \delta\,\vec{n}\times\vec{x} + O(\delta^2)$ : $\vec{n}$ with $\vec{n}^2 = 1$ : rotation axis

$\delta$ : rotation angle

$x_i \longmapsto x_i + \delta\,\varepsilon_{ijk}\,n_j\,x_k = x_i + \delta\,n_j\,(T_j)_{ik}\,x_k \Leftrightarrow$

$\vec{x} \longmapsto \vec{x} + \delta\,n_j\,T_j\,\vec{x}$ , $\{T_j\}$ : 3x3 matrix generators

$(T_j)_{ik} = \varepsilon_{ijk}$

$R \cong \mathbb{1} + \delta\,\vec{n}\cdot\vec{T}$

$$T_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad T_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad T_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$(T_j)^T = -T_j$ antisymmetric

$\{T_j\}$ satisfy the commutation relations

$$[T_i, T_j] = \varepsilon_{ijk} T_k$$

Proof: $[T_i, T_j]_{mn} = \varepsilon_{mir}\varepsilon_{rjn} - \varepsilon_{mjr}\varepsilon_{rin} = \varepsilon_{mir}\varepsilon_{jnr} - (i \Leftrightarrow j)$

$$= (\delta_{mj}\delta_{in} - \delta_{mn}\delta_{ij}) - (i \Leftrightarrow j)$$

$$= \delta_{mj}\delta_{in} - \delta_{mi}\delta_{jn} = \varepsilon_{kmn}\varepsilon_{kji} = \varepsilon_{ijk}\varepsilon_{mkn}$$

$$= \varepsilon_{ijk}(T_k)_{mn}$$ ☒

Commutation relations characterizes the group of rotations.

Rotations induce transformations in the Hilbert space $\mathcal{H}$:

$$\langle \vec{x}_1 \dots \vec{x}_n | \Psi_R \rangle := \langle R^{-1}\vec{x}_1 \dots R^{-1}\vec{x}_n | \Psi \rangle \qquad \overset{\shortparallel}{\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n}$$

infinitesimal

$$\cong \langle (\vec{x}_1 - \delta\vec{n}\times\vec{x}_1) \dots (\vec{x}_n - \delta\vec{n}\times\vec{x}_n) | \Psi \rangle$$

$$\cong \Big(\mathbb{1} - \sum_{k=1}^{n} \delta \underbrace{(\vec{n}\times\vec{x}_k)\cdot\vec{\nabla}_{x_k}}_{=\vec{n}\cdot(\vec{x}_k \times \vec{\nabla}_{x_k})}\Big) \langle \vec{x}_1 \dots \vec{x}_n | \Psi \rangle$$

$$= \langle \vec{x}_1 \dots \vec{x}_n | \Big(\mathbb{1} - \frac{i}{\hbar}\delta\vec{n}\cdot\sum_{k=1}^{n} \underbrace{\hat{\vec{x}}_k \times \hat{\vec{p}}_k}_{(\mathbb{1}\otimes\dots\otimes\underbrace{\hat{\vec{x}}\times\hat{\vec{p}}}_{k\text{th factor (particle)}}\otimes\dots\otimes\mathbb{1})}\Big) |\Psi\rangle$$

$\Rightarrow |\Psi_R\rangle = \mathcal{U}(R)|\Psi\rangle$

infinitesimal: $\mathcal{U}(R) = \mathbb{1} - \frac{i}{\hbar}\delta\vec{n}\cdot\vec{L}$

$\vec{L} = \sum_{k=1}^{n} \hat{\vec{x}}_k \times \hat{\vec{p}}_k$ is the total angular momentum

System of $n$ particles has a rotation symmetry if $V(\vec{x}_1, \dots, \vec{x}_n) = V(R\vec{x}_1, \dots, R\vec{x}_n)$, then

$$[\mathcal{U}(R), H] = 0 \quad \text{and}$$

$$[L_j, H] = 0 \quad j = 1,2,3$$

$\mathcal{U}(R)$ is unitary, $\vec{L}$ is Hermitian $(\hat{x}_k \hat{p}_\ell = \hat{p}_\ell \hat{x}_k$ if $k \neq \ell)$

Components of $\vec{L}$ have the same commutation relations as $i\hbar\vec{T}$:

$$[i\hbar T_i, i\hbar T_j] = i\hbar\, \varepsilon_{ijk} (i\hbar T_k)$$

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk}\, L_k \quad \text{(please verify)}$$

This is not by chance: $\mathcal{U}(R)$ = representation of $SO(3)$ on $\mathcal{H}$

$\{L_i\}$ cannot be simultaneously diagonal, $[L_i, L_j] \neq 0$

$[L_j, H] = 0 \Rightarrow [f(L_j), H] = 0$ (only one component $j$)

$\{L_3, \vec{L}^2 = L_1^2 + L_2^2 + L_3^2, H\}$ commute pairwise $\Rightarrow$ have a common set of eigenvectors (see hydrogen atom)

## 2.2 Transformation of Observables

active transformation $\mathcal{T}$: $|\psi\rangle \xmapsto{\mathcal{T}} |\psi'\rangle = \mathcal{U}|\psi\rangle$

If the measurement apparatus ($\Leftrightarrow$ observables) remain unchanged:

$$\langle\psi|A|\psi\rangle \xmapsto{\mathcal{T}} \langle\psi'|A|\psi'\rangle = \langle\psi|\mathcal{U}^\dagger A\,\mathcal{U}|\psi\rangle$$

For some set of observables $\{A_i\}$, $\mathcal{U}^\dagger A_i \mathcal{U}$ $(\langle\psi'|A_i|\psi'\rangle)$ can be again expressed in terms of $\{A_i\}$ $(\{\langle\psi|A|\psi\rangle\})$.

Example: $\vec{x}$, rotations $\mathcal{U} \simeq \mathbb{1} - \frac{i}{\hbar}\delta\, \vec{n}\cdot\vec{L}$ :

$$\mathcal{U}^{\dagger}\,\hat{x}_j\,\mathcal{U} \cong \left(\mathbb{1} + \frac{i}{\hbar}\,\delta\,\vec{n}\cdot\vec{L}\right)\hat{x}_j\left(\mathbb{1} - \frac{i}{\hbar}\,\delta\,\vec{n}\cdot\vec{L}\right)$$

$$\cong \hat{x}_j + \frac{i}{\hbar}\,\delta\, n_k\left[L_k , \hat{x}_j\right]$$

$$\left[L_k , \hat{x}_j\right] = \varepsilon_{k\ell m}\left[\hat{x}_\ell\,\hat{p}_m , \hat{x}_j\right] \underset{\substack{\uparrow \\ \text{components of } \hat{x} \text{ commute}}}{=} \varepsilon_{k\ell m}\,\hat{x}_\ell\,\underbrace{\left[\hat{p}_m , \hat{x}_j\right]}_{=\frac{\hbar}{i}\delta_{mj}} = \frac{\hbar}{i}\,\varepsilon_{k\ell j}\,\hat{x}_\ell$$

$$\Rightarrow \mathcal{U}^{\dagger}\,\hat{x}_j\,\mathcal{U} \cong \hat{x}_j + \delta\, n_k\,\varepsilon_{k\ell j}\,\hat{x}_\ell = \left(\mathbb{1} + \delta\, n_k\, T_k\right)_{j\ell}\hat{x}_\ell$$

Finite transformations:

$$\mathcal{U}^{\dagger}\,\hat{x}_j\,\underset{\substack{\uparrow \\ \text{Hilbert space}}}{\mathcal{U}} = \underset{\substack{\uparrow \\ SO(3) \text{ matrix}}}{R_{j\ell}}\,\hat{x}_\ell$$

This means: $\langle\psi'|\hat{x}_j|\psi'\rangle = R_{j\ell}\,\langle\psi|\hat{x}_\ell|\psi\rangle$.

"rotated position expectation values in the rotated state"

Definition: $\vec{\hat{x}}$ is a vector operator. $\vec{\hat{p}}$ too.

Dynamics is invariant under rotations $\Leftrightarrow \mathcal{U}^{\dagger} H\,\mathcal{U} = H$

$\Leftrightarrow$ Hamilton operator $H$ is a scalar operator.

Other (than scalar, vector) tensor operators exist.

## 2.3 Groups and Representations

Concept of a group, for example $SO(3)$

$$\vec{x} \longmapsto R_1\vec{x} \longmapsto R_2R_1\vec{x}\,, \quad R_3 = R_2R_1 \in SO(3)$$

rotation $R_i$ is determined by axis $\vec{n}_i$ ($\vec{n}_i^{\,2} = 1$) and angle $\alpha_i$

$$\left.\begin{aligned} \Rightarrow \alpha_3 &= \alpha_3\left(\alpha_1, \alpha_2, \vec{n}_1\cdot\vec{n}_2\right) \\ \vec{n}_3 &= \vec{n}_3\left(\alpha_1, \alpha_2, \vec{n}_1, \vec{n}_2\right) \end{aligned}\right\}\ \text{complicated functions}$$

$R^{-1} \in SO(3)$ with $(-\alpha, \vec{n})$ , $\mathbb{1}_{3\times 3} \in SO(3)$ identity

SO(3) is an example of a Lie group.

$$\frac{\partial R}{\partial \alpha}\Big|_{\alpha=0} = \vec{n}\cdot\vec{T} \quad , \quad R = \mathbb{1} + \alpha\, \vec{n}\cdot\vec{T} + O(\alpha^2)$$

$$\Rightarrow R = \lim_{N\to\infty} \left(R\left(\frac{\alpha}{N}, \vec{n}\right)\right)^N = \lim_{N\to\infty} \left(\mathbb{1} + \frac{\alpha}{N}\vec{n}\cdot\vec{T}\right)^N = e^{\alpha \vec{n}\cdot\vec{T}}$$

* $R^T = e^{\alpha \vec{n}\cdot\vec{T}^T} = e^{-\alpha \vec{n}\cdot\vec{T}} = R^{-1}$
* $\det R = e^{\operatorname{tr}\ln R} = e^{\operatorname{tr}(\alpha \vec{n}\cdot\vec{T})} = 0$
* each element $R \in SO(3)$ can be expressed this way
* $\{T_1, T_2, T_2\}$ are a basis of the Lie algebra so(3)
* commutation relations determine the group multiplication (Baker, Campbell, Hausdorff)

  $$e^A \cdot e^B = e^C$$

  $$C = A + B + \frac{1}{2}[A,B] + \frac{1}{12}\left\{[A,[A,B]] + [B,[B,A]]\right\} + \dots$$

  only commutators $\Rightarrow$ $C \in so(3)$
* analogously for other Lie groups like SU(3) (quarks)

Representation : unitary, in Hilbert space :

$R \longmapsto \mathcal{U}(R)$ , $\mathcal{U} : \mathcal{H} \to \mathcal{H}$

$$\mathcal{U}(R_1 \cdot R_2) = \mathcal{U}(R_1)\cdot\mathcal{U}(R_2)$$

$$\mathcal{U}(R^{-1}) = \mathcal{U}(R)^{-1} = \mathcal{U}(R)^{+}$$

$$\mathcal{U}(\mathbb{1}) = \mathbb{1}$$

Our example, n=1 particles:

$$\langle \vec{x} | \mathcal{U}(R_2)\,\mathcal{U}(R_1)\,|\psi\rangle = \langle R_2^{-1}\vec{x}|\,\mathcal{U}(R_1)\,|\psi\rangle = \langle R_1^{-1}R_2^{-1}\vec{x}\,|\psi\rangle$$

$$= \langle (R_2R_1)^{-1}\vec{x}\,|\psi\rangle = \langle \vec{x}\,|\,\mathcal{U}(R_2\cdot R_1)\,|\psi\rangle$$

Inverse, identity: straightforward.

* $\{R\}$ and $\{\mathcal{U}(R)\}$ have the same multiplication rules as specified above

* $\frac{\partial}{\partial\alpha} R\Big|_{\alpha=0} = \vec{n}\cdot\vec{T} = n_k T_k$

$\frac{\partial}{\partial\alpha}\,\mathcal{U}(R)\Big|_{\alpha=0} = -\frac{i}{\hbar}\,\vec{n}\cdot\vec{L}$ $\Rightarrow$ $\{T_k\}$, $\{-\frac{i}{\hbar}L_k\}$ have the algebra of commutation relations

* $R \leftrightarrow \alpha, \vec{n}$ $(\vec{n}^2 = 1)$ $\leftrightarrow$ 3 real parameters

$\mathcal{U}(R)$ is defined in infinite dimensional Hilbert space: do subspaces exist, which are invariant under <u>all</u> $\{\mathcal{U}(R)\}$? ($\Leftrightarrow$ invariant under $\vec{L}$) Irreducible representations (irreps)

## 2.4 Representations of the Rotation Group

Goal: find the irreps in the Hilbert space of the algebra

$$[J_i, J_j] = i\hbar\,\varepsilon_{ijk}\,J_k$$

Procedure: find the simultaneous eigenvectors of $J_3, \vec{J}^2$:

$$[J_i, J_kJ_k] = J_k[J_i, J_k] + [J_i, J_k]J_k = i\hbar\,(J_k\varepsilon_{ikl}J_l + \varepsilon_{ikl}J_lJ_k)$$

$$= i\hbar\,\underbrace{\varepsilon_{ikl}}_{\text{antisymmetric}}\,\underset{\text{symmetric when } k\leftrightarrow l}{(J_kJ_l + J_lJ_k)} = 0$$

$$\vec{J}^2\,|jm\rangle = \hbar^2\alpha_j\,|jm\rangle\,;\quad \alpha_j \geq 0,\ \text{real}$$ ($\hbar^2$ because of dimension)

$$J_3\,|jm\rangle = \hbar\, m\,|jm\rangle$$

Values of $m, \alpha_j$ still undetermined.

$\{|jm\rangle\}$ is a CON. Since $[J_i, \vec{J}^2] = 0$ it follows

$$J_i |jm\rangle = \sum_{m'} c^{j}_{i,m,m'} |jm'\rangle \qquad (j \Leftrightarrow \alpha_j \text{ unchanged})$$

$$\langle jm'|jm\rangle = \delta_{mm'}$$

Instead of $J_1, J_2 \to J_\pm = J_1 \pm i J_2$ , $J_+^\dagger = J_-$ .

$$\langle jm'|J_3|jm\rangle = \hbar m \, \delta_{mm'}$$

$$\langle jm'|J_\pm|jm\rangle = \hbar \times ?$$

* $\hbar^2 m^2 = \langle jm|J_3^2|jm\rangle \leq \langle jm|\vec{J}^2|jm\rangle = \hbar \alpha_j \Rightarrow m^2 \leq \alpha_j$

* $[J_3, J_\pm] = [J_3, J_1 \pm i J_2] = i\hbar (J_2 \mp i J_1) = \pm\hbar (J_1 \pm i J_2) = \pm\hbar J_\pm$

$\Rightarrow J_3 J_\pm |jm\rangle = \left([J_3, J_\pm] + J_\pm J_3\right)|jm\rangle = \hbar (m \pm 1) J_\pm |jm\rangle$

$\Rightarrow J_\pm |jm\rangle$ is eigenvector of $J_3$ with eigenvalue $\hbar(m \pm 1)$

$\Rightarrow J_3 (J_\pm)^n |jm\rangle = \hbar (m \pm n) (J_\pm)^n |jm\rangle$

It is possible that $(J_\pm)^n |jm\rangle = 0$ for some $n$.

* Since $m^2 \leq \alpha_j$, $\exists\, |j\, m_{max}\rangle$ with $J_+ |j\, m_{max}\rangle = 0$

Convention: $j = m_{max}$ ( $j$ is not the eigenvalue $\alpha_j$ )

$J_+ |jj\rangle = 0$

* Again, since $m^2 \leq \alpha_j$, $\exists\, n$ such that $(J_-)^{n+1} |jj\rangle = 0$, $(J_-)^n |jj\rangle \neq 0$

$|j\, j-k\rangle := c_k (J_-)^k |jj\rangle$ , $k = 0, 1, \dots, n$

dimension of the representation $= n + 1$

$\langle jm|jm'\rangle \overset{!}{=} \delta_{mm'}$ , $c_k > 0$

fixes $c_k$ uniquely, only phase of $|jj\rangle$ (global phase for all $|jm\rangle$) is still free.

* from the commutation relations $[J_i, J_j] = i\hbar\varepsilon_{ijk} J_k$ it follows

$$J_+ J_- = \vec{J}^2 - J_3^2 + \hbar J_3$$
$$J_- J_+ = \vec{J}^2 - J_3^2 - \hbar J_3$$

* computation of $j\ (= m_{max})$, $n$, $\alpha_j$ and matrix elements :

$$0 = J_- J_+ |jj\rangle = \hbar^2 (\alpha_j - j^2 - j)\, |jj\rangle \qquad (1)$$

with $m_{min} = m_{max} - n$ :

$$0 = J_+ J_- |j\, m_{min}\rangle = \hbar^2 (\alpha_j - m_{min}^2 + m_{min})\, |j\, m_{min}\rangle \qquad (2)$$

$$(1) \text{ and } (2) \Rightarrow \quad j(j+1) = m_{min}(m_{min} - 1) = \alpha_j$$

$$m_{min} = \left\{ \begin{array}{l} \cancel{j+1} \\ -j \end{array} \right.$$

$$n = m_{max} - m_{min} = 2j$$

$$\Rightarrow \left\{ \begin{array}{ll} m = j, j-1, \ldots, -j+1, -j & : \ 2j+1 \text{ values} \\ 2j = n \quad \text{integer} & \\ j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots & : \ j \text{ (and } m\text{) must be an integer or} \\ \alpha_j = j(j+1) & \quad \text{a half integer !} \end{array} \right.$$

Matrix elements :

$$|\, J_- |jm\rangle \,|^2 = \langle jm | J_+ J_- | jm\rangle = \langle jm | \vec{J}^2 - J_3^2 + \hbar J_3 | jm \rangle$$
$$= \hbar^2 \left[ j(j+1) - m(m-1) \right]$$

$$\Rightarrow \quad J_- |jm\rangle = \hbar \sqrt{j(j+1) - m(m-1)}\ |j\, m-1\rangle \qquad \text{real and positive}$$
$$= \hbar \sqrt{(j+m)(j-m+1)}\ |j\, m-1\rangle \qquad \text{phase}$$
$$(= 0 \quad \text{for } m = -j)$$

analogously: $J_+ |jm\rangle = \hbar \sqrt{(j-m)(j+m+1)}\ |j\ m+1\rangle$

$$(= 0 \quad \text{for } m = j)$$

$$\langle jm' | J_- | jm \rangle = \sqrt{(j+m)(j-m+1)}\, \hbar\, \delta_{m', m-1} \qquad \langle jm' | J_3 | jm\rangle = \hbar m\, \delta_{m', m}$$

$$\langle jm' | J_+ | jm \rangle = \sqrt{(j-m)(j+m+1)}\, \hbar\, \delta_{m', m+1} \qquad \langle jm' | \vec{J}^2 | jm \rangle = \hbar^2 j(j+1)\, \delta_{m', m}$$

## 2.4.1 Spin $j = \frac{1}{2}$

$j = 0$ : trivial irrep, one-dimensional : $|00\rangle$

$$\vec{J}^2 |00\rangle = 0 \quad , \quad J_3 |00\rangle = 0$$

$j = \frac{1}{2}$ : $m = \frac{1}{2}, -\frac{1}{2}$ : $|\frac{1}{2}\ \frac{1}{2}\rangle =: |+\rangle$ , $|\frac{1}{2}\ -\frac{1}{2}\rangle =: |-\rangle$ , two-dimensional

$$J_3 \longrightarrow \langle j m' | J_3 | j m \rangle = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$J_+ \longrightarrow \qquad = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \langle +|J_+|+\rangle & \langle +|J_+|-\rangle \\ \langle -|J_+|+\rangle & \langle -|J_+|-\rangle \end{pmatrix}$$

$$J_- \longrightarrow \qquad = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$J_1 = \frac{1}{2}(J_+ + J_-) \longrightarrow \quad = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$J_2 = \frac{1}{2i}(J_+ - J_-) \longrightarrow \quad = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$J_k \longrightarrow \qquad \langle \tfrac{1}{2} m' | J_k | \tfrac{1}{2} m \rangle = \frac{\hbar}{2} (\sigma_k)_{m'm} \quad , \quad k = 1,2,3$$

$$\{\sigma_1, \sigma_2, \sigma_3\} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \text{ Pauli matrices}$$

* basis of Hermitian traceless 2x2 matrices

* $\sigma_i \sigma_j = \delta_{ij} + i \varepsilon_{ijk} \sigma_k$ (multiplication table)

$\Rightarrow [\sigma_i, \sigma_j] = 2i \varepsilon_{ijk} \sigma_k$ ( commutator algebra)

$\{\sigma_i, \sigma_j\} = 2\delta_{ij}$

$\Rightarrow \left[\frac{\hbar}{2}\sigma_i, \frac{\hbar}{2}\sigma_j\right] = i\hbar \varepsilon_{ijk} \frac{\hbar}{2}\sigma_k \Rightarrow \{\frac{\hbar}{2}\sigma_k\}$ obey algebra of angular momentum

* two-dimensional irrep of angular momentum
it does <u>not</u> occur among the irreps of $U(R)$ (orbital angular momentum), see book of G. Münster.

## 2.4.2 Spin 1

$j = 1 \quad , \quad m = 1, 0, -1$

$$J_- \longrightarrow \langle 1\, m' | J_- | 1\, m \rangle = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \qquad \left[\begin{array}{c|ccc} & & \xrightarrow{m} & \\ & 1 & 0 & -1 \\ m' \downarrow\; 1 & & & \\ 0 & & & \\ -1 & & & \end{array}\right]$$

$$J_+ \longrightarrow \qquad = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$$

$$J_3 \longrightarrow \qquad = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$J_1 = \frac{1}{2}\left(J_+ + J_-\right) \longrightarrow \qquad = \hbar \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$J_2 = \frac{1}{2i}\left(J_+ - J_-\right) \longrightarrow \qquad = \hbar \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

Spin 1 representation matrices, fulfill algebra of angular momentum.

$i\hbar\vec{T}$ , $(T_i)_{jk} = \varepsilon_{jik}$ fulfill algebra of angular momentum and are $3\times3$ matrices, too. Yet a different representation? No, they are equivalent up to a unitary similarity transformation

# 3. The Electron Spin

## 3.1. Particles in the Electromagnetic Field

The electromagnetic field can be expressed in terms of potentials $(\phi, \vec{A})$ as

$$\begin{aligned} \vec{E} &= -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} \\ \vec{B} &= \vec{\nabla}\times\vec{A} \end{aligned} \quad \Longrightarrow \quad \begin{aligned} \vec{\nabla}\times\vec{E} &= -\frac{\partial \vec{B}}{\partial t} && \text{(Faraday's law)} \\ \vec{\nabla}\cdot\vec{B} &= 0 && \text{(absence of free magnetic poles} \end{aligned}$$

* $\Rightarrow$ : automatically fulfill Maxwell's equation

* $\vec{E}, \vec{B}$ are invariant under the gauge transformations:

$$\begin{aligned} \phi &\longmapsto \phi' = \phi - \frac{\partial \alpha}{\partial t} \qquad \alpha = \alpha(\vec{x}, t) \text{ real function} \\ \vec{A} &\longmapsto \vec{A}' = \vec{A} + \vec{\nabla}\alpha \end{aligned}$$

$$H = \frac{1}{2m}\Big(\vec{p} - q\underset{\substack{\uparrow \\ \text{operator } \vec{A}(\vec{x},t)}}{\vec{A}}\Big)^2 + q\phi$$

: Hamiltonian of a non-relativistic particle in the electromagnetic field

$\psi(\vec{x}, t)$ is a solution of Schrödinger's equation with $\phi, \vec{A}$ $\Longleftrightarrow$
$\psi'(\vec{x}, t) = \Omega(\vec{x}, t)\,\psi(\vec{x}, t)$ is a solution of Schrödinger's equation with gauge transformed $\phi', \vec{A}'$ and

$$\Omega(\vec{x}, t) = e^{i\frac{q}{\hbar}\alpha(\vec{x}, t)}$$

: gauge transformation

$$\rho = |\psi|^2 \,, \quad \vec{j} = \frac{\hbar}{2mi}\left\{\psi^*\left(\vec{\nabla} - \frac{iq}{\hbar}\vec{A}\right)\psi - \psi\left(\vec{\nabla} + \frac{iq}{\hbar}\vec{A}\right)\psi^*\right\}$$

$$\left.\begin{aligned} q\cdot\rho &= \text{charge density} \\ q\cdot\vec{j} &= \text{electrical current density} \end{aligned}\right\} \text{ are invariant under gauge transformations}$$

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0$$

Example : electron in a homogeneous magnetic field $\vec{B}(\vec{x}) = \vec{B} = \text{const}$, $q = -e$

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{x} \quad \Rightarrow \quad \vec{\nabla} \times \vec{A} = \vec{B}$$

$$\left(\hat{\vec{p}} + e\vec{A}\right)^2 = \hat{\vec{p}}^2 + e^2 \vec{A}^2 + e\left(\hat{\vec{p}} \cdot \vec{A} + \vec{A} \cdot \hat{\vec{p}}\right)$$

last term : it holds $\left[\hat{p}_k, f(\hat{\vec{x}})\right] = \frac{\hbar}{i}\frac{\partial f}{\partial x_k}(\hat{\vec{x}})$

proof : $\langle \vec{y} | \left[\hat{p}_k, f(\hat{\vec{x}})\right] | \psi \rangle = \langle \vec{y} | \hat{p}_k f(\hat{\vec{x}}) | \psi \rangle - \langle \vec{y} | f(\hat{\vec{x}}) \hat{p}_k | \psi \rangle$

$$= \frac{\hbar}{i}\frac{\partial}{\partial y_k} \underbrace{\langle \vec{y} | f(\hat{\vec{x}}) | \psi \rangle}_{= f(\vec{y}) \langle \vec{y} | \psi \rangle} - f(\vec{y}) \frac{\hbar}{i}\frac{\partial}{\partial y_k} \langle \vec{y} | \psi \rangle$$

$$= \frac{\hbar}{i}\frac{\partial f}{\partial y_k}(\vec{y}) \langle \vec{y} | \psi \rangle = \langle \vec{y} | \frac{\hbar}{i}\frac{\partial f}{\partial x_k}(\hat{\vec{x}}) | \psi \rangle \quad \square$$

$$\Rightarrow \hat{\vec{p}} \cdot \vec{A} = \vec{A} \cdot \hat{\vec{p}} + \left[\hat{p}_k, A_k\right] = \vec{A} \cdot \hat{\vec{p}} + \frac{\hbar}{i}\frac{\partial A_k}{\partial x_k}$$

$$= \vec{A} \cdot \hat{\vec{p}} + \frac{\hbar}{i}\vec{\nabla} \cdot \vec{A}$$

due to $\vec{A} = \frac{1}{2}\vec{B} \times \vec{x}$ : $\vec{\nabla} \cdot \vec{A} = \frac{1}{2}\varepsilon_{ijk} \underbrace{\frac{\partial}{\partial x_i} B_j x_k}_{= \delta_{ik}} = 0$ Coulomb gauge

$$\Rightarrow \hat{\vec{p}} \cdot \vec{A} + \vec{A} \cdot \hat{\vec{p}} = 2\vec{A} \cdot \hat{\vec{p}} = \left(\vec{B} \times \hat{\vec{x}}\right) \cdot \hat{\vec{p}} = \vec{B} \cdot \left(\hat{\vec{x}} \times \hat{\vec{p}}\right) = \vec{B} \cdot \vec{L}$$

$$\Rightarrow H = \frac{\hat{\vec{p}}^2}{2m} + \frac{e}{2m}\vec{B} \cdot \vec{L} + \frac{e^2}{8m}\left(\vec{B} \times \hat{\vec{x}}\right) - e\phi$$

## 3.2 The Zeeman Effect

$\frac{e}{2m}\vec{B} \cdot \vec{L}$ paramagnetic term

$= -\vec{\mu} \cdot \vec{B}$ with $\vec{\mu} = -\frac{e}{2m}\vec{L}$ = magnetic moment ($q = -e$)

( permanent, results from the motion of the particle, exists also if $\vec{B} = 0$ )

if $\vec{\mu}$ is parallel to $\vec{B}$ $\Rightarrow$ energy decreases

$\mu_B = \frac{e}{2m}\hbar = 0.579 \times 10^{-4} \frac{eV}{T}$ = Bohr's magneton
↖ Tesla

$\frac{e^2}{8m}(\vec{B} \times \vec{x})^2$ diamagnetic term

(magnetic field changes the particle's motion and induces a extra magnetic moment $\propto B$)

Orders of magnitude: $\frac{e^2}{m} B^2 a_B^2 \sim (\mu_B B)^2 \frac{m a_B^2}{\hbar^2}$

$\sim \mu_B B \cdot \frac{\mu_B}{E_R} \cdot B$

$\frac{\mu_B}{E_R} \sim \frac{10^{-5}}{T}$

in the lab usually $B \sim 1T \Rightarrow$ diamagnetic $\sim 10^{-5} \times$ paramagnetic, diamagnetic term can be neglected compared to $\mu_B B$

With $\vec{B} = B\vec{e}_3$: $H \cong H_0 + \frac{\mu_B}{\hbar} B L_3$

$H_0$: hydrogen-atom-like, $\phi = \frac{Ze}{4\pi\epsilon_0} \frac{1}{|\vec{x}|}$

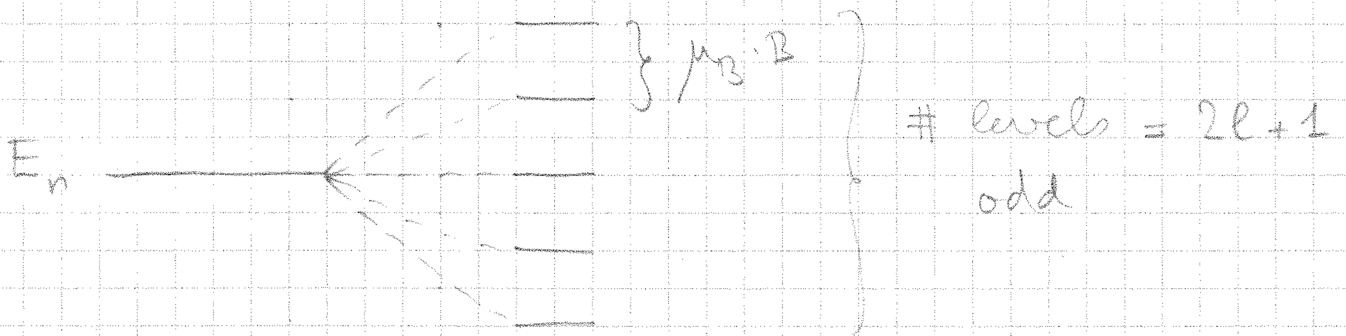
$H \psi_{n\ell m} = E_{nm} \psi_{n\ell m}$

$E_{nm} = -\frac{E_R Z^2}{n^2} + \mu_B B \underset{\uparrow}{m}$

m-quantum number: $L_3 \psi_{n\ell m} = \hbar m \psi_{n\ell m}$

easy because $\{H_0, \vec{L}^2, L_3\}$ simultaneously diagonal

* m-degeneracy of $E_n$ is split by $B \neq 0$
* m = magnetic quantum number



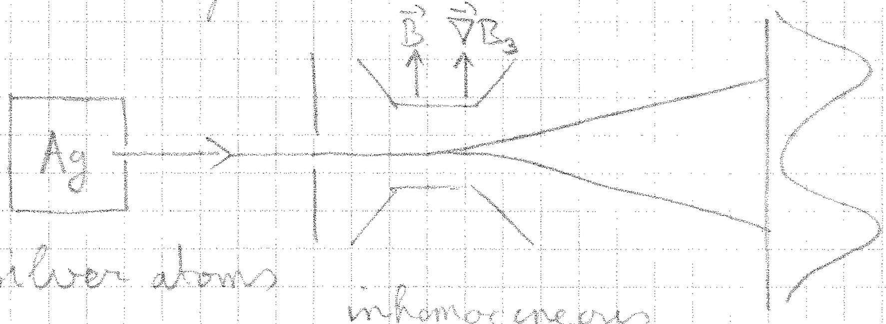
Zeeman effect

Effect was observed in the 1890's by the spectroscopist Pieter Zeeman (splitting of the D spectral lines of sodium)

* m-degeneracy ↔ rotational invariance ($L_\pm$ change m) broken by external magnetic field $\vec{B} \neq 0$

Experimental observations:

- ground state of hydrogen atom has $l=0$, $m=0$
  ⇒ no Zeeman splitting
  but: energy level is doubled
- Stern-Gerlach experiment:
  Walter Gerlach and Otto Stern, in 1922



Splitting is not observed with $Ag^+$ ions

- in general: even splitting for atoms with a odd number of electrons
- splittings $g\mu_B B$ with $g = O(1)$ = Landé factor or gyromagnetic factor depend on the multiplet

seems like half-integer $l, m$ although they do not occur for orbital angular momentum $\vec{L} = \vec{x} \times \vec{p}$

Interpretation by George Uhlenbeck and Samuel Goudsmit, 1925: splitting is due to spin, intrinsic angular momentum of the electron with $j = \frac{1}{2}$, independently of the orbital motion

permanent magnetic moment $\vec{\mu} = \frac{-e}{2m} g \vec{S}$ , $m_s = \pm \frac{\hbar}{2}$

## 3.3 The Electron with Spin $\frac{1}{2}$

$\mathcal{H} = \mathcal{H}_{\vec{x}} \otimes \mathcal{H}_S$

$\mathcal{H}_{\vec{x}}$ like so far, basis $|\vec{x}\rangle$

$\mathcal{H}_S \cong \mathbb{C}^2$ Hilbert space where spin operator $\vec{S}$ acts

Basis $\{ |\frac{1}{2}\ m\rangle , m = +\frac{1}{2}, -\frac{1}{2} \}$

$[S_i, S_j] = i\hbar\, \varepsilon_{ijk} S_k$

$\vec{S}^2 |\frac{1}{2}\ m\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right) |\frac{1}{2}\ m\rangle = \hbar^2 \frac{3}{4} |\frac{1}{2}\ m\rangle$

$S_3 |\frac{1}{2}\ m\rangle = \hbar m |\frac{1}{2}\ m\rangle$

simplified notation: $|+\rangle := |\frac{1}{2}\ \frac{1}{2}\rangle$ , $|-\rangle := |\frac{1}{2}\ -\frac{1}{2}\rangle$

$\langle \varepsilon' | \vec{S} | \varepsilon \rangle = \frac{\hbar}{2} (\vec{\sigma})_{\varepsilon'\varepsilon}$ , $\varepsilon', \varepsilon = +, -$

$\vec{\sigma}$ : Pauli matrices

basis in $\mathcal{H}$ : $\{ |\vec{x}\ \varepsilon\rangle = |\vec{x}\rangle \otimes |\varepsilon\rangle \}$

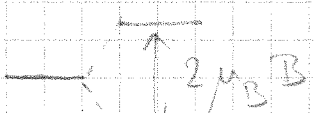
$|\psi\rangle = \int d^3x \, \{ |\vec{x}\, +\rangle \psi_+(\vec{x}) + |\vec{x}\, -\rangle \psi_-(\vec{x}) \}$

$\begin{pmatrix} \psi_+(\vec{x}) \\ \psi_-(\vec{x}) \end{pmatrix}$ two-component wave function, Pauli spinor

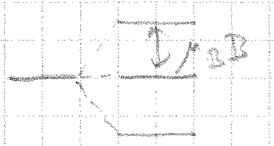
$H = H_{\text{Schrödinger}} \otimes \mathbb{1} + \frac{\mu_B}{\hbar} g_e \vec{B} \cdot \left( \mathbb{1} \otimes \vec{S} \right)$

- yields the correct splittings

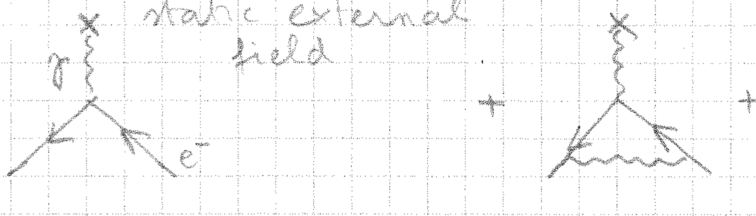
- $g_e \approx 2$ : $\Rightarrow$ eigenvalues of $g_e S_3$ : $\pm 2 \cdot \frac{\hbar}{2}$



$g_e \simeq 2 \Rightarrow$ spacing of energy levels $\simeq$ like for
$l = 1$ : $\mu_B B m$ , $m = +1, 0, -1$



later: relativistic Dirac - theory of the electron yields $g_e = 2$.
Corrections due to processes like the emission and absorption of photons shift $g_e = 2.002322\ldots$ (quantum electrodynamics)



$+ \ldots \quad g = 2 + \frac{\alpha}{\pi} + \ldots$

$\uparrow$ Schwinger, 1948

fine structure constant $\frac{e^2}{4\pi\varepsilon_0 \hbar c} \simeq \frac{1}{137}$

remark: there are many other particles with spin $\frac{1}{2}$, for example the proton: $\vec{\mu}_S = g_p \frac{\mu_p}{\hbar} \vec{S}$

$\mu_p = \frac{e\hbar}{2m_p} \simeq \frac{\mu_B}{1836}$

$g_p \simeq 5.59$ (complicated internal structure)

$g_n \simeq -3.83$ (neutron)

## 3.4 The Pauli Equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

position-spin basis : $\psi(\vec{x}, t) = \begin{pmatrix} \psi_+(\vec{x}, t) \\ \psi_-(\vec{x}, t) \end{pmatrix}$

$$H = \frac{1}{2m} \left( \frac{\hbar}{i} \vec{\nabla} + e \vec{A}(\vec{x}, t) \right)^2 - e \phi(\vec{x}, t) + \mu_B \vec{B} \cdot \vec{\sigma} \quad (g_e = 2)$$

It can be shown:

$$H = \frac{1}{2m}\left[\vec{\sigma}\cdot\left(\frac{\hbar}{i}\vec{\nabla} + e\vec{A}\right)\right]^2 - e\phi$$

For bound states: $1 = \int d^3x\, \psi^\dagger \psi = \int d^3x \left(|\psi_+|^2 + |\psi_-|^2\right)$

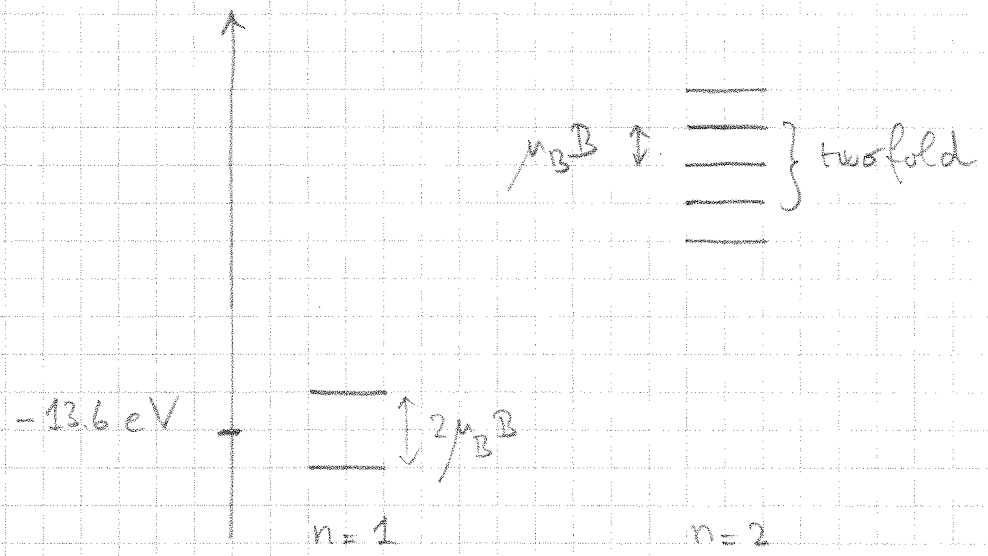
$|\psi_\pm|^2$ = probability density for electron with $S_3 = \pm\frac{\hbar}{2}$

Eigenfunctions ( $\vec{B} = B\vec{e}_3$ , no diamagnetic term,
hydrogen-atom-like as in 3.2 ) :

$$R_{nl} Y_{lm} \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad R_{nl} Y_{lm} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$E = -\frac{E_R Z^2}{n^2} + \underbrace{\mu_B B\,(m \pm 1)}$$

$2l+1$ states with $S_3 = +\frac{\hbar}{2}$
and $2l+1$ states with $S_3 = -\frac{\hbar}{2}$



partially
degenerate
levels even
with $B \neq 0$

degeneracy for $B = 0$ : $2n^2$

Complete set of commuting observables in the Pauli theory:

$$H,\ \vec{L}^2,\ L_3,\ \vec{S}^2 = \frac{\hbar^2}{4}\vec{\sigma}^2 = \frac{3\hbar^2}{4}\cdot \mathbb{1},\ S_3$$

Relativistic ( $\frac{v}{c}$ not negligible) : $[H, L_3] \neq 0$ , $[H, S_3] \neq 0$
because $H$ contains a term $\vec{S}\cdot\vec{L}\cdot O\left(\frac{v^2}{c^2}\right)$

$$\rightarrow H,\ \vec{J}^2,\ J_3,\ \vec{L}^2,\ \vec{S}^2 = \frac{3\hbar^2}{4}\cdot\mathbb{1}$$

$$\vec{J} = \vec{L} + \vec{S} = \vec{L} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{S} \quad , \quad [\vec{J}, \vec{S}\cdot\vec{L}] = 0$$

## 3.5 Rotations of Spinors

We show: the total angular momentum $\vec{J} = \vec{L} + \vec{S}$ is the generator of rotations in the Pauli theory:

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk}\, L_k \qquad [S_i, S_j] = i\hbar\, \varepsilon_{ijk}\, S_k$$

$[S_i, L_j] = 0$ (different factors of tensor product)

$$\Rightarrow \quad [J_i, J_j] = i\hbar\, \varepsilon_{ijk}\, J_k$$

For $R = 1 + \delta\, \vec{n}\cdot\vec{T}$ : $|\psi'\rangle \approx \left(\mathbb{1} - \delta \frac{i}{\hbar}\, \vec{n}\cdot\vec{J}\right)|\psi\rangle$ infinitesimal

finite : $|\psi'\rangle = e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{J}}\, |\psi\rangle = e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{L}}\, e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{S}}\, |\psi\rangle$

$$=: \mathcal{U}(R)\, |\psi\rangle$$

$$\langle \vec{x}\, \varepsilon | \psi' \rangle = \langle R^{-1}\vec{x}\ \varepsilon |\, e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{S}}\, |\psi\rangle = \langle R^{-1}\vec{x}| \otimes \langle \varepsilon |\, e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{S}}\, |\psi\rangle$$

$$= \int d^3y \sum_{\varepsilon'} \langle R^{-1}\vec{x}| \otimes \langle\varepsilon|\, e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{S}}\, |\varepsilon'\rangle \otimes |\vec{y}\rangle\, \langle \vec{y}\,\varepsilon' | \psi\rangle$$

$$= \sum_{\varepsilon'} \langle \varepsilon |\, e^{-\alpha\frac{i}{\hbar}\vec{n}\cdot\vec{S}}\, | \varepsilon' \rangle\, \langle R^{-1}\vec{x}\ \varepsilon' | \psi \rangle$$

$$= \sum_{\varepsilon'} \left( e^{-i\frac{\alpha}{2}\vec{n}\cdot\vec{\sigma}} \right)_{\varepsilon\varepsilon'} \langle R^{-1}\vec{x}\ \varepsilon' | \psi\rangle$$

$$\Rightarrow \begin{pmatrix} \psi'_+(\vec{x}) \\ \psi'_-(\vec{x}) \end{pmatrix} = e^{-i\frac{\alpha}{2}\vec{n}\cdot\vec{\sigma}} \begin{pmatrix} \psi_+(R^{-1}\vec{x}) \\ \psi_-(R^{-1}\vec{x}) \end{pmatrix}$$

* transformation of the argument and of the spinor components

* $(\vec{n}\cdot\vec{\sigma})^2 = n_i n_j \sigma_i \sigma_j = n_i n_i = 1$ since $\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$

$$\Rightarrow e^{-i\frac{\alpha}{2}\vec{n}\cdot\vec{\sigma}} = \cos\left(\frac{\alpha}{2}\right)\mathbb{1} - i \sin\left(\frac{\alpha}{2}\right)\vec{n}\cdot\vec{\sigma}$$

Special case $\alpha = 2\pi$ : $e^{-i\pi\vec{n}\cdot\vec{\sigma}} = \cos(\pi)\mathbb{1} = -\mathbb{1}$

$\Rightarrow$ $\mathcal{U}(R)\,|\psi\rangle = -\,|\psi\rangle$ under rotation by $2\pi$

* $\vec{S}$ is a vector operator $\Leftrightarrow$ $\mathcal{U}^{\dagger}(R)\,S_i\,\mathcal{U}(R) = R_{ik}\,S_k$

Proof : infinitesimal :

$$\mathcal{U}^{\dagger}(R)\,S_i\,\mathcal{U}(R) \cong \left(\mathbb{1} + \delta\frac{i}{\hbar}\vec{n}\cdot\vec{J}\right) S_i \left(\mathbb{1} - \delta\frac{i}{\hbar}\vec{n}\cdot\vec{J}\right)$$

$$= S_i + \delta\frac{i}{\hbar}\,n_j\,[J_j, S_i]$$

$\vec{L}$ commutes with $\vec{S}$ $\curvearrowright$

$$= S_i + \delta\frac{i}{\hbar}\,n_j\,[S_j, S_i]$$

$$= S_i - \delta\,n_j\,\epsilon_{jik}\,S_k = S_i + \delta\,n_j\,(T_j)_{ik}\,S_k$$

$$= \left(\delta_{ik} + \delta(\vec{n}\cdot\vec{T})_{ik}\right) S_k$$

$$\cong R_{ik}\,S_k \quad \boxed{\xi}$$

$\Rightarrow$ terms like $\langle\psi|\vec{B}\cdot\vec{S}\,|\psi\rangle$ are invariant (scalar product of two vectors), when

- * $|\psi\rangle \longmapsto \mathcal{U}(R)\,|\psi\rangle$
- * external field $\vec{B} \longmapsto R\vec{B}$

# 4. Addition of Angular Momenta

## 4.1 Addition of Two Angular Momenta

### 4.1.1 Motivation

Angular momenta $\vec{j} \hat{=} (\vec{j} \otimes \mathbb{1})$ and $\vec{j}' \hat{=} (\mathbb{1} \otimes \vec{j}')$ in state space $\mathcal{H} \otimes \mathcal{H}'$ with

$$[j_i, j_k] = i\hbar \varepsilon_{ikl} j_l \text{ , similarly } \vec{j}' \text{, } [j_i, j'_k] = 0$$

Examples:

- $\vec{j} = \vec{S}_1$, $\vec{j}' = \vec{S}_2$ spins of two electrons in the ground state of the helium atom, no orbital angular momentum
- $\vec{j} = \vec{L}$, $\vec{j}' = \vec{S}$ for the Pauli electron

Presence of interaction between angular momenta usually has the effect that they are not separately conserved

Example: term $\vec{j} \cdot \vec{j}'$ in $H \Rightarrow [\vec{j}, H] \neq 0$ , $[\vec{j}', H] \neq 0$

Total angular momentum: $\vec{J} = \vec{j} + \vec{j}'$ in $\mathcal{H} \otimes \mathcal{H}'$

$$[\vec{J}, \vec{j} \cdot \vec{j}'] = 0$$

$$[J_i, j_k j'_k] = [j_i, j_k] j'_k + j_k [j'_i, j'_k] = i\hbar \varepsilon_{ikl} (j_l j'_k + j_k j'_l) = 0$$

$\vec{J}$ commutes with $H \rightarrow$ diagonalize $\vec{J}^2$ and $J_z$ !

Problem: how do we express the eigenstates of $\vec{J}$ in terms of the eigenstates of $\vec{j}$ and $\vec{j}'$?

Tensor-product basis $|r j m\rangle \otimes |r' j' m'\rangle = |r r' j j' m m'\rangle$

diagonalizes $\vec{j}^2$, $j_z$, $\vec{j}'^2$, $j'_z$, ...

Shorthand notation: $|r r' j j' m m'\rangle \to |m m'\rangle$

since we stay in the eigenspace with values $\hbar^2 j(j+1)$ for $\vec{j}^2$ and $\hbar^2 j'(j'+1)$ for $\vec{j}'^2$ and $r, r'$ for ... $\left( [\vec{J}, \vec{j}^2] = 0 = [\vec{J}, \vec{j}'^2] \right)$

$\Rightarrow \quad \{ |m m'\rangle \}$ dimension $(2j+1)\cdot(2j'+1)$

$$J_3 \, |m m'\rangle = (j_3 + j_3') \, |m m'\rangle = \hbar \, (m + m') \, |m m'\rangle$$

$$\vec{J}^2 \, |m m'\rangle = \left( \vec{j}^2 + \vec{j}'^2 + 2 \, \vec{j} \cdot \vec{j}' \right) |m m'\rangle$$

$$= \left[ \hbar^2 j(j+1) + \hbar^2 j'(j'+1) + (j_+ j_-' + j_- j_+' + 2\hbar^2 m m') \right] |m m'\rangle$$

$$= a \, |m m'\rangle + b \, |m+1 \; m'-1\rangle + c \, |m-1 \; m'+1\rangle$$

not diagonal

$$2 \, \vec{j} \cdot \vec{j}' = j_+ j_-' + j_- j_+' + 2 j_3 j_3' \, , \quad j_\pm = j_1 \pm i j_2 \, , \quad j_\pm' = j_1' \pm i j_2'$$

Construct $|J M\rangle = \sum_{m,m'} |m m'\rangle \underbrace{\langle m m' | J M \rangle}$

$\vec{J}^2 \, |J M\rangle = \hbar J (J+1) \, |J M\rangle$ Clebsch-Gordan coefficients

$J_3 \, |J M\rangle = \hbar M \, |J M\rangle$ which $J, M$ values?

### 4.1.2 $j = \frac{1}{2}$ + $j' = \frac{1}{2}$

In the tensor basis $|1\rangle := |++\rangle$, $|2\rangle := |+-\rangle$, $|3\rangle := |-+\rangle$, $|4\rangle := |--\rangle$

$$\langle i | \frac{J_3}{\hbar} | k \rangle = \begin{pmatrix} 1 & & & \\ & 0 & & \Large 0 \\ \Large 0 & & 0 & \\ & & & -1 \end{pmatrix}$$

$$j_+ \, |- m'\rangle = \hbar \, |+ m'\rangle$$

$$j_- \, |+ m'\rangle = \hbar \, |- m'\rangle \quad \text{etc.}$$

$$\langle i | \frac{1}{\hbar^2} \vec{J}^2 | k \rangle = 2 \times \frac{3}{4} \delta_{ik} + \begin{pmatrix} \frac{1}{2} & & & 0 \\ & -\frac{1}{2} & \boxed{1} & \\ & 1 & -\frac{1}{2} & \\ 0 & & & \frac{1}{2} \end{pmatrix}$$

$\langle +- | 2 j_3 j_3' | +- \rangle$

$\langle +- | j_+ j_-' | -+ \rangle$

$$= \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

$\Rightarrow$ $|++\rangle$ and $|--\rangle$ have $J = 1 \Rightarrow J(J+1) = 2$ therefore

$|J=1 \; M=1\rangle = |++\rangle = |1\rangle$

$|J=1 \; M=-1\rangle = |--\rangle = |4\rangle$

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 1 \end{pmatrix} , \quad \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = 0$$

$\Rightarrow \frac{1}{\sqrt{2}} \left( |+-\rangle - |-+\rangle \right) = \frac{1}{\sqrt{2}} \left( |2\rangle - |3\rangle \right) = |J=0 \; M=0\rangle$

antisymmetric $\Leftrightarrow$ total spin is zero

$\frac{1}{\sqrt{2}} \left( |+-\rangle + |-+\rangle \right) = \frac{1}{\sqrt{2}} \left( |2\rangle + |3\rangle \right) = |J=1 \; M=0\rangle$

symmetric

Standard procedure to construct $\vec{J}^2$ multiplets:

$J_- |++\rangle = (j_- + j_-') |++\rangle = \hbar |-+\rangle + \hbar |+-\rangle \overset{!}{=} c \cdot |J=1 \; M=0\rangle$

with $c > 0$. $|J=0 \; M=0\rangle$ is a state orthogonal to $|J=1 \; M=0\rangle$.

$\Rightarrow$ several $J$-values, 0 and 1, when adding $\frac{1}{2} + \frac{1}{2}$.

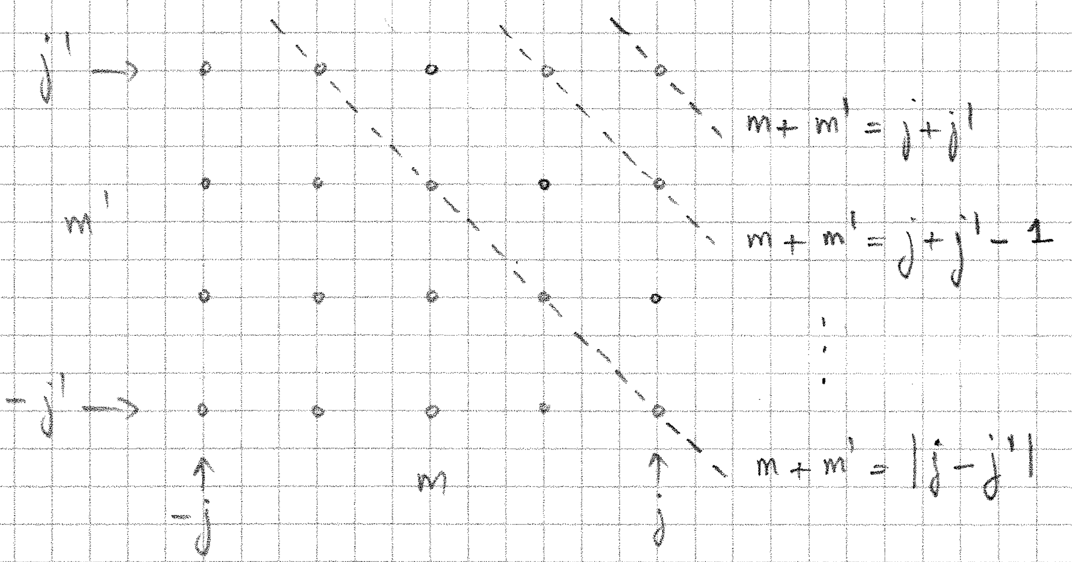
### 4.1.3 General Case

Since $J_3 |mm'\rangle = \hbar (m+m') |mm'\rangle$ it holds :

$M = m + m' \Rightarrow -j - j' \leq M \leq j + j'$

$\Rightarrow \mathcal{J} \leq j + j'$

$\langle \mathcal{J} M | m m' \rangle \propto \delta_{M,\, m+m'}$ (calculate $\langle \mathcal{J} M | \mathcal{J}_3 | m m' \rangle$ )



* maximal $M$ : $|m = j\ m' = j'\rangle = |\mathcal{J} = j + j'\ \ M = \mathcal{J}\rangle$

"highest" state of the multiplet $|\mathcal{J} M\rangle$, $M = \mathcal{J}, \dots, -\mathcal{J}$, with $\mathcal{J} = j + j'$

apply $(\mathcal{J}_-)^k$ on $|\mathcal{J}\mathcal{J}\rangle \rightarrow$ all $|\mathcal{J} M\rangle$ ($\mathcal{J} = j + j'$ fixed)

$$\mathcal{J}_\pm |\mathcal{J} M\rangle = \hbar \sqrt{(\mathcal{J} \mp M)(\mathcal{J} \pm M + 1)}\ |\mathcal{J}\ M \pm 1\rangle \quad , \quad \mathcal{J}_\pm = \mathcal{J}_1 \pm i \mathcal{J}_2$$

4.1.4 ←

$$\mathcal{J}_- |\mathcal{J}\ \mathcal{J}\rangle = \hbar \sqrt{2\mathcal{J}}\ |\mathcal{J}\ \mathcal{J} - 1\rangle$$

$$= (j_- + j'_-)\ |m = j\ m' = j'\rangle = \hbar\sqrt{2j}\ |j-1\ j'\rangle + \hbar\sqrt{2j'}\ |j\ j'-1$$

* choose $|\mathcal{J} = j + j' - 1\ \ M = \mathcal{J}\rangle$ as a linear combination of the states on the "line" with $m + m' = j + j' - 1$ such that

$$\mathcal{J}_+ |\mathcal{J} = j + j' - 1\ \ M = \mathcal{J}\rangle = 0$$

$\Rightarrow$ highest state $|\mathcal{J}\ M = \mathcal{J}\rangle$ of the multiplet with $\mathcal{J} = j + j' - 1$, other states in the multiplet obtained by $\mathcal{J}_-$

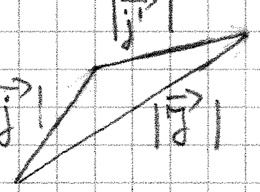
* multiplets $J = j+j'$, $J = j+j'-1$, $J = j+j'-2$, ...
as long as there is one more state on the lines with
$M = m+m'$ fixed when $J_-$ is applied $(M \to M-1)$

* algorithm terminates when a corner is reached
$\Leftrightarrow$ $M = |j-j'|$ = smallest value of $J$

* $|J\,M\rangle$ with $J = j+j',\ j+j'-1,\ \dots,\ |j-j'|$ and
$M = J,\ J-1,\ \dots,\ -J$ (for each $J$)

* complete set of states (given $j, j'$) : for example $j' \leq j$

$$\sum_{J=j-j'}^{j+j'} (2J+1) = (2j'+1)\,\frac{1}{2}\left[2(j+j')+1 + 2(j-j')+1\right] = (2j'+1)(2j+1)$$



* $|j-j'| \leq J \leq |j+j'|$

$\Rightarrow \sqrt{J(J+1)} < \sqrt{j(j+1)} + \sqrt{j'(j'+1)}$ triangle inequality

$j = j' = \frac{1}{2} \Rightarrow J = 0, 1$ , $\sqrt{2} < \sqrt{\frac{3}{4}} + \sqrt{\frac{3}{4}} = \sqrt{3}$

### ↳ 1.4 Computation of Clebsch-Gordan coefficients

$$|J\,M\rangle = \sum_{m,m'} |mm'\rangle \langle mm'|JM\rangle$$

$\langle \underbrace{mm'}_{\nwarrow} | \underbrace{JM}_{\uparrow} \rangle$ : unitary matrix , size : $\left[(2j+1)(2j'+1)\right]^2$

indices, $(2j+1)\cdot(2j'+1)$ values

$$\sum_{mm'} \langle mm'|JM\rangle^* \langle mm'|J'M'\rangle = \delta_{JJ'}\,\delta_{MM'}$$

$$\sum_{JM} \langle mm'|JM\rangle^* \langle nn'|JM\rangle = \delta_{mn}\,\delta_{m'n'}$$

Remark : it will be shown that $\langle mm'|JM\rangle$ can be chosen to be real

Phase convention :

- inside each "ladder" the phase is fixed :

$J_- |J M\rangle = c \, |J \; M-1\rangle$ with c real and positive

all states $\| \, | \, \rangle \|^2 \overset{!}{=} 1 \Rightarrow c = +\hbar \sqrt{(J+M)(J-M+1)}$

- the overall phase of the multiplet is not fixed

convention of spherical harmonics :

$Y_{\ell 0}(0,0)$ = real positive

convention of Clebsch-Gordan coefficients :

$\langle m \, m' | J J \rangle$ = real positive for all $|j-j'| \le J \le j+j'$

at $\underline{m=j}$, $m' = J-j$

→ "entry point on the J-ladder"

⟹ all $\langle m m' | J M \rangle$ real

This phase convention is asymmetric under $\vec{j} \leftrightarrow \vec{j}'$

Firstly : $\boxed{J = j + j'}$

$$|J J\rangle = |m=j \; m'=j'\rangle \Rightarrow \langle j j' | J J \rangle = +1$$

Application of $J_- = j_- + j'_-$ on both sides :

$$J_- |J J\rangle = \hbar \sqrt{(J+J)(J-J+1)} \, |J \; J-1\rangle = \hbar \sqrt{2J} \, |J \; J-1\rangle$$

$$= (j_- + j'_-) \, |m=j \; m'=j'\rangle = \hbar \sqrt{2j} \, |j-1 \; j'\rangle + \hbar \sqrt{2j'} \, |j \; j'-1\rangle$$

$$\Rightarrow |J \; J-1\rangle = \sqrt{\frac{j}{J}} \, |j-1 \; j'\rangle + \sqrt{\frac{j'}{J}} \, |j \; j'-1\rangle$$

$$\langle j-1 \; j' | J=j+j' \; M=J-1 \rangle = \sqrt{\frac{j}{j+j'}}$$

$$\langle j \; j'-1 | \quad '' \quad \rangle = \sqrt{\frac{j'}{j+j'}}$$

etc. until $\langle -j \; -j' | J=j+j' \; M=-J \rangle = +1$

Afterwards : $\boxed{J = j + j' - 1}$

$|J\, J\rangle = \alpha\, |j\; j'-1\rangle + \beta\, |j-1\; j'\rangle$ , $\alpha > 0$ real (our phase convention)

$\alpha^2 + |\beta|^2 = 1$

$$0 \overset{!}{=} J_+ |J\, J\rangle = \beta\, j_+ |j-1\;\, j'\rangle + \alpha\, j'_+ |j\;\, j'-1\rangle$$
$$= \left(\hbar\beta\sqrt{2j} + \hbar\alpha\sqrt{2j'}\right) |j\;\, j'\rangle$$

$$\Rightarrow \alpha = \sqrt{\frac{j}{j+j'}} \quad , \quad \beta = -\sqrt{\frac{j'}{j+j'}}$$

$$\langle j-1\;\, j' |\, J = j+j'-1 \quad M = J\rangle = -\sqrt{\frac{j'}{j+j'}}$$

$$\langle j\;\, j'-1 | \qquad '' \qquad \rangle = \sqrt{\frac{j}{j+j'}}$$

other $|J\, M\rangle$ from application of $J_- = j_- + j'_-$ .

- tables (cf. Weinberg's book)
- tricks, recursion formulae, symmetries between Clebsch-Gordan coefficients
- computer

4.1.5 Example : $1 + \frac{1}{2}$ → exercises

For example Pauli electron with $l = 1$ , $S = \frac{1}{2}$ , $\vec{J} = \vec{L} + \vec{S}$ :

$|m\; s\rangle$ , $m = 1, 0, -1$ , $s = \frac{1}{2}, -\frac{1}{2}$

Dimension = dim = 6

Expect : $J = \frac{3}{2}$ (dim = 4) and $J = \frac{1}{2}$ (dim = 2)

$\boxed{J = \frac{3}{2}}$ :

$$|J = \tfrac{3}{2} \quad M = \tfrac{3}{2}\rangle = |m = 1 \quad s = \tfrac{1}{2}\rangle$$

on the left : $J_- \, |\frac{3}{2}\;\, \frac{3}{2}\rangle = \hbar\sqrt{3}\, |\frac{3}{2}\;\, \frac{1}{2}\rangle$

on the right : $(L_- + S_-)\, |1\;\, \frac{1}{2}\rangle = \hbar\sqrt{2}\, |0\;\, \frac{1}{2}\rangle + \hbar\, |1\;\, -\frac{1}{2}\rangle$

$$\Rightarrow \left|J=\tfrac{3}{2}\;\; M=\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}}\left|0\;\; \tfrac{1}{2}\right\rangle + \sqrt{\tfrac{1}{3}}\left|1\;\; -\tfrac{1}{2}\right\rangle$$

on the left: $J_-\left|\tfrac{3}{2}\;\; \tfrac{1}{2}\right\rangle = \hbar\, 2\left|\tfrac{3}{2}\;\; -\tfrac{1}{2}\right\rangle$

on the right: $\left(L_- + S_-\right)\left(\sqrt{\tfrac{2}{3}}\left|0\;\; \tfrac{1}{2}\right\rangle + \sqrt{\tfrac{1}{3}}\left|1\;\; -\tfrac{1}{2}\right\rangle\right) =$

$$= \sqrt{\tfrac{2}{3}}\left(\hbar\sqrt{2}\left|-1\;\; \tfrac{1}{2}\right\rangle + \hbar\left|0\;\; -\tfrac{1}{2}\right\rangle\right) + \sqrt{\tfrac{1}{3}}\,\hbar\sqrt{2}\left|0\;\; -\tfrac{1}{2}\right\rangle$$

$$= \frac{2}{\sqrt{3}}\,\hbar\left|-1\;\; \tfrac{1}{2}\right\rangle + 2\sqrt{\tfrac{2}{3}}\,\hbar\left|0\;\; -\tfrac{1}{2}\right\rangle$$

$$\Rightarrow \left|J=\tfrac{3}{2}\;\; M=-\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}}\left|0\;\; -\tfrac{1}{2}\right\rangle + \sqrt{\tfrac{1}{3}}\left|-1\;\; \tfrac{1}{2}\right\rangle$$

on the left: $J_-\left|\tfrac{3}{2}\;\; -\tfrac{1}{2}\right\rangle = \hbar\sqrt{3}\left|\tfrac{3}{2}\;\; -\tfrac{3}{2}\right\rangle$

on the right: $\left(L_- + S_-\right)\left(\sqrt{\tfrac{2}{3}}\left|0\;\; -\tfrac{1}{2}\right\rangle + \sqrt{\tfrac{1}{3}}\left|-1\;\; \tfrac{1}{2}\right\rangle\right) =$

$$= \sqrt{\tfrac{2}{3}}\left(\hbar\sqrt{2}\left|-1\;\; -\tfrac{1}{2}\right\rangle\right) + \sqrt{\tfrac{1}{3}}\left(\hbar\left|-1\;\; -\tfrac{1}{2}\right\rangle\right) = \sqrt{3}\,\hbar\left|-1\;\; -\tfrac{1}{2}\right\rangle$$

$$\Rightarrow \left|J=\tfrac{3}{2}\;\; M=-\tfrac{3}{2}\right\rangle = \left|-1\;\; -\tfrac{1}{2}\right\rangle$$

$\boxed{J=\tfrac{1}{2}}$ :

Claim: $\left|J=\tfrac{1}{2}\;\; M=\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}}\left|1\;\; -\tfrac{1}{2}\right\rangle - \sqrt{\tfrac{1}{3}}\left|0\;\; \tfrac{1}{2}\right\rangle$

Proof: $J_+$ " $= \left(L_+ + S_+\right)\left|J=\tfrac{1}{2}\;\; M=\tfrac{1}{2}\right\rangle$

$$= \sqrt{\tfrac{2}{3}}\left(\hbar\left|1\;\; \tfrac{1}{2}\right\rangle\right) - \sqrt{\tfrac{1}{3}}\left(\sqrt{2}\,\hbar\left|1\;\; \tfrac{1}{2}\right\rangle\right) = 0 \quad \square$$

$$\Rightarrow \left|J=\tfrac{1}{2}\;\; M=-\tfrac{1}{2}\right\rangle = \frac{1}{\hbar}\, J_-\left|J=\tfrac{1}{2}\;\; M=\tfrac{1}{2}\right\rangle$$

$$= \sqrt{\tfrac{2}{3}}\left(\sqrt{2}\left|0\;\; -\tfrac{1}{2}\right\rangle\right) - \sqrt{\tfrac{1}{3}}\left(\sqrt{2}\left|-1\;\; \tfrac{1}{2}\right\rangle + \left|0\;\; -\tfrac{1}{2}\right\rangle\right)$$

$$= \sqrt{\tfrac{1}{3}}\left|0\;\; -\tfrac{1}{2}\right\rangle - \sqrt{\tfrac{2}{3}}\left|-1\;\; \tfrac{1}{2}\right\rangle$$

## 4.2 Addition of > 2 Angular Momenta

$$\vec{J} = \vec{j_1} + \vec{j_2} + \vec{j_3}$$

Tensor-product basis $|j_1 j_2 j_3 m_1 m_2 m_3\rangle$

Coupling $- \; \vec{j_1} + \vec{j_2} = \vec{J}_{12}$

$- \; \vec{J}_{12} + \vec{j_3} = \vec{J}$

$$|j_1 j_2 j_3 J_{12} M_{12} m_3\rangle =$$

$$\sum_{m_1, m_2} |j_1 j_2 j_3 m_1 m_2 m_3\rangle \underbrace{\langle j_1 j_2 m_1 m_2 | j_1 j_2 J_{12} M_{12}\rangle}_{\text{Clebsch-Gordan from } \vec{j_1}+\vec{j_2}=\vec{J}_{12}\text{, does not depend on } m_3}$$

then:

$$|j_1 j_2 j_3 J_{12} J M\rangle =$$

$$\sum_{M_{12}, m_3} |j_1 j_2 j_3 J_{12} M_{12} m_3\rangle \underbrace{\langle J_{12} j_3 M_{12} m_3 | J_{12} j_3 J M\rangle}_{\text{Clebsch-Gordan from } \vec{J}_{12}+\vec{j_3}=\vec{J}}$$

$$= \sum_{\substack{m_1 m_2 m_3 \\ M_{12}}} |j_1 j_2 j_3 m_1 m_2 m_3\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 J_{12} M_{12}\rangle \langle J_{12} j_3 M_{12} m_3 | J_{12} j_3 J M\rangle$$

$$J_{12} = |j_1 - j_2| \ldots j_1 + j_2$$

$$J = |J_{12} - j_3| \ldots J_{12} + j_3 \Rightarrow \text{maximal } J = j_1 + j_2 + j_3$$

Alternatively:

Coupling $\vec{J}_{13} = \vec{j_1} + \vec{j_3} \rightarrow |j_1 j_2 j_3 J_{13} J M\rangle$,

or $\vec{J}_{23} = \vec{j_2} + \vec{j_3} \rightarrow |j_1 j_2 j_3 J_{23} J M\rangle$

$$|j_1 j_2 j_3 J_{23} J M\rangle = \sum_{J_{12}} |j_1 j_2 j_3 J_{12} J M\rangle \cdot \underbrace{\langle j_1 j_2 j_3 J_{12} J | j_1 j_2 j_3 J_{23} J\rangle}_{\text{independent of } M}$$

Change of coupling → recoupling : Racah W-coefficients, Wigner 6-j symbols

4 angular momenta → 9-j symbols

## 4.3 The Wigner - Eckart Theorem

### 4.3.1 Selection Rules

System with angular momentum $\vec{J}$ and basis $|r j m\rangle$
( r other quantum numbers)

A is a scalar observable : $[A, \vec{J}] = 0$

Implications for matrix elements (ME) :

$$\langle r j m | A | r' j' m'\rangle = a_j(r, r')\, \delta_{jj'}\, \delta_{mm'}$$

Proof : for example $\delta_{jj'}$ :

$$0 = \langle r j m | \vec{J}^2 A - A \vec{J}^2 | r' j' m'\rangle$$

$$= \big( j(j+1) - j'(j'+1) \big) \hbar^2 \langle r j m | A | r' j' m'\rangle$$

$\Rightarrow$ ME is zero unless $j = j'$ ☒

→ several ME = 0 , others are equal

$\Rightarrow$ predictions through symmetry without solving the problem

$\vec{V}$ is a vector operator : $[J_i, V_k] = i\hbar\, \varepsilon_{ikl} V_l$

for example $\vec{x}, \vec{p}, \vec{L}, \vec{S}$

$$\Leftrightarrow \langle \psi_R | V_i | \psi_R \rangle = \langle \psi | \mathcal{U}^\dagger(R) V_i\, \mathcal{U}(R) | \psi \rangle = R_{ik} \langle \psi | V_k | \psi \rangle$$

Proof: $\mathcal{U}(R) = e^{-\frac{i}{\hbar}\alpha\,\vec{n}\cdot\vec{J}}$, infinitesimal ($\delta = \alpha$):

$$\mathcal{U}(R)^{+} V_i\, \mathcal{U}(R) \cong \left(\mathbb{1} + \frac{i}{\hbar}\delta\,\vec{n}\cdot\vec{J}\right) V_i \left(\mathbb{1} - \frac{i}{\hbar}\delta\,\vec{n}\cdot\vec{J}\right)$$

$$\cong V_i + \frac{i}{\hbar}\delta\, n_k \underbrace{[J_k, V_i]}$$

$$= i\hbar\,\varepsilon_{kil} V_l = -i\hbar\,\varepsilon_{ikl} V_l = -i\hbar \left(T_k\right)_{il} V_l$$

$$= \left(\delta_{il} + \delta\left(\vec{n}\cdot\vec{T}\right)_{il}\right) V_l \cong R_{il} V_l \qquad \blacksquare$$

Proportionality between ME of $\vec{J}$ and $\vec{V}$: it holds

$$\langle r j m | \vec{V} | r' j m' \rangle = v(r, r', j)\ \langle j m | \vec{J} | j m' \rangle$$

Proof: application of algebra, see Cohen-Tannoudji volume 2

### 4.3.2 Irreducible Tensor Operators

Other than scalar, vector operators: there exists more general operators $T^k_q$ with a well-defined transformation under rotation analogous to the states $|j m\rangle \to |k q\rangle$:

$$[J_3, T^k_q] = \hbar q\, T^k_q$$

$$[J_\pm, T^k_q] = \hbar \sqrt{k(k+1) - q(q\pm 1)}\ T^k_{q\pm 1} \quad , \quad -k \leq q \leq k$$

vector operator corresponds to $k = 1$:

$$T^1_0 = V_3 \quad , \quad T^1_\pm = \mp \frac{1}{\sqrt{2}}\left(V_1 \pm i V_2\right)$$

Proof: for example

$$[J_+, T^1_-] = \left[J_1 + iJ_2, \frac{1}{\sqrt{2}}(V_1 - iV_2)\right] = \frac{1}{\sqrt{2}}\left([J_1, -iV_2] + [iJ_2, V_1]\right)$$

$$= \frac{1}{\sqrt{2}}\left(-i\, i\hbar\,\varepsilon_{123} V_3 + i\, i\hbar\,\varepsilon_{213} V_3\right) = \hbar\sqrt{2}\, V_3 = \hbar\sqrt{2}\, T^1_0 \qquad \blacksquare$$

$\Rightarrow$ $T^k_q |j m\rangle$ have the same transformation properties under rotations as $|k q\rangle \otimes |j m\rangle$

(addition of angular momenta "$k + j$")

$$\Rightarrow \sum_{q,m} T_k^q \, | j \, m \rangle \; \langle \underbrace{(k \, j)}_{\text{dropped so far}} q \, m \, | \, J \, M \rangle$$

rotates like $|J \, M\rangle$ $\quad ( k+j \geq M \geq |k-j| )$

$$\text{cf.} \quad |J \, M\rangle = \sum_{m,m'} |(j j') \, m m'\rangle \; \langle (j j') \, m m' \, | \, J \, M \rangle$$

## 4.3.3 The Theorem

$$\langle r \, J \, M \, | \, T_q^k \, | \, r' J' M' \rangle =$$

$$\underset{\substack{\uparrow \\ \text{convention}}}{\frac{1}{\sqrt{2J+1}}} \quad \underset{\substack{\uparrow \\ \text{"reduced} \\ \text{matrix elements",} \\ \text{independent of} \\ M,\, M',\, q}}{\langle r \, J \, \| \, T^k \, \| \, r' \, J' \rangle} \cdot \underset{\substack{\uparrow \\ \text{Clebsch-Gordan,} \\ \propto \, \delta_{q,\, M-M'}}}{\langle (J' k) \, M' q \, | \, J \, M \rangle}$$

→ ratios of ME are determined in terms of Clebsch-Gordan coefficients

→ selection rules, for example $k + J' \geq J \geq |k - J'|$

# 5. Approximation Methods

Recapitulation of time-independent perturbation theory:

$H(\lambda) = H_0 + \lambda H_1 \quad (\lambda \to 1$ at the end$)$

$H_0 \, |k\rangle^{(0)} = E_0 \, |k\rangle^{(0)} \quad , \quad k = 1, \dots, d \;\to\; d$-fold degeneracy

$H(\lambda) \, |k, \lambda\rangle = E^{(k)}(\lambda) \, |k, \lambda\rangle$

Perturbation of a set of degenerate states $\{|k\rangle^{(0)}\}$ :

$$\begin{cases} E^{(k)}(\lambda) = E_0 + E_1^{(k)} \cdot \lambda + E_2^{(k)} \cdot \lambda^2 + \dots \\ |k, \lambda\rangle = |k\rangle^{(0)} + |k\rangle^{(1)} \cdot \lambda + |k\rangle^{(2)} \cdot \lambda^2 + \dots \end{cases} \qquad k = 1, \dots, d$$

The states $\{|k\rangle^{(0)}\}$ have to be chosen such that

$${}^{(0)}\langle \ell | H_1 | k\rangle^{(0)} = \text{diagonal} = \underline{\underline{E_1^{(k)}}} \cdot \delta_{k\ell}$$

( $\to$ diagonalize the matrix ${}^{(0)}\langle \ell | H_1 | k\rangle^{(0)}$ if it is not the case )

$$\Rightarrow \; |k\rangle^{(1)} = - \underset{\substack{\uparrow \\ \text{okay, since } {}^{(0)}\langle \ell | H_1 - E_1^{(k)} | k\rangle^{(0)} = 0}}{\left(H_0 - E_0\right)^{-1}} \left(H_1 - E_1^{(k)}\right) |k\rangle^{(0)}$$

Proof: insert the expansions in $\lambda$, compare powers of $\lambda$ till 1st order: $(H_0 + \lambda H_1) \left( |k\rangle^{(0)} + \lambda \, |k\rangle^{(1)} \right) =$

$$\left( E_0 + \lambda E_1^{(k)} \right) \left( |k\rangle^{(0)} + \lambda \, |k\rangle^{(1)} \right)$$

$$\Rightarrow \mathcal{O}(\lambda^1): \quad H_1 |k\rangle^{(0)} + H_0 |k\rangle^{(1)} = E_1^{(k)} \, |k\rangle^{(0)} + E_0 \, |k\rangle^{(1)}$$

$$(H_0 - E_0) \, |k\rangle^{(1)} = - \left( H_1 - E_1^{(k)} \right) |k\rangle^{(0)} \qquad \square$$

Explicitely: $|k\rangle^{(1)} = \sum_m{}' \dfrac{|m\rangle \, \langle m | H_1 - E_1^{(k)} | k\rangle^{(0)}}{E_0 - E_m}$ , sum over eigenstates of $H_0$ other than $\{|k\rangle^{(0)}\}$.

## 5.1 Time-dependent Perturbation Theory

$H(t) = H_0 + H_1(t)$

$\frac{\partial H_0}{\partial t} = 0$ ;

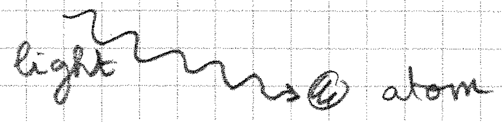
$H_0 |n\rangle = \varepsilon_n |n\rangle$

$\langle n|m\rangle = \delta_{nm}$ , $\mathbb{1} = \sum_n |n\rangle\langle n|$

$H_0$ : stationary system
- here : discrete spectrum
- later : continuum spectrum of final states

$H_1(t)$ : perturbation
- activation operation, for example $H_1(t) = 0$ for $t \leq 0$
- external fields

transition probabilities between stationary states without $H_1$, for example radiative transitions



### 5.1.1 Perturbation Theory in the Schrödinger Picture

$H_1(t) = 0$ for $t \leq 0$

$|\Psi(t=0)\rangle = |i\rangle$ initial state

$\rightarrow$ solve $i\hbar \frac{d}{dt} |\Psi(t)\rangle = (H_0 + H_1(t)) |\Psi(t)\rangle$ for $t \geq 0$

$P_{if}(t) = |\langle f|\Psi(t)\rangle|^2$ = transition probability

Matrix representation in the basis of $H_0$-eigenstates :

$|\Psi(t)\rangle = \sum_n c_n(t) |n\rangle$ , $c_n(t) = \langle n|\Psi(t)\rangle$

$$\langle m | H_0 | n \rangle = \varepsilon_m \delta_{mn}$$

$$\langle m | H_1(t) | n \rangle =: W_{mn}(t)$$

$$\Rightarrow i\hbar \sum_m \dot{c}_m(t) |m\rangle = \sum_m c_m(t) \left( \varepsilon_m |m\rangle + H_1(t) |m\rangle \right) \qquad \left( \dot{} \equiv \frac{d}{dt} \right)$$

$$\overset{\langle n|}{\Rightarrow} i\hbar \dot{c}_n = \varepsilon_n c_n + \sum_m W_{nm}(t) c_m \qquad (*)$$

$$c_n(0) = \delta_{ni}$$

$$P_{if} = |c_f(t)|^2$$

Solution of $(*)$: write $c_n(t) = \underset{\substack{\uparrow \\ \text{solution without } H_1}}{e^{-\frac{i}{\hbar}\varepsilon_n t}} b_n(t)$

Insert into $(*)$ and multiply by $e^{+\frac{i}{\hbar}\varepsilon_n t}$:

$$\Rightarrow i\hbar \dot{b}_n = \sum_m W_{nm}(t) e^{i\omega_{nm} t} b_m(t)$$

$$\omega_{nm} = \frac{\varepsilon_n - \varepsilon_m}{\hbar} = \text{Bohr frequencies}$$

Expansion in powers of $H_1$ ($H_1 \to \lambda H_1$ in $\lambda$):

$$b_n(t) = b_n^{(0)}(t) + b_n^{(1)}(t) + b_n^{(2)}(t) + \dots$$

$$\left( O(\lambda^0) \qquad O(\lambda) \qquad O(\lambda^2) \qquad \dots \right)$$

$$i\hbar \left( \dot{b}_n^{(0)}(t) + \dot{b}_n^{(1)}(t) + \dots \right) = \sum_m \underset{(O(\lambda))}{W_{nm}(t)} e^{i\omega_{nm} t} \left( b_m^{(0)}(t) + \dots \right)$$

$$\Rightarrow O(\lambda^0) : \dot{b}_n^{(0)}(t) = 0$$

$$O(\lambda^r) : i\hbar \dot{b}_n^{(r)}(t) = \sum_m W_{nm}(t) e^{i\omega_{nm} t} b_m^{(r-1)}(t)$$

Initial condition: $b_n^{(0)}(0) = \delta_{ni}$ , $b_n^{(r)}(0) = 0$ for $r > 0$.

$$\Rightarrow O(\lambda^0) : b_n^{(0)}(t) = \delta_{ni}$$

$$O(\lambda^1) : i\hbar \dot{b}_n^{(1)}(t) = W_{ni}(t) \cdot e^{i\omega_{ni} t}$$

In leading order for $n \neq i$:

$$b_n^{(1)}(t) = -\frac{i}{\hbar} \int_0^t dt' \, W_{ni}(t') \, e^{i\omega_{ni} \cdot t'}$$

$$P_{if}(t) \underset{\underset{f \neq i}{\uparrow}}{=} |b_f^{(1)}(t)|^2 = \frac{1}{\hbar^2} \left| \int_0^t dt' \, W_{fi}(t') \, e^{i\omega_{fi} \cdot t'} \right|^2 + O(H_1^3) \quad (f \neq i)$$

## 5.1.2 The Interaction Picture

Time-evolution operator: $|\psi(t)\rangle = \mathcal{U}(t,t_0) \, |\psi(t_0)\rangle$

defined through:

- $\mathcal{U}(t_0,t_0) = \mathbb{1}$
- $i\hbar \frac{\partial}{\partial t} \mathcal{U}(t,t_0) = H(t) \, \mathcal{U}(t,t_0)$ (Schrödinger's equation)

$\Rightarrow$ $\mathcal{U}$ is unitary: $\mathcal{U}^+(t_0,t_0) \, \mathcal{U}(t_0,t_0) = \mathbb{1}$

$$\frac{\partial}{\partial t} \mathcal{U}^+(t,t_0) \, \mathcal{U}(t,t_0) = 0 \quad \left( \Leftarrow \frac{\partial}{\partial t} \mathcal{U}^+ = \frac{i}{\hbar} \mathcal{U}^+ H \right)$$

similarly for $\mathcal{U}\mathcal{U}^+$

$$\Rightarrow \mathcal{U}(t_3,t_2) \, \mathcal{U}(t_2,t_1) = \mathcal{U}(t_3,t_1)$$

$$\Rightarrow \mathcal{U}^{-1}(t,t_0) = \mathcal{U}^+(t,t_0) = \mathcal{U}(t_0,t)$$

$$\Rightarrow \mathcal{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar} \int_0^t dt' \, H(t') \, \mathcal{U}(t',t_0)$$

(integral representation)

Special case: $H = H_0$ time-independent:

$$\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar} H_0 (t-t_0)} = \sum_n e^{-\frac{i}{\hbar} \varepsilon_n (t-t_0)} \, |n\rangle\langle n|$$

In general:

$$\mathcal{U} = \mathbb{1} + \sum_{n=1}^{\infty} \mathcal{U}^{(n)} \quad \text{with}$$

$$\mathcal{U}^{(n)}(t,t_0) = \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \; H(t_1)\, H(t_2) \cdots H(t_n)$$

Dyson perturbation theory (F. J. Dyson, Phy. Rev. 75, 1949)

Proof: recursive use of the integral representation:

$$\mathcal{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^{t} dt_1 \; H(t_1)\, \mathcal{U}(t_1,t_0)$$

$$= \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^{t} dt_1 \; H(t_1) \left( \mathbb{1} - \int_{t_0}^{t_1} dt_2 \; H(t_2)\, \mathcal{U}(t_2,t_0) \right)$$

$$= \cdots$$

$\square$

We can rewrite

$$\mathcal{U}^{(n)}(t,t_0) = \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \; T\left( H(t_1)\, H(t_2) \cdots H(t_n) \right)$$

$T$ : time-ordering operator

$$T\left( H(t_1) \cdots H(t_n) \right) = H(t_{\pi(1)})\, H(t_{\pi(2)}) \cdots H(t_{\pi(n)})$$

where $\pi$ = permutation of the indices $1, 2, \ldots, n$ such that

$$t_{\pi(1)} \geqslant t_{\pi(2)} \geqslant \ldots \geqslant t_{\pi(n)}$$

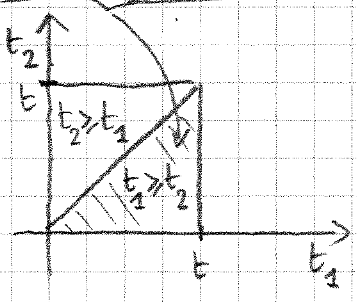
- $T\left( H(t_1) \cdots H(t_n) \right)$ is symmetric with respect to the sequence of the arguments $t_1 \ldots t_n$ by construction
- $$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \; F(t_1, \ldots, t_n) \underset{\substack{\uparrow \\ F \text{ symmetric}}}{=} \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \; F$$

Proof:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \; H(t_1) H(t_2) = \frac{1}{2}\Bigg( \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \; H(t_1)H(t_2) \quad \} \; t_1 \geq t_2$$

$$+ \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1 \; H(t_2)H(t_1) \Bigg) \quad \} \; t_2 \geq t_1$$

$$= \frac{1}{2} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \; T\big(H(t_1)H(t_2)\big)$$



generalize in $n$, **$n!$** = number of permutations of $t_1, \ldots, t_n$. $\boxed{\xi}$

$$\Rightarrow \mathcal{U}(t,t_0) = T\left( e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')} \right)$$

So far: Schrödinger picture: $|\psi_S(t)\rangle$, $\frac{\partial A_S}{\partial t} = 0$ ($A_S$ = observable)

Heisenberg picture:

$$|\psi_H\rangle = \mathcal{U}^{+}(t,t_0)\,|\psi_S(t)\rangle = |\psi_S(t_0)\rangle$$

$$A_H(t) = \mathcal{U}^{+}(t,t_0)\, A_S\, \mathcal{U}(t,t_0)$$

$i\hbar \frac{\partial A_H}{\partial t} = \left[ A_H(t), H_H(t) \right]$ Heisenberg equation

(if $\frac{\partial H}{\partial t} = 0$, then $H_H = H$)

Equal matrix elements: $\langle \psi_H | A_H(t) | \varphi_H \rangle = \langle \psi_S(t) | A_S | \varphi_S(t) \rangle$

Dirac or Interaction picture:

$\mathcal{U}_0(t,t_0) = e^{-\frac{i}{\hbar} H_0 \cdot (t-t_0)}$ free dynamics

$$A_D(t) = \mathcal{U}_0^{+}(t,t_0)\, A_S\, \mathcal{U}_0(t,t_0)$$

Require $\langle \psi_D(t) | A_D(t) | \varphi_D(t) \rangle = \langle \psi_S(t) | A_S | \varphi_S(t) \rangle$

$$\Rightarrow |\psi_D(t)\rangle = \mathcal{U}_0^{+}(t,t_0)\,|\psi_S(t)\rangle = \mathcal{U}_0^{+}(t,t_0)\,\mathcal{U}(t,t_0)\,|\psi_H\rangle$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} |\psi_D(t)\rangle = \mathcal{U}_0^+(t,t_0) \Big( \underbrace{H - H_0}_{= H_1} \Big) \mathcal{U}(t,t_0) \, |\psi_H\rangle$$

$$=: H_D(t) \, |\psi_D(t)\rangle$$

$$H_D(t) = \mathcal{U}_0^+(t,t_0) \, H_1(t) \, \mathcal{U}_0(t,t_0)$$

Define $\mathcal{U}_D(t,t_0) = \mathcal{U}_0^+(t,t_0)\,\mathcal{U}(t,t_0)$ ; then $|\psi_D(t)\rangle = \mathcal{U}_D(t,t_0)\,|\psi_H\rangle$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} \mathcal{U}_D(t,t_0) = H_D(t) \, \mathcal{U}_D(t,t_0)$$

$$\Rightarrow \quad \mathcal{U}_D(t,t_0) = T\left( e^{-\frac{i}{\hbar}\int_0^t dt' \, H_D(t')} \right)$$

Expansion yields formally all orders of perturbation theory.

## 5.1.3 The Perturbation Series in the Interaction Picture

$$P_{if}(t) = \left| \langle f | \psi_S(t)\rangle \right|^2$$

$$= \left| \langle f | \mathcal{U}(t,0) | i\rangle \right|^2$$

$$= \Big| \underbrace{\langle f | \mathcal{U}_0^+(t,0)}_{= e^{+\frac{i}{\hbar}\varepsilon_f t} \langle f|} \mathcal{U}(t,0) | i \rangle \Big|^2 = \left| \langle f | \mathcal{U}_D(t,0) | i\rangle \right|^2$$

With Dyson perturbation series:

$$\langle f | \mathcal{U}_D | i\rangle = \delta_{fi} + \sum_{n=1}^{\infty} \langle f | \mathcal{U}_D^{(n)} | i \rangle$$

1st order:

$$\langle f | \mathcal{U}_D^{(1)} | i\rangle = -\frac{i}{\hbar} \int_0^t dt' \, \langle f | H_D(t') | i\rangle$$

$$= -\frac{i}{\hbar} \int_0^t dt' \, e^{+\frac{i}{\hbar}\varepsilon_f t'} \langle f | H_1(t') | i \rangle \, e^{-\frac{i}{\hbar}\varepsilon_i t'}$$

$$= -\frac{i}{\hbar} \int_0^t dt' \, e^{i\omega_{fi} t'} \, W_{fi}(t') \, , \quad \omega_{fi} = \frac{\varepsilon_f - \varepsilon_i}{\hbar} \, , \text{ like before}$$

2nd order:

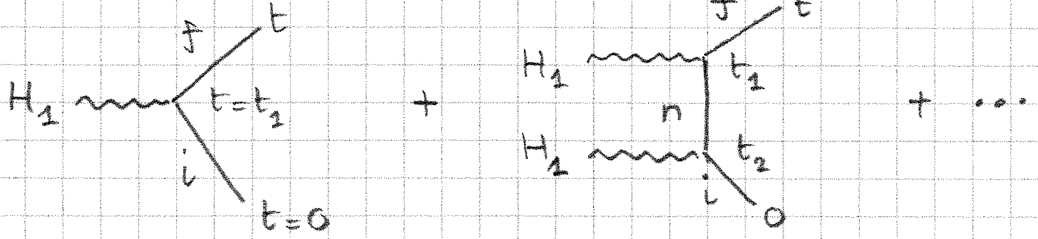
$$\langle f | \mathcal{U}_D^{(2)} | i \rangle = \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \; \langle f | H_D(t_1) \, H_D(t_2) | i \rangle$$

$$= \left(\frac{i}{\hbar}\right)^2 \sum_n \int_0^t dt_1 \int_0^{t_1} dt_2 \; e^{+\frac{i}{\hbar}\varepsilon_f \cdot t_1} \langle f | H_1(t_1) | n \rangle \, e^{-\frac{i}{\hbar}\varepsilon_n \cdot t_1} \times$$

$$e^{+\frac{i}{\hbar}\varepsilon_n \cdot t_2} \langle n | H_1(t_2) | i \rangle \, e^{-\frac{i}{\hbar}\varepsilon_i \cdot t_2}$$

$$= \left(\frac{i}{\hbar}\right)^2 \sum_n \int_0^t dt_1 \int_0^{t_1} dt_2 \; e^{i\omega_{fn} \cdot t_1} \, W_{fn}(t_1) \, e^{i\omega_{ni} \cdot t_2} \, W_{ni}(t_2)$$

etc.



Sum over discrete scatterings ; virtual intermediate states.

2nd order:

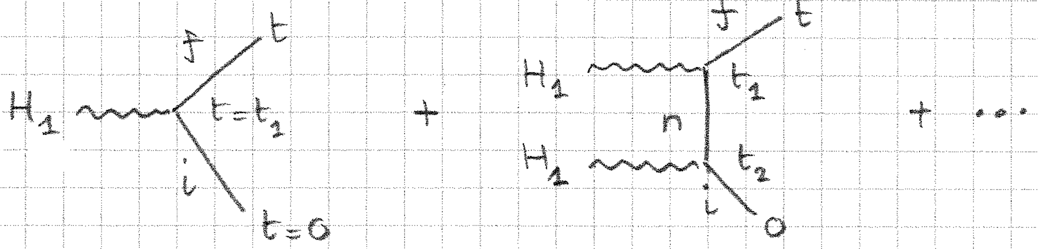
$$\langle f | \mathcal{U}_D^{(2)} | i \rangle = \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \; \langle f | H_D(t_1) \, H_D(t_2) | i \rangle$$

$$= \left(\frac{i}{\hbar}\right)^2 \sum_n \int_0^t dt_1 \int_0^{t_1} dt_2 \; e^{+\frac{i}{\hbar}\varepsilon_f \cdot t_1} \langle f | H_1(t_1) | n \rangle \, e^{-\frac{i}{\hbar}\varepsilon_n \cdot t_1} \times$$

$$e^{+\frac{i}{\hbar}\varepsilon_n \cdot t_2} \langle n | H_1(t_2) | i \rangle \, e^{-\frac{i}{\hbar}\varepsilon_i \cdot t_2}$$

$$= \left(\frac{i}{\hbar}\right)^2 \sum_n \int_0^t dt_1 \int_0^{t_1} dt_2 \; e^{i\omega_{fn} \cdot t_1} \, W_{fn}(t_1) \, e^{i\omega_{ni} \cdot t_2} \, W_{ni}(t_2)$$

etc.



Sum over discrete scatterings, virtual intermediate states.

Stopping criterium (sufficient):

$$\frac{t}{\hbar} \left| \langle m | H_1(t) | n \rangle \right| \ll 1$$

## 5.1.4 Fermi's Golden Rule

Let $\langle f | i \rangle = 0$, transition $i \to f$ occurs at 1st order

$H_1$ is independent of t, or rather

$$H_1(t) = \begin{cases} H_1 & \text{for } 0 \leq t \leq T \\ 0 & \text{otherwise} \end{cases}$$

→ then it is natural to consider eigenstates of $H_0$ at $t = 0, T$

$$P_{if} \cong \frac{1}{\hbar^2} \left| \langle f | H_1 | i \rangle \right|^2 f\left(T, \frac{\varepsilon_f - \varepsilon_i}{\hbar}\right)$$

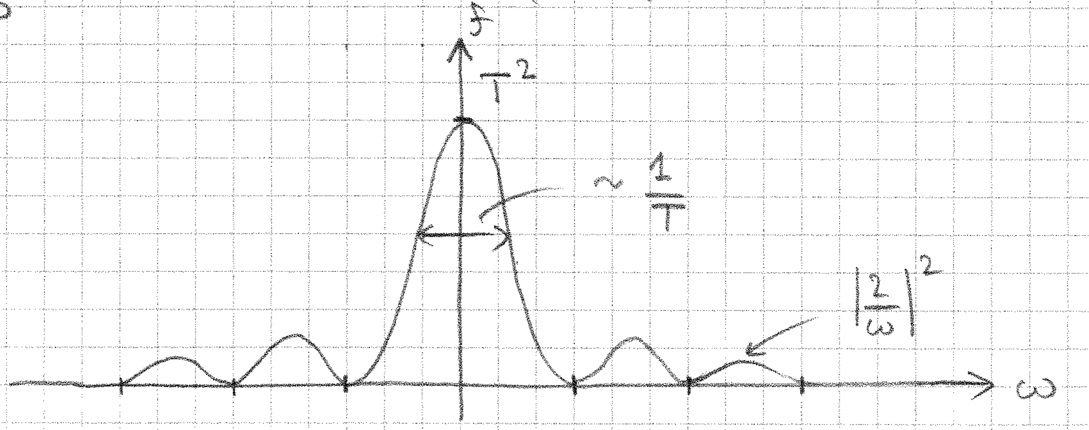
$$f(T, \omega) = \left| \int_0^T dt \; e^{it\omega} \right|^2 = \left| \frac{2}{\omega} \sin\left(\frac{\omega T}{2}\right) \right|^2$$

(1st order)

$$\lim_{\omega\to 0} f(T,\omega) =: f(T,0) = T^2$$

$f(T,\omega) = 0$ for $\omega = \frac{2\pi}{T}\cdot n$

$$\int_{-\infty}^{\infty} d\omega\, f(T,\omega) = 2\pi T \quad \left( \leftrightarrow \int d\omega\, e^{i(t-t')\omega} = 2\pi\,\delta(t-t') \right)$$



$$\Rightarrow \frac{1}{2\pi T} f(T,\omega) \xrightarrow{T\to\infty} \delta(\omega)$$

↳ representation of δ-function with height $\sim \frac{T}{2\pi}$

width $\sim \frac{1}{T}$

⇒ for large T transitions with

$|\varepsilon_f - \varepsilon_i| \lesssim \frac{\hbar}{T}$ are favoured

there: $P_{if} \cong \frac{1}{\hbar^2} \left|\langle f|H_1|i\rangle\right|^2 T^2$

$\ll 1$ (validity condition of 1st order)

$\lim\limits_{T\to\infty}$ is meaningful for transitions to a continuum of states:

(since for discrete states it holds $\lim\limits_{T\to\infty} \frac{1}{T} P_{if} \sim \delta_{fi}$)

let $F$ be a continuum of final states with energies close to $\varepsilon_f$:

$P_F = \int df\, |f\rangle\langle f|$ = projector on $F$

$\Gamma_{i\to F} = \frac{1}{T} \int_F df\, P_{if}$ : $\frac{\text{transitions}}{\text{time}}$ = rate

$$T^1_{i\to F} \overset{T\to\infty}{=} \int_F df \, \frac{1}{\hbar^2} \left|\langle f|H_1|i\rangle\right|^2 \underbrace{2\pi\,\delta\left(\frac{\varepsilon_f-\varepsilon_i}{\hbar}\right)}_{=\frac{f}{T}}$$

$$= \frac{2\pi}{\hbar} \left|\langle f|H_2|i\rangle\right|^2 \rho(\varepsilon_i) \quad \text{Fermi's golden rule}$$

$$\rho(\varepsilon) = \int_F df \, \delta(\varepsilon-\varepsilon_f) = \text{density of states}$$

We used the assumption : $|\langle f|H_1|i\rangle|$ is constant on the "shell" of $|f\rangle$ with $\varepsilon_f = \varepsilon_i$

## 5.1.5 Periodic Perturbation

Example : atom in the electromagnetic field

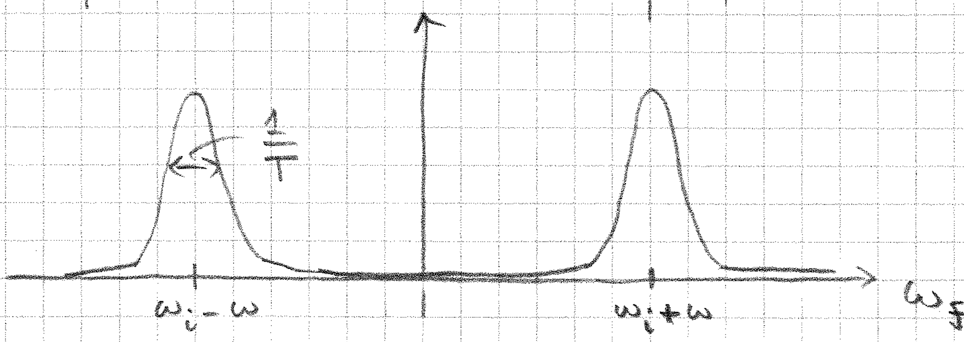
$H_1(t) = V\cos(\omega t)$ (monochromatic perturbation)

$$P_{if} = \frac{1}{\hbar^2}\left|\int_0^T dt \, e^{\frac{i}{\hbar}(\varepsilon_f-\varepsilon_i)\cdot t} \cos(\omega t) \langle f|V|i\rangle\right|^2$$

$$= \frac{1}{4\hbar^2}\left|\langle f|V|i\rangle\right|^2 \left|\int_0^T dt \left\{ e^{i(\omega_{fi}+\omega)t} + e^{i(\omega_{fi}-\omega)t}\right\}\right|^2$$

$\omega_{fi} = \frac{\varepsilon_f-\varepsilon_i}{\hbar}$ Bohr frequency

- integrals are similar as before
- contributions when $\omega_{fi}+\omega = O\left(\frac{1}{T}\right)$ or $\omega_{fi}-\omega = O\left(\frac{1}{T}\right)$
- well separated when $\omega \gg \frac{1}{T}$, no mixing contributions



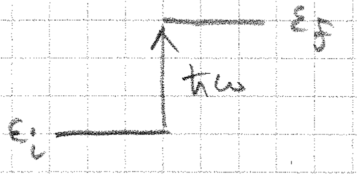
- therefore peaks when $\varepsilon_f = \varepsilon_i \pm \hbar\omega$

$$P_{if} \approx \frac{1}{4\hbar^2} \left|\langle f|V|i\rangle\right|^2 \left( f(T, \omega_{fi}+\omega) + f(T, \omega_{fi}-\omega) \right)$$

Consider groups of continuum final states $F_\pm$ with energies $\approx \varepsilon_i \pm \hbar\omega$

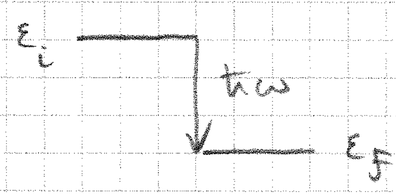
$$T_{i\to F_+} = \frac{\pi}{2\hbar} \left|\langle f_+|V|i\rangle\right|^2 \rho(\varepsilon_i + \hbar\omega)$$

absorption



$$T_{i\to F_-} = \frac{\pi}{2\hbar} \left|\langle f_-|V|i\rangle\right|^2 \rho(\varepsilon_i - \hbar\omega)$$

stimulated emission



This works provided that $\rho(\varepsilon_i \pm \hbar\omega)$ is large: resonance, depends on the spectrum

# 6. Quantum Mechanics as a Path Integral

Formalism proposed by R. P. Feynman in his Ph.D. thesis

- alternative but equivalent representation of QM
- no operators! instead functional integrals
- some problems are easier to handle
- classical limit: very intuitive
- starting point for several approximation methods and numerical simulations, in particular for Quantum Field Theories

In the following: $H = \frac{\hat{p}^2}{2m} + \underbrace{V(\hat{x})}_{\text{time-independent}}$, for now $D = 1$ (dimensions)

$H\,|n\rangle = E_n\,|n\rangle$ energie-eigenstates $|n\rangle, |m\rangle, \dots$ (notation)

$\hat{x}\,|y\rangle = y\,|y\rangle$ position-eigenstates $|x\rangle, |y\rangle, |z\rangle, \dots$

$\hat{p}\,|q\rangle = q\,|q\rangle$ momentum-eigenstates $|p\rangle, |q\rangle, \dots$

Normalization and completeness:

$$\langle n|m\rangle = \delta_{nm} \;, \quad \mathbb{1} = \sum_n |n\rangle\langle n|$$

$$\langle x|y\rangle = \delta(x-y) \;, \quad \mathbb{1} = \int dx\, |x\rangle\langle x|$$

$$\langle p|q\rangle = \delta(p-q) \;, \quad \mathbb{1} = \int dp\, |p\rangle\langle p|$$

Wave functions of the momentum-eigenstates: plane waves

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar} p\cdot x}$$

Remark: non-normalizable continuum states like $|x\rangle$, $|p\rangle$ are easier to manipulate than physical wave packets.

## 6.1. The Path Integral Representation of Transition Amplitudes

$$\mathcal{U}(t_f, x_f ; t_i, x_i) := \langle x_f | e^{-\frac{i}{\hbar} H (t_f - t_i)} | x_i \rangle$$

also called: propagator or evolution kernel

Wave function: $\psi(t_f, x_f) = \int dx_i \, \mathcal{U}(t_f, x_f ; t_i, x_i) \, \psi(t_i, x_i)$

since $\langle x_f | \psi(t_f) \rangle = \langle x_f | e^{-\frac{i}{\hbar} H (t_f - t_i)} | \psi(t_i) \rangle$

$$= \int dx_i \underbrace{\langle x_f | e^{-\frac{i}{\hbar} H (t_f - t_i)} | x_i \rangle}_{\mathcal{U}} \underbrace{\langle x_i | \psi(t_i) \rangle}_{\psi(t_i, x_i)}$$

Example: the free particle : $H = \frac{\hat{p}^2}{2m}$

$$\mathcal{U} = \langle x_f | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} T} | x_i \rangle \quad , \quad T = t_f - t_i$$

$$= \int dp \, \langle x_f | p \rangle \, e^{-\frac{i}{\hbar} \frac{p^2}{2m} T} \langle p | x_i \rangle$$

$$= \frac{1}{2\pi \hbar} \int dp \, e^{-\frac{i}{\hbar} \frac{p^2}{2m} T + \frac{i}{\hbar} p (x_f - x_i)}$$

Gauss integral with imaginary exponent

Classic Gauss integrals: $\int_{-\infty}^{\infty} dx \, e^{-\frac{x^2}{2}} = \sqrt{2\pi}$

$$\Rightarrow \int_{-\infty}^{\infty} dx \, e^{-a \frac{x^2}{2}} = \sqrt{\frac{2\pi}{a}} \quad \text{for } a > 0$$

Can be analytically continued in the domain $a \in \mathbb{C}$, $\operatorname{Re} a > 0$. The boundary value with $a = iA$ is

$$\int_{-\infty}^{\infty} dx \, e^{-iA \frac{x^2}{2}} = \sqrt{\frac{2\pi}{iA}} \, , \quad A \in \mathbb{R} .$$

With an additional linear term in the exponent (completing the square)

$$\int_{-\infty}^{\infty} dx \, e^{-a \frac{x^2}{2} + bx} = \int_{-\infty}^{\infty} dx \, e^{-\frac{a}{2} \left(x - \frac{b}{a}\right)^2 + \frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} \, e^{\frac{b^2}{2a}}$$

$$\Rightarrow \mathcal{U} = \langle x_f | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}T} | x_i \rangle = \left( \frac{2\pi i \hbar T}{m} \right)^{-1/2} e^{\frac{im}{2\hbar T}(x_f - x_i)^2}$$

$$\left( a = i \frac{T}{\hbar m} \quad , \quad b = \frac{i}{\hbar}(x_f - x_i) \quad \text{above} \right)$$

Now $V(\hat{x}) \neq 0$:

There is no simple spectral representation for $e^{-\frac{i}{\hbar}HT}$.

For small $T = \tau$:

$$e^{-\frac{i}{\hbar}\tau\left[\frac{\hat{p}^2}{2m} + V\right]} \cong e^{-\frac{i}{\hbar 2}\tau V} \; e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\tau} \; e^{-\frac{i}{\hbar 2}\tau V} + O(\tau^3)$$

(Baker, Campbell, Hausdorff → exercises)

$$\langle x_f | e^{-\frac{i}{\hbar}H\tau} | x_i \rangle \cong \langle x_f | e^{-\frac{i}{\hbar 2}\tau V} \; e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\tau} \; e^{-\frac{i}{\hbar 2}\tau V} | x_i \rangle$$

$$= \left( \frac{2\pi i \hbar \tau}{m} \right)^{-\frac{1}{2}} e^{\frac{im}{2\hbar\tau}(x_f - x_i)^2 - \frac{i}{\hbar}\frac{\tau}{2}(V(x_i) + V(x_f))}$$

calculation as before: result valid only for $\tau \to 0$

Partition of the time interval $[t_i, t_f]$ in N subintervals

$$T = t_f - t_i = N \cdot \tau$$

$$\Rightarrow \mathcal{U} = \langle x_f | e^{-\frac{i}{\hbar}HT} | x_i \rangle = \langle x_f | \left( e^{-\frac{i}{\hbar}H\tau} \right)^N | x_i \rangle$$

$$\underset{\substack{\text{completeness}\\\text{relations}}}{=} \int dx_1 \dots \int dx_{N-1} \langle x_f | e^{-\frac{i}{\hbar}H\tau} | x_{N-1} \rangle \langle x_{N-1} | e^{-\frac{i}{\hbar}H\tau} | x_{N-2} \rangle$$

$$\langle x_{N-2} | \dots | x_1 \rangle \langle x_1 | e^{-\frac{i}{\hbar}H\tau} | x_i \rangle$$

$$\cong \left( \frac{2\pi i \hbar \tau}{m} \right)^{-\frac{N}{2}} \int \left( \prod_{k=1}^{N-1} dx_k \right) \prod_{k=0}^{N-1} e^{\frac{im}{2\hbar\tau}(x_{k+1} - x_k)^2 - \frac{i}{\hbar}\frac{\tau}{2}(V(x_{k+1}) + V(x_k))}$$

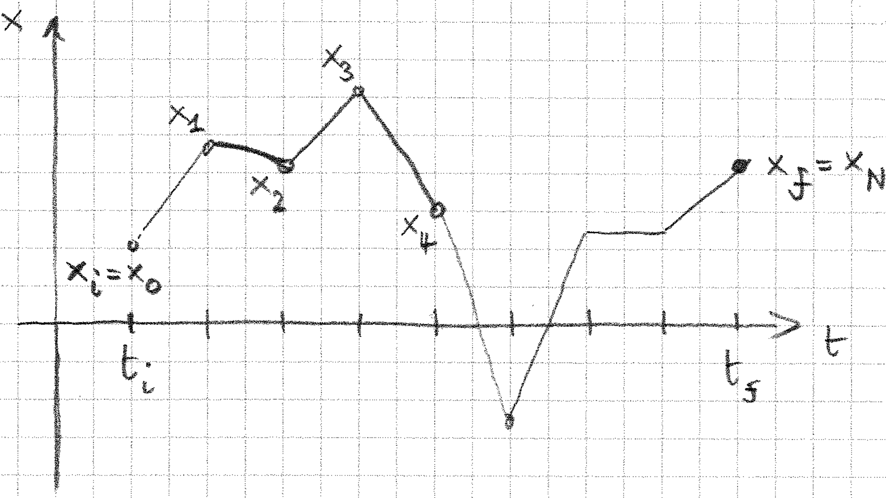
with $|x_i\rangle \equiv |x_0\rangle$

$|x_f\rangle \equiv |x_N\rangle$

$$+ \underbrace{O(N \cdot \tau^3)}_{= O(\tau^2)}$$

(Lie - Kato - Trotter product formula)

Interpretation for $N \to \infty$, $\tau \to 0$, $T = N \cdot \tau$ fixed :



$x(t) \approx$ trajectory or path

Integration over all paths :

$$\Big[\underset{\substack{\uparrow \\ \tau}}{\;}\Big]^{-\frac{N}{2}} \int_{-\infty}^{\infty} \prod_k dx_k =: \int \mathcal{D}x \quad \text{or} \quad \int \mathcal{D}[x(t)]$$

$\tau \to 0$ : functional integral : integration over all continuous functions $x(t)$ with $x(t_i) = x_i$ and $x(t_f) = x_f$

Integrand : $\prod_k e^{\cdots} = e^{\sum_k \cdots}$

$$\sum_k \tau \cdot f(x_k) \xrightarrow{\tau \to 0} \int_{t_i}^{t_f} dt \; f(x(t))$$

$$\frac{x_{k+1} - x_k}{\tau} \xrightarrow{\tau \to 0} \dot{x}(t)$$

$$\Rightarrow \mathcal{U} = \int \mathcal{D}x \; e^{\frac{i}{\hbar} \int_{t_i}^{t_f} \left(\frac{m}{2}\dot{x}^2 - V(x)\right) dt}$$

Classical mechanics : action along a trajectory

$$S[x(t)] = \int_{t_i}^{t_f} \left[\frac{m}{2}\dot{x}^2(t) - V(x(t))\right] dt$$

$$\Rightarrow \boxed{\mathcal{U} = \langle x_f | \, e^{-\frac{i}{\hbar} H (t_f - t_i)} \, | x_i \rangle = \int \mathcal{D}x \; e^{\frac{i}{\hbar} S[x(t)]}}$$

- $\lim\limits_{\tau \to 0}$ is mathematically problematic:
  - $x(t)$ continuous but in general not differentiable → what is $\dot{x}$?
  - in Quantum Mechanics: Wiener measure
  - for QFT the existence of $\tau \to 0$ is in general not proven

- classical limit: $S \gg \hbar$ or "$\hbar \to 0$"

dominant contribution comes from the trajectories for which $e^{\frac{i}{\hbar}S}$ has the slowest oscillations

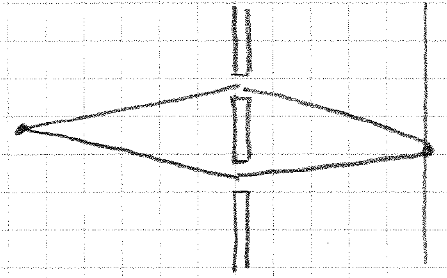
$$\to \left.\frac{\delta S}{\delta x(t)}\right|_{x(t_i)=x_i,\, x(t_f)=x_f} = 0$$ = classical principle of least action

$$\Rightarrow \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \quad , \quad L = \frac{m}{2}\dot{x}^2 - V(x)$$

Euler-Lagrange eqs. Lagrange function

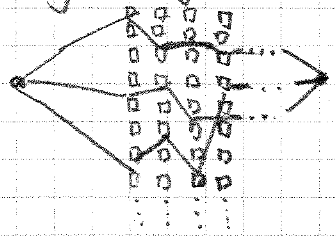
In QM all paths contribute even the classically forbidden → tunneling etc.

Illustration of the principle: double-slit experiment:



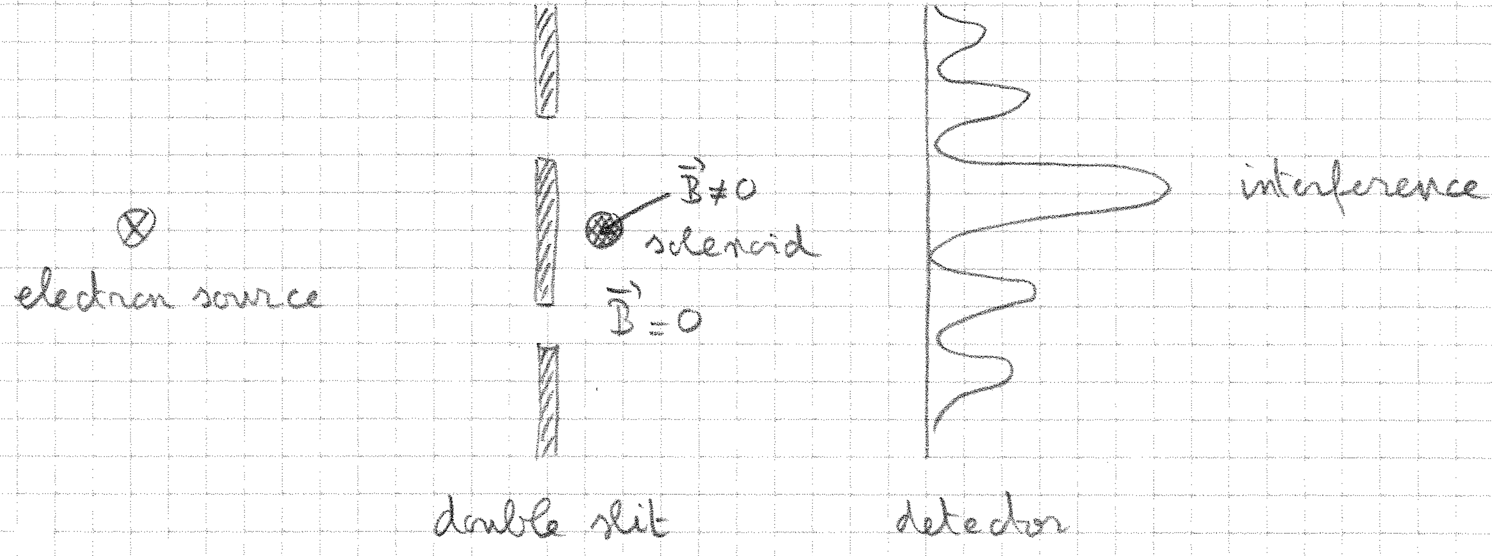
interference between paths

Limit of infinitely many "infinite-slit" experiments:



# 6.2 The Aharonov - Bohm Effect

D. Bohm and Y. Aharonov, 1959 prediction



* magnetic solenoid behind the slit generates $\vec{B} \neq 0$, $\vec{B}$ parallel to slit confined inside the solenoid, outside $\vec{B} = 0$

* solenoid is much smaller than distance of the slit, wave function of electron is practically zero there

* $\vec{B}$ on or $\vec{B}$ out changes the interference pattern!

* this effect has been observed in several experiments

$\vec{B} = \vec{\nabla} \times \vec{A}$ ; outside the solenoid is $\vec{B} = 0$ but for example

$$\vec{A}(\vec{x}) = \frac{\Phi}{2\pi} \frac{1}{x_1^2 + x_2^2} \begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix} \Rightarrow \vec{B} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Does $\vec{A}$ perhaps affect the interference pattern? But $\vec{A}$ unphysical.

Classical mechanics: no effect, since $m\ddot{\vec{x}} = e\,\dot{\vec{x}} \times \vec{B}$

$\Rightarrow$ $\vec{B} = 0$ $\Leftrightarrow$ no force on the electrons

Lagrange function and action:

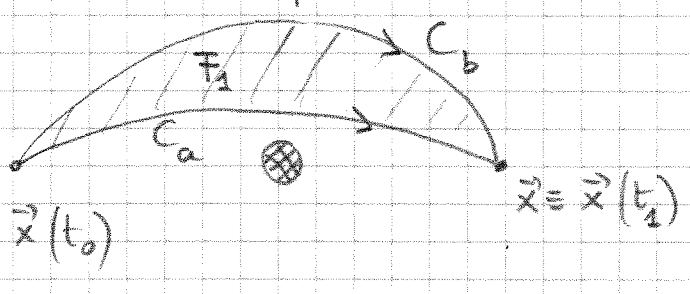
$$L = \frac{m}{2}\dot{\vec{x}}^2 + e\,\dot{\vec{x}}\cdot\vec{A}(\vec{x}) = \underbrace{L_0}_{\text{free electron}} + e\,\dot{\vec{x}}\cdot\vec{A}(\vec{x})$$

$$\Rightarrow S = S_0 + e\int_{t_1}^{t_2}\vec{A}(\vec{x}(t))\cdot\dot{\vec{x}}(t)\,dt$$

$$= S_0 + e\int_{\vec{x}(t_1)}^{\vec{x}(t_2)}\vec{A}(\vec{x})\cdot d\vec{x} \quad \text{line integral}$$

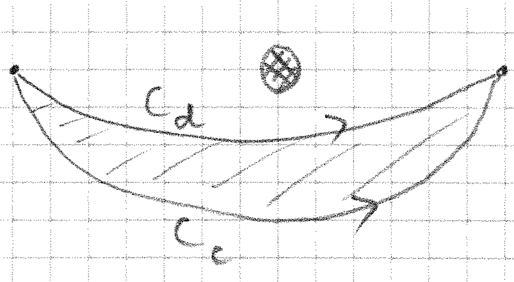
QM: all paths contribute to path integral
We can distinguish two categories of paths, (1) an (2), depending whether they go left or right of the solenoid

① consider two paths $C_a$ and $C_b$ of type (1):



$F_1$ = enclosed surface

② consider two paths $C_c$ and $C_d$ of type (2):



$F_2$ = enclosed surface

$$① : \int_{C_a}\vec{A}\cdot d\vec{x} - \int_{C_b}\vec{A}\cdot d\vec{x} = \oint_{C_a - C_b}\vec{A}\cdot d\vec{x} \underset{\substack{\uparrow \\ \text{Stokes' theorem}}}{=} \int_{F_1}(\vec{\nabla}\times\vec{A})\cdot d\vec{F}$$

$$= \int_{F_1}\vec{B}\cdot d\vec{F} = 0$$

$$\Rightarrow \int_{C_a}\vec{A}\cdot d\vec{x} = \int_{C_b}\vec{A}\cdot d\vec{x} =: \alpha_1$$

Paths of type (1) have the same action independent of the path

②: analogously: $\int_{C_c} \vec{A}\cdot d\vec{x} = \int_{C_d} \vec{A}\cdot d\vec{x} =: \alpha_2$

In the path integral:

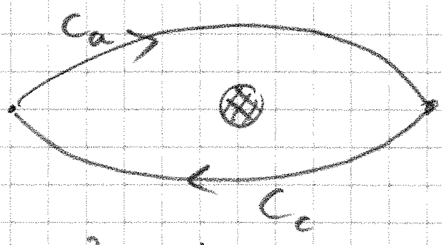
$$\langle \vec{x}, t_1 | \vec{y}, t_0 \rangle = \int \mathcal{D}x \, e^{\frac{i}{\hbar}S} = \underbrace{\int^{(1)} \mathcal{D}x \, e^{\frac{i}{\hbar}S}}_{\text{paths of type (1)}} + \underbrace{\int^{(2)} \mathcal{D}x \, e^{\frac{i}{\hbar}S}}_{\text{type (2)}}$$

$$= \underbrace{\int^{(1)} \mathcal{D}x \, e^{\frac{i}{\hbar}S_0}}_{=K_1} e^{\frac{ie}{\hbar}\alpha_1} + \underbrace{\int^{(2)} \mathcal{D}x \, e^{\frac{i}{\hbar}S_0}}_{=K_2} e^{\frac{ie}{\hbar}\alpha_2}$$

$$\Rightarrow \langle \vec{x}, t_1 | \vec{y}, t_0 \rangle = K_1 e^{\frac{ie}{\hbar}\alpha_1} + K_2 e^{\frac{ie}{\hbar}\alpha_2} = e^{\frac{ie}{\hbar}\alpha_2}\left(K_1 + K_2 e^{\frac{ie}{\hbar}(\alpha_2-\alpha_1)}\right),$$

The interference pattern is determined by $|\langle \ \rangle|^2$ and depends on

$$\alpha_2 - \alpha_1 = \int_{C_a} \vec{A}\cdot d\vec{x} - \int_{C_c} \vec{A}\cdot d\vec{x} = \oint_{C_a - C_c} \vec{A}\cdot d\vec{x} = \int \vec{B}\cdot d\vec{f} = \underbrace{\Phi}_{\text{magnetic flux}}$$

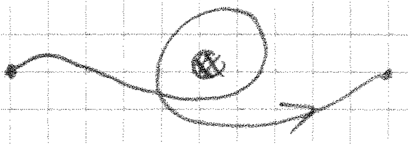


$$|\langle \vec{x}, t_1 | \vec{y}, t_0 \rangle|^2 = \left| K_1 + K_2 e^{\frac{ie}{\hbar}\Phi} \right|^2$$

Remarks:

* $\vec{A}$ depends on the gauge but $\oint \vec{A}\cdot d\vec{x}$ is gauge invariant

* the decomposition in $\int^{(1)} + \int^{(2)}$ was incomplete, for example



, if we consider such paths ($n$ windings)

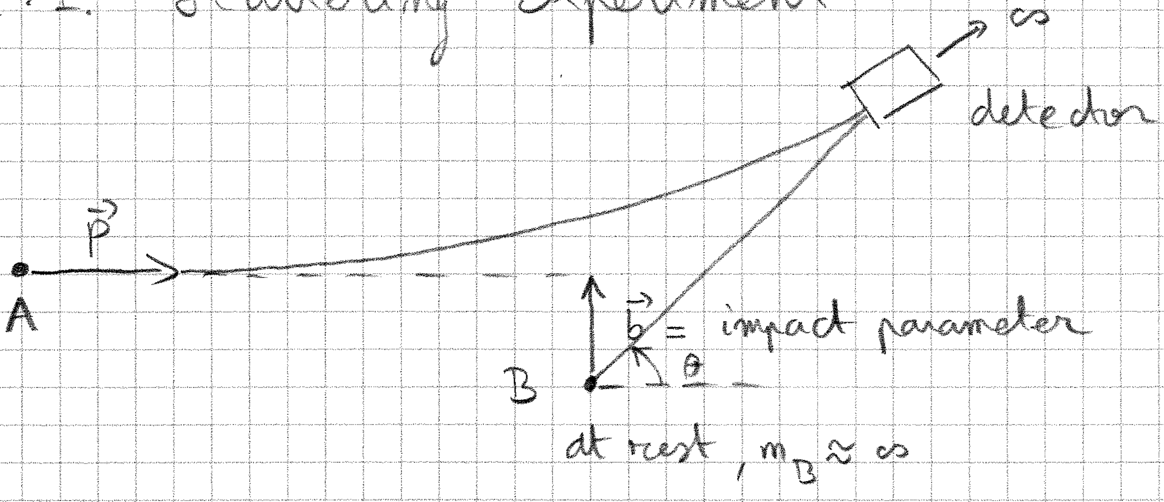
$$|\langle \vec{x}, t_1 | \vec{y}, t_0 \rangle|^2 = \left| \sum_{n\in\mathbb{Z}} K_n e^{\frac{ine}{\hbar}\Phi} \right|^2$$

# 7. Scattering

So far: spectroscopy:
transitions between discrete states

Scattering: continuum of states (at beginning and end)
- form superposition of states

## 7.1. Scattering Experiment

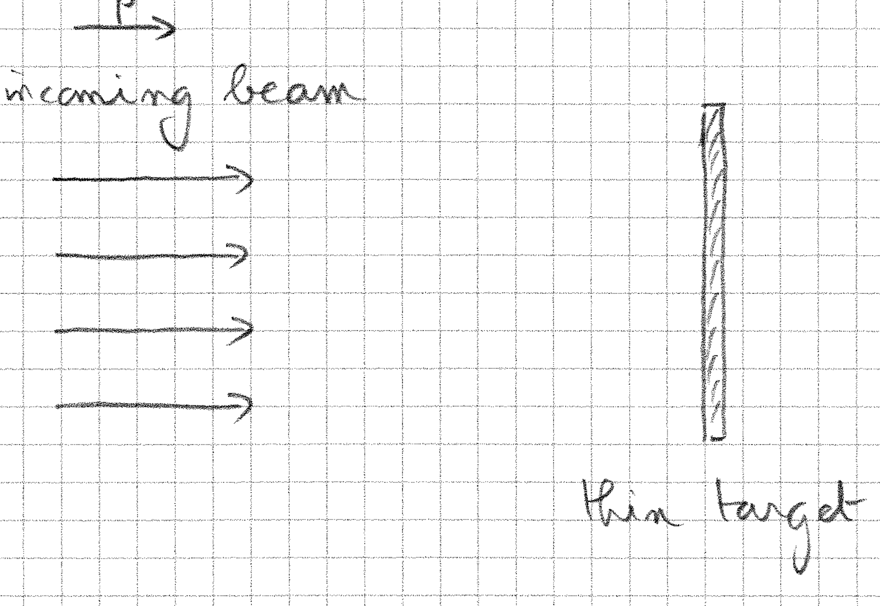


$t \to \pm\infty$: interaction between A and B can be neglected
$\to$ uniform (straight line) motion

$V(\vec{x}_A - \vec{x}_B) \cong$ constant for $|\vec{x}_A - \vec{x}_B| \to \infty$

detector $\to$ infinitely distant

more realistic:



impact parameter $\vec{b}$
and position of B
in the plane $\perp$ $\vec{p}$
are statistically
distributed (even
classically)

The detector counts the incoherent superposition of scatterings of particles A's in the beam at particles B's in the target without multiple scatterings
QM: wave packets, $\vec{p}, \vec{b}$ are not sharp, target density, ...

Choose dimensions of the system such that
- classical treatment is asymptotically meaningful
- uncertainty relation OK, i.e. $\vec{p}$ and $\vec{x}$ are sufficiently well determined

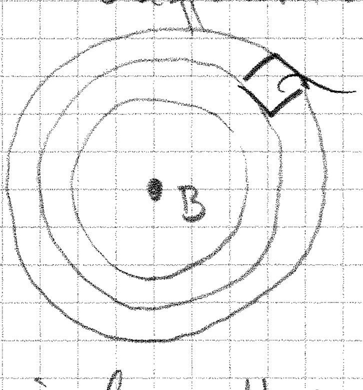
Counting rate $\left[\frac{\text{clicks}}{\text{sec}}\right]$ in the detector

$$R(d\Omega) \propto J_{in} \cdot \#(\text{involved scattering centers})$$

$$J_{in} = \frac{\#\text{ incoming particles}}{\text{sec} \cdot \text{area } (\perp \vec{p})} \qquad \left[\frac{1}{\text{sec} \cdot m^2}\right]$$

$$d\sigma := \frac{R}{J_{in} \cdot \#(\text{scattering centers})} = f(\theta, \varphi)\, d\Omega \qquad [m^2]$$

differential cross section



$d\sigma$: particles incoming here land asymptotically in $d\Omega$ (classically)

- classical scattering is described statistically because of beam, scattering centers (impact parameter cannot be determined)
- same for the QM description ("rate of clicks in $d\Omega$"), although there are no trajectories any more

$$\sigma_{tot} = \int d\sigma = \int d(\cos\theta)\, d\varphi\, F(\theta, \varphi)$$

total cross section

$\sigma_{tot}$ : surface around B, where particles are deflected = experience a force

$\sigma_{tot} \sim (\text{range of interaction})^2$ if finite

otherwise : more complicated

Nuclear physics : range $1\,\mathrm{Fm} = 10^{-13}$ cm

Unit for cross section : $1\,\text{barn} = 10^{-24}\,\mathrm{cm}^2$

mb, μb, pb, $\mathrm{fb} = 10^{-12}$ barn

Here we consider only elastic scattering : the particle changes its direction but not its kinetic energy

We do not consider inelastic scattering $A + B \to \underset{\overset{\downarrow}{\text{different internal state, e.g. atom}}}{A^*} + B^*$

Goal : infer information about the potential V from $\frac{d\sigma(\theta,\varphi)}{d\Omega} = F$

Remark :

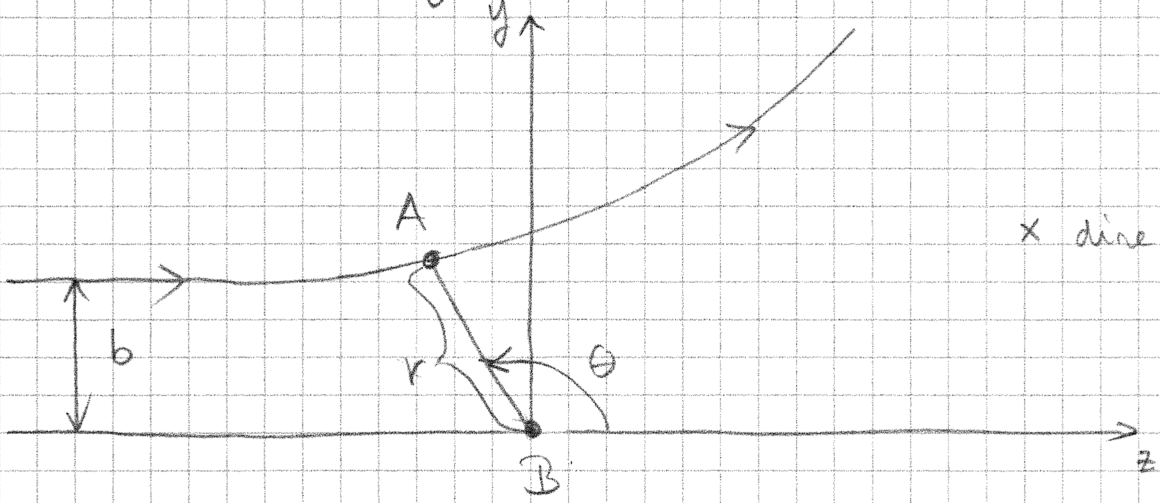
new particles (relativistic, $E > mc^2$) : $A + B \to X$

$\sigma_X$ = "cross section for X-production"

$\frac{\sigma_X}{\sigma_{anything}}$ = X-branching ratio

Constraints : conservation laws (can be tested)

# 7.2 Scattering classical



x direction : ⊗ "down"

effective "1-body in potential" problem

$m\ddot{\vec{r}} = -\vec{\nabla} V(|\vec{r}|)$ ; $V = V(|\vec{r}|)$ central potential, well-behaved

$\vec{r}(t) \simeq \vec{v}_{in} \cdot t + \vec{r}_{in}$ for $t \to -\infty$

$\vec{r}(t) \simeq \vec{v}_{out} \cdot t + \vec{r}_{out}$ for $t \to +\infty$

$\vec{L} = \vec{r} \times \vec{p} = \vec{r}_{in} \times m\vec{v}_{in} = \vec{r}_{out} \times m\vec{v}_{out}$

$\vec{L}$ is conserved $\Rightarrow$ motion in the $(y,z)$-plane:

$\vec{r} = (0, r\sin\theta, r\cos\theta)$

$\vec{v}_{in} = (0, 0, v)$

$$\Rightarrow \left.\begin{array}{l} r(t) \simeq -v \cdot t \\ \pi - \theta(t) \simeq \dfrac{b}{-vt} \end{array}\right\} t \to -\infty$$

Energy:

$$E = \frac{m}{2}\Big(\underbrace{\dot{r}^2 + r^2\dot{\theta}^2}_{= \dot{\vec{r}}^2}\Big) + V(r) \underset{t \to -\infty}{\overset{\uparrow}{=}} \frac{m}{2} v^2$$

Angular momentum:

$$\vec{L} = \vec{r} \times \vec{p} =: \begin{pmatrix} l \\ 0 \\ 0 \end{pmatrix} , \quad l = -mr^2\dot{\theta} \underset{t \to -\infty}{\overset{\uparrow}{=}} -m(-vt)^2\left(\frac{-b}{vt^2}\right) = +mbv = b\sqrt{2mE}$$

$\Rightarrow$

$$\dot{r}^2 = \frac{2}{m}\left[E\left(1-\frac{b^2}{r^2}\right) - V(r)\right]$$

$\uparrow$ centrifugal term $\frac{\ell^2}{2mr^2}$

for $t \leq t_0$:

$$\dot{r} = -\sqrt{\frac{2}{m}}\left[E\left(1-\frac{b^2}{r^2}\right) - V(r)\right]^{1/2}$$

$r$ decreases till the right hand side becomes zero for $t=t_0$, $r=r_0$

afterwards

$$\dot{r} = +\sqrt{\frac{2}{m}}\left[E\left(1-\frac{b^2}{r^2}\right) - V(r)\right]^{1/2} \quad \text{for } t \geq t_0$$

$r(t_0+\Delta t) = r(t_0-\Delta t)$ (symmetry)

$r_0 = r(t_0)$ : turning point for $r$

$t \to \infty$ : $r(t) = r(t_0 + t - t_0) = r(t_0 - (t-t_0)) = r(\underbrace{2t_0 - t}_{\to -\infty}) \simeq v\cdot(t-2t_0$

Conservation of angular momentum $\Rightarrow \dot{\theta} = -\frac{bv}{r(t)^2}$

$$\theta_{out} - \theta_{in} = \theta_{out} - \pi$$

$$= \int_{-\infty}^{\infty} dt\, \dot{\theta}(t) = -bv\int_{-\infty}^{\infty}\frac{dt}{r(t)^2} = -2bv\int_{t_0}^{\infty}\frac{dt}{r(t)^2} \qquad \left[\frac{dr}{dt} = \dot{r}\right]$$

$$= -2bv\int_{r_0}^{\infty}\frac{dr}{\dot{r}\,r^2} = -2b\sqrt{E}\int_{r_0}^{\infty}\frac{dr}{r}\left[E(r^2-b^2) - r^2V(r)\right]^{-1/2}$$

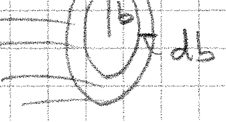
$\theta_{out}$ = scattering angle

given $b, E \to$ find $r_0$ ($\dot{r}=0$) $\to$ compute $\theta_{out}$

$\theta_{out} =: \theta = f(b)$ for fixed $E$

Cross section:

$J_{in}\, 2\pi b\, db\, \frac{\text{particles}}{\text{sec}}$ incoming in the ring



⇒ these particle are deflected in the interval $[\theta(b), \theta(b+db)]$

$\frac{\#\text{particles}}{\text{sec}}$ in $d\Omega$ $= j_{in}\, b\, db\, d\varphi \qquad (2\pi = \int d\varphi)$

$= j_{in}\, b(\theta)\, \frac{db}{d\theta}\, \frac{d\Omega}{\sin\theta} \qquad (d\Omega = \sin\theta\, d\theta\, d\varphi)$

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = \frac{b(\theta)}{\sin\theta}\,\frac{db}{d\theta}$$

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega}\, d\Omega = 2\pi \int_{0 \leftrightarrow \theta=\pi}^{b_{max} \leftrightarrow \theta=0} b\, db = \pi b_{max}^2 = \text{surface,}$$

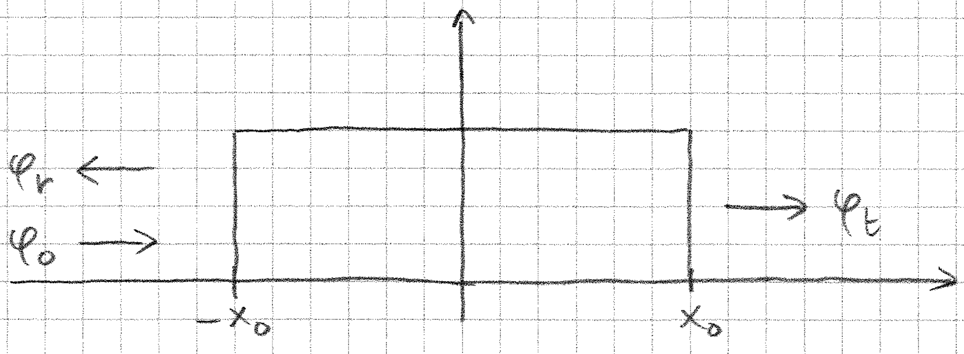
where scattering occurs

$\sigma_{tot} < \infty$ only when $V(r) = 0$ for $r \geqslant R$

## 7.3 Scattering QM

### 7.3.1 Asymptotic Solution for rotationally invariant potentials

Reminder: dimension $d=1$



$\varphi_0$ : incoming wave } for $x_0 < -x_0$ : $\varphi_0 + \varphi_r$
$\varphi_r$ : reflected wave
$\varphi_t$ : transmitted wave for $x_0 > x_0$ : $\varphi_t$

stationary scattering solution:

$$\varphi_0 + \varphi_r = e^{ikx} + \alpha_-(k)\, e^{-ikx}$$

$$\varphi_t = \gamma_+(k)\, e^{ikx} \qquad E = \frac{(\hbar k)^2}{2m}$$

general scattering solution for $x \notin [-x_0, x_0]$:

$$\Psi(x,t) = \int dk \, \tilde{\varphi}(k) \, e^{-\frac{i}{\hbar} E(k) \cdot t} \begin{cases} \varphi_0 + \varphi_r , & x < -x_0 \\ \varphi_t & x > x_0 \end{cases}$$

- time dependent solution of the Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

- no fixed energy, momentum
- localized, for example incoming wave packet

In $d=3$ dimensions we look for stationary scattering solutions

$$\varphi(\vec{x}) = \varphi_0(\vec{x}) + \varphi_s(\vec{x})$$

$$\left( -\frac{\hbar^2}{2m} \Delta + V(|\vec{x}|) - E \right) \varphi(\vec{x}) = 0$$

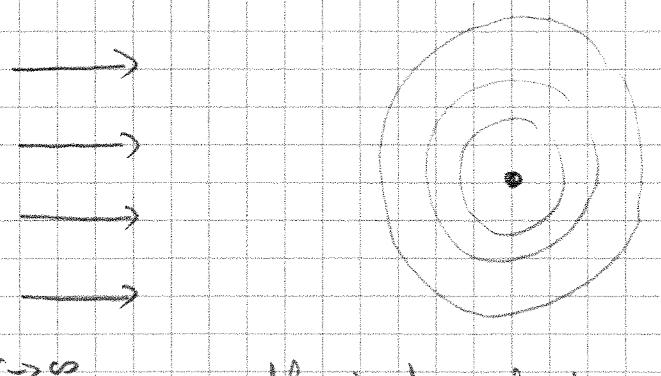
with $\varphi_0 = e^{i \vec{k} \cdot \vec{x}}$ : incoming

Particle current:

$$\vec{j}_0 = \frac{\hbar}{2mi} \left( \varphi_0^* \vec{\nabla} \varphi_0 - \varphi_0 \vec{\nabla} \varphi_0^* \right) = \frac{\hbar \vec{k}}{m}$$

in direction of $\vec{k} = (0,0,k)$

to be determined: $\varphi_s$ : scattering wave $(\leftrightarrow V(r))$



$V(r) \xrightarrow{r \to \infty} 0$ sufficiently fast, such that:

$\lim_{r \to \infty} r V(r) = 0$, i.e. $V \propto \frac{1}{r^{1+\varepsilon}}$, not Coulomb

$\Rightarrow$ $\varphi_0 + \varphi_s$ is asymptotically $(r \to \infty)$ a solution of the free Schrödinger equation with suitable boundary conditions : $\varphi_s$ outgoing scattering wave

$\varphi_0 = e^{ikz}$ = solution of the free $(V=0)$ Schrödinger equation

$$\underset{\substack{\uparrow\\ \text{polar coordinates}}}{=} e^{ikr\cos(\theta)} = f(r,\theta,\underset{\substack{\uparrow\\ \text{symmetry}}}{\cancel{\varphi}}) = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta)$$

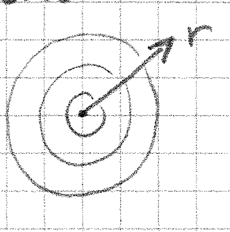
$j_l(z) = (-z)^l \left(\frac{1}{z}\frac{d}{dz}\right)^l \frac{\sin z}{z}$ : spherical Bessel function

asymptotically :

$$j_l(kr) \xrightarrow{r\to\infty} \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right) = \frac{1}{2ikr}\Big[\underset{\substack{\uparrow\\ \text{outgoing}}}{e^{i(kr-\frac{l\pi}{2})}} - \underset{\substack{\uparrow\\ \text{incoming}}}{e^{-i(kr-\frac{l\pi}{2})}}\Big]$$

spherical wave

$e^{-\frac{i}{\hbar}Et}\, e^{ikr}$ has constant phase for $r = \frac{E\cdot t}{\hbar k}$



Ansatz: $\varphi_s = f(\theta)\,\frac{e^{ikr}}{r}$

= modification of the outgoing component

It is indeed an asymtotic solution for $r \to \infty$ :

$$\Delta\varphi_0 = -k^2\varphi_0$$

$$\Delta\varphi_s = \left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\vec{L}^2}{r^2\hbar^2}\right) f(\theta)\,\frac{e^{ikr}}{r}$$

$$= \left(-k^2 + O\left(\frac{1}{r^2}\right)\right)\varphi_s$$

$$\Rightarrow \left(-\frac{\hbar^2}{2m}\Delta + V(r)\right)(\varphi_0+\varphi_s) = \left(\frac{\hbar^2k^2}{2m} + O\Big(\underset{\substack{\uparrow\\ \text{assumption!}}}{\frac{1}{r^{1+\varepsilon}}}\Big)\right)\varphi \overset{!}{=} E\varphi$$

$$\Rightarrow E = \frac{(\hbar k)^2}{2m} = \text{energy of the incoming particles}$$

Particle current of the scattering wave:

$$\vec{j}_s = \frac{\hbar}{2im}\left(\varphi_s^* \vec{\nabla}\varphi_s - \varphi_s \vec{\nabla}\varphi_s^*\right)$$

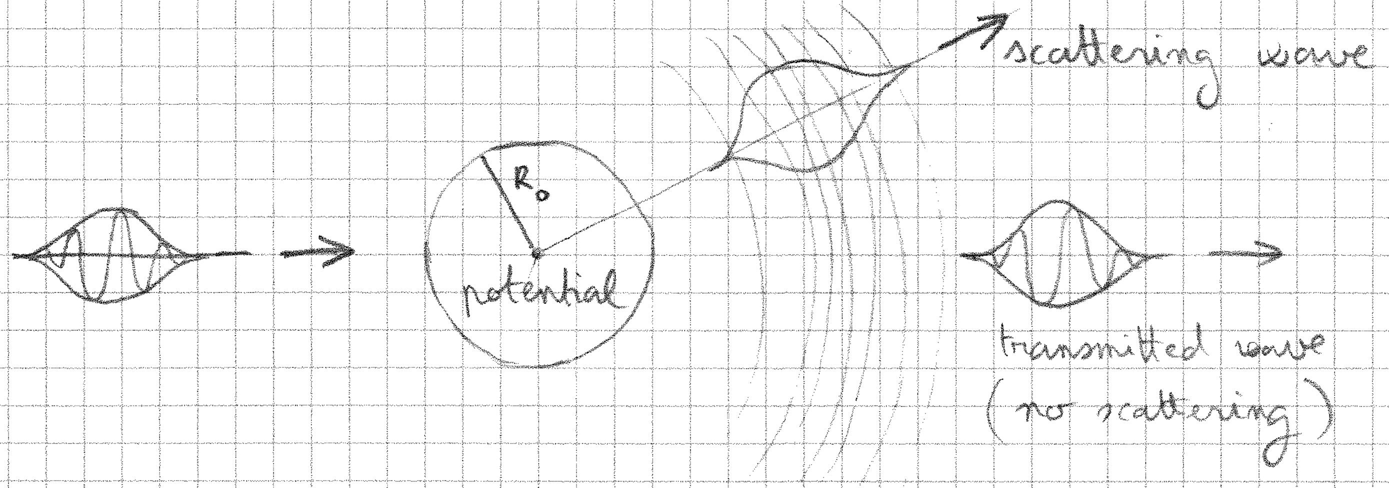
$$= \frac{\hbar k}{m}\,\frac{|f(\theta)|^2}{r^2}\,\vec{e}_r + \mathcal{O}\left(\frac{1}{r^3}\right), \quad \vec{r} = r\,\vec{e}_r$$

because $\vec{\nabla} = \vec{e}_r \underset{\hookrightarrow\, ik}{\frac{\partial}{\partial r}} + \frac{1}{r}\,\vec{e}_\theta \frac{\partial}{\partial \theta} + \frac{1}{r\sin\theta}\,\vec{e}_\varphi \frac{\partial}{\partial \varphi}$

- We assume that there is no interference between $\varphi_0$ and $\varphi_s$,

$$\vec{j}_{0+s} = \vec{j}_0 + \vec{j}_s$$

This can be achieved through the construction of wavepackets

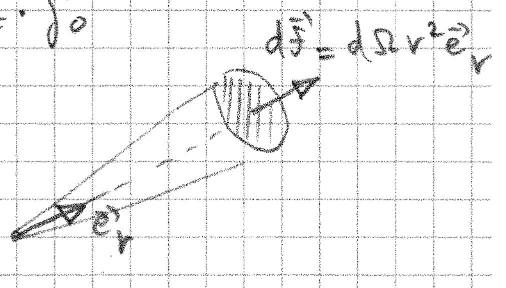


$$\frac{\#\text{ particle in detector}}{\text{sec}} = \int_{\text{sphere }(R)} \vec{j}_s \cdot d\vec{f} = \underbrace{\frac{2\pi\hbar k}{m}\int_{-1}^{1} d(\cos\theta)\,|f(\theta)|^2}_{\text{independent of } R} + \mathcal{O}\left(\frac{1}{R}\right)$$

$\Rightarrow$ conservation of number of particles of the asymptotic solution

$$d\sigma(\theta,\varphi) = \lim_{r\to\infty} \frac{\vec{j}_s \cdot d\vec{f}}{\vec{e}_z \cdot \vec{j}_0} = \lim_{r\to\infty} \frac{\vec{j}_s \cdot (d\Omega\, r^2 \vec{e}_r)}{\vec{e}_z \cdot \vec{j}_0}$$

$$= |f(\theta)|^2\, d\Omega$$



$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

- look for solutions with asymptotics $\varphi_s$

## 7.3.2 Partial Waves

From asymptotics of the solution in full space we determine $f(\theta)$

$V(|\vec{x}|) \rightarrow$ separation in polar coordinates $\rightarrow$ effective $d=1$ problem

General ansatz: $\varphi(r,\theta) = \sum_{\ell=0}^{\infty} \frac{u_\ell(r)}{r} P_\ell(\cos\theta)$

- only $P_\ell \propto Y_{\ell 0}$ because of symmetry in the azimuthal angle $\phi$ $\left( Y_{\ell m} \propto e^{im\phi} \right)$

Stationary Schrödinger equation:

$$\left( -\frac{\hbar^2}{2m} \Delta + V(r) - E \right) \varphi = 0$$

Ansatz is solution, if for each $\ell$ it holds

$$u_\ell'' + \left( k^2 - v_{eff}(r) \right) u_\ell = 0$$

$$k^2 = \frac{2m}{\hbar^2} E$$

$$v_{eff} = \frac{2m}{\hbar^2} \left[ V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \right] \qquad \left( \Delta = \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{\vec{L}^2}{r^2 \hbar^2} \right)$$

$\varphi(0,\theta)$ regular $\Rightarrow$ $u_\ell(0) = 0$ boundary condition (b.c.)

- unique solution up to a complex factor of the differential equation of 2nd order and b.c. at $r=0$
- for each $\ell$ one free constant ($=$ factor in $u_\ell$) for the general solution

$\rightarrow$ compute $u_\ell$ for a given $V(r)$

→ fit to asymptotics $\varphi_0 + \varphi_s = e^{ikz} + f(\theta)\,\frac{e^{ikr}}{r}$ for $r \to \infty$

→ determine $f(\theta)$

For $V = 0$ the solution is $\varphi = \varphi_0 \; \forall r$ with $\frac{u_\ell}{r} \propto j_\ell(kr)$

$\Rightarrow$ solves $u_\ell'' + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right) u_\ell = 0$ with $u_\ell(0) = 0$

$\ell = 0$ : $u_0 = kr\, j_0(kr) = \sin(kr)$

$\ell > 0$ : $u_\ell = kr\, j_\ell(kr) \overset{r\to\infty}{\approx} \sin\left(kr - \frac{\ell\pi}{2}\right)$

$-\frac{\ell\pi}{2}$ : phase shift due to centrifugal potential

For $V \neq 0$ but $V \xrightarrow{r\to\infty} 0$ fast enough it must hold

$$u_\ell \overset{r\to\infty}{\approx} \alpha_\ell \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)$$

$\delta_\ell$ : phase shift due to $V$

Determine $\{\alpha_\ell\}$ through asymptotics $\varphi_0 + \varphi_s$ :
$\alpha_\ell$ can be chosen such that

$$u_\ell \overset{r\to\infty}{\approx} \frac{1}{k}\, i^\ell (2\ell+1)\, e^{i\delta_\ell} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)$$

$$\Rightarrow \varphi(r,\theta) \overset{r\to\infty}{\approx} \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) P_\ell(\cos\theta) \frac{1}{2ikr} \left[ e^{2i\delta_\ell} e^{i\left(kr - \frac{\ell\pi}{2}\right)} - e^{-i\left(kr - \frac{\ell\pi}{2}\right)} \right]$$

- in the representation of $e^{ikz}$ in terms of spherical waves only the outgoing wave changes by a factor $S_\ell = e^{2i\delta_\ell}$ = phase

$$\Rightarrow f(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \frac{1}{2i} \left(S_\ell - 1\right) P_\ell(\cos\theta)$$

$\Rightarrow$ $S_\ell$ contain precisely the information about the effect of the potential

$\delta_\ell$ = phase shift of the $\ell$ partial wave

$|S_\ell| = 1$ (phase) $\Longrightarrow$ scattering is elastic : it holds

$$\int_{\partial V} \vec{j} \cdot d\vec{f} = 0$$ : no particle of the type considered is lost

$\partial V$ = sphere of radius $R \to \infty$

Proof :

$$\vec{j} = \frac{\hbar}{m} \Im m \left( \varphi^* \vec{\nabla} \varphi \right) \quad ; \quad \varphi = \sum_{\ell=0}^{\infty} \frac{u_\ell(r)}{r} P_\ell(\cos\theta)$$

$$\vec{\nabla}\varphi = \frac{\partial \varphi}{\partial r} \vec{e}_r + \dots \qquad u_\ell \overset{r\to\infty}{\approx} \frac{i^\ell (2\ell+1)}{2ik} \left[ S_\ell e^{i(kr - \frac{\ell\pi}{2})} - e^{-i(kr-\frac{\ell\pi}{2})} \right]$$

$$\int_{\partial V} \vec{j} \cdot d\vec{f} = \int d\Omega \, r^2 \vec{e}_r \cdot \vec{j} =$$

$$= \sum_{\ell,\ell'} \underbrace{\int d\Omega \, P_\ell(\cos\theta) P_{\ell'}(\cos\theta)}_{= \delta_{\ell\ell'} \frac{4\pi}{2\ell+1}} \frac{\hbar}{m} \Im m \left( u_\ell^* \frac{d}{dr} u_\ell \right)$$

$$= \sum_\ell 4\pi (2\ell+1) \frac{\hbar}{m} \frac{1}{4k} \left( \underset{\substack{\uparrow \\ \text{outgoing}}}{|S_\ell|^2} - \underset{\substack{\uparrow \\ \text{incoming}}}{1} \right) = 0$$

$\Longrightarrow$ conservation of particle current for each partial wave

$$f(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell} \sin(\delta_\ell) P_\ell(\cos\theta)$$

classically : $L = bp \leq R_0 \sqrt{2mE}$ ($R_0$ = range of $V$)

$\rightarrow$ does this imply only a finite number of $\ell$-values in QM?

# 7.3.3 The Optical Theorem

$$\frac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2$$

$$\sigma = \int d\Omega \, \frac{d\sigma}{d\Omega} = \frac{1}{k^2} \sum_{l,l'} (2l+1)(2l'+1) \, e^{i(\delta_l - \delta_{l'})} \sin(\delta_l) \sin(\delta_{l'}) \underbrace{\int d\Omega \, P_l(\cos\theta) P_{l'}(\cos\theta)}_{= \frac{4\pi}{2l+1} \delta_{ll'}}$$

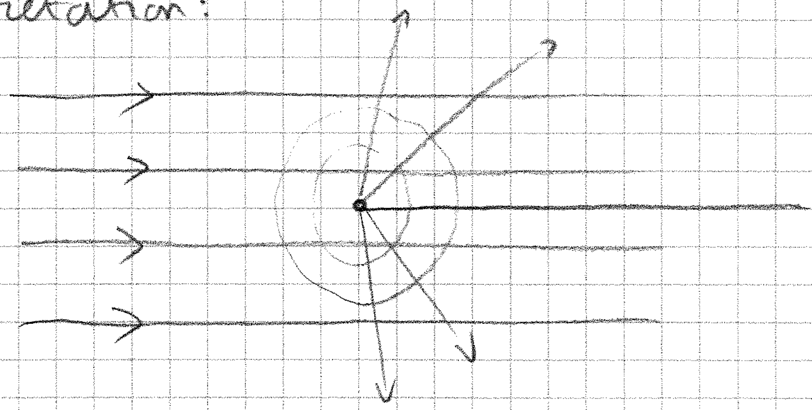
$$\Rightarrow \sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2(\delta_l)$$

$$f(0) = \frac{1}{k} \sum_l (2l+1) \, e^{i\delta_l} \sin \delta_l \qquad \left( P_l(1) = 1 \right)$$

$$\Rightarrow \sigma = \frac{4\pi}{k} \, \mathrm{Im} \, f(0)$$

This relation holds in general, even without rotational invarianc

Interpretation:



$\theta = 0$ : interference of $\varphi_s$ and $\varphi_0$

$f(\theta) \rightarrow$ scattering current deriving from $\varphi_0$ in direction $\theta = 0$ must be cancelled by interference ("shadow") because of conservation of the total current

# 7.4 Example: The Potential Well

$$V(r) = \begin{cases} -V_0 & \text{for } r<a \\ 0 & \text{for } r\geq a \end{cases} \quad , \quad q(r)^2 = \begin{cases} k_0^2 = \frac{2m}{\hbar^2}(E+V_0) & \text{for } r<a \\ k^2 = \frac{2m}{\hbar^2}E & \text{for } r\geq a \end{cases}$$

$$u_l'' + \left(q^2 - \frac{l(l+1)}{r^2}\right)u_l = 0 \quad , \quad \varphi = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos\theta)$$

Solution with $u_l(0)=0$:

$$\frac{u_l(r)}{r} = \begin{cases} c_l\, j_l(k_0 r) & \text{for } r<a \\ \alpha_l\, j_l(kr) + \beta_l\, n_l(kr) & \text{for } r\geq a \end{cases}$$

Neumann functions (irregular at $r=0$)

basis for general solution ($\to$ sin, cos asymptotically)

$c_l$ are arbitrary (Normalization), then $\alpha_l, \beta_l$ fixed by continuity at $r=a$

For $r\to\infty$:

$$u_l \overset{r\to\infty}{\approx} \frac{\alpha_l}{k}\sin\left(kr-\frac{l\pi}{2}\right) - \frac{\beta_l}{k}\cos\left(kr-\frac{l\pi}{2}\right)$$

$$\overset{!}{\propto} \sin\left(kr-\frac{l\pi}{2}+\delta_l\right) =$$

$$\cos\delta_l \sin\left(kr-\frac{l\pi}{2}\right) + \sin\delta_l \cos\left(kr-\frac{l\pi}{2}\right)$$

$$\Rightarrow \tan\delta_l = -\frac{\beta_l}{\alpha_l}$$

$\frac{d}{dr}\ln\left(\frac{u_l}{r}\right)$ continuous at $r=a$ ($\Leftrightarrow \frac{u_l}{r}$ and $\frac{d}{dr}\left(\frac{u_l}{r}\right)$ continuous):

$$k_0 \left.\frac{j_l'}{j_l}\right|_{r=k_0 a} = k \left.\frac{\alpha_l j_l' + \beta_l n_l'}{\alpha_l j_l + \beta_l n_l}\right|_{r=ka}$$

$$\Rightarrow \tan\delta_l = \frac{k j_l'(ka) j_l(k_0 a) - k_0 j_l'(k_0 a) j_l(ka)}{k n_l'(ka) j_l(k_0 a) - k_0 j_l'(k_0 a) n_l(ka)}$$

## 7.4.1 Low-Energy Limit

$z = k \cdot a \to 0$ (not $k_0 \cdot a \to 0$ !)

for small argument $z$ : $j_\ell(z) = \frac{z^\ell}{(2\ell+1)!!}\left(1 + O(z^2)\right)$

$$n_\ell(z) = -\frac{(2\ell-1)!!}{z^{\ell+1}}\left(1 + O(z^2)\right)$$

$(2\ell \pm 1)!! = 1 \cdot 3 \cdot 5 \cdot \ldots \cdot (2\ell \pm 1)$

Therefore:

$$\tan\delta_\ell = \frac{1}{(2\ell+1)!!\,(2\ell-1)!!}\,\frac{\ell z^\ell j_\ell(k_0a) - z^\ell a k_0 j_\ell'(k_0a)}{(\ell+1) z^{-\ell-1} j_\ell(k_0a) + z^{-\ell-1} a k_0 j_\ell'(k_0a)}$$

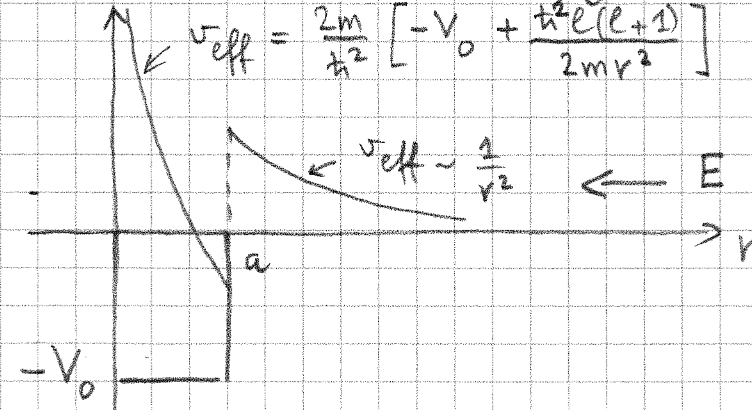
$$= \frac{z^{2\ell+1}}{(2\ell+1)!!\,(2\ell-1)!!}\,\frac{\ell j_\ell - a k_0 j_\ell'}{(\ell+1) j_\ell + a k_0 j_\ell'}\Bigg|_{\text{all arguments } = k_0 a}$$

If the denominator $\neq 0$ (see resonance):

$\tan\delta_\ell \propto (ka)^{2\ell+1}$

dominated by $\ell = 0$, s-wave scattering

other $\ell$ values: centrifugal repulsion, particles do not "see" $V(r)$ at low energy:



$$\tan\delta_0 = -ka\,\frac{a k_0 j_0'(k_0a)}{j_0(k_0a) + a k_0 j_0'(k_0a)}$$

with $j_0(z) = \frac{\sin(z)}{z}$ : $\tan\delta_0 = ka\left(\frac{\tan(k_0 a)}{k_0 a} - 1\right)$

## 7.4.2 Resonance

$$0 = (\ell+1)\, j_\ell(k_0 a) + k_0 a\, j_\ell'(k_0 a)\Big|_{E=E_R} \quad , \quad k_0^2 = \frac{2m}{\hbar^2}(E+V_0)$$

In the case $y = k_0 a \gg \ell \gg 1$ (deep well):

$$j_\ell(y) \approx \frac{1}{y}\sin\left(y - \frac{\ell\pi}{2}\right)$$

$$j_\ell'(y) \approx -\frac{1}{y^2}\sin\left(y-\frac{\ell\pi}{2}\right) + \frac{1}{y}\cos\left(y-\frac{\ell\pi}{2}\right)$$

$$0 = \frac{\ell}{k_0 a}\sin\left(k_0 a - \frac{\ell\pi}{2}\right) + \cos\left(k_0 a - \frac{\ell\pi}{2}\right)$$

$$-\cot\left(k_0 a - \frac{\ell\pi}{2}\right) = \frac{\ell}{k_0 a} \ll 1$$

$$= \tan\Big(\underbrace{k_0 a - (\ell+1)\frac{\pi}{2}}_{\text{close to } n\cdot\pi}\Big)$$

$$\Rightarrow \underbrace{k_0 a - \ell\frac{\pi}{2} \approx \left(n+\frac{1}{2}\right)\pi}_{} + \frac{\ell}{k_0 a} \qquad n = 0,1,2,\dots$$

condition for binding energy in the deep 3d potential well

since $\frac{\ell}{k_0 a} \ll 1$, $n < 0$ is not possible

Scattering phase at $E_R$:

for $E \neq E_R$, $\tan\delta_\ell \approx (ka)^{2\ell+1} \ll 1$, $\delta_\ell \approx m\cdot\pi$

at $E_R$: $\tan\delta_\ell$ diverges, $\delta_\ell(E_R) = \left(m \pm \frac{1}{2}\right)\pi$,

$\delta_\ell$ makes a jump $\delta_\ell \to (m\pm 1)\cdot\pi$

Taylor expansion of denominator at $E \approx E_R$, replace $E \to E_R$ in the numerator $\Longrightarrow$

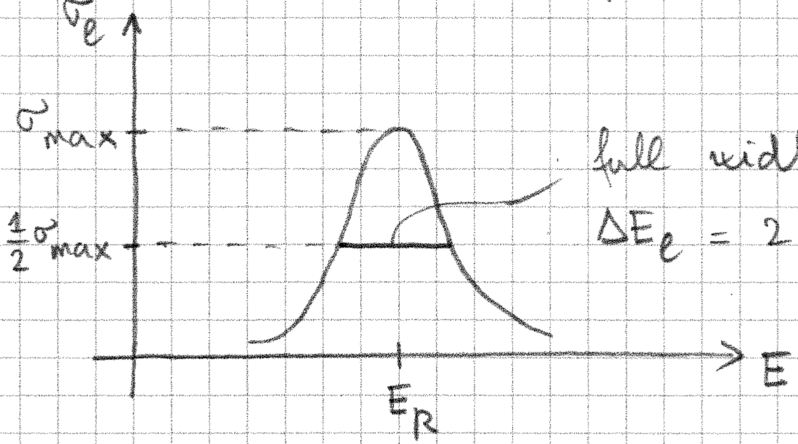
$$\tan\delta_\ell \approx \gamma_\ell \frac{(ka)^{2\ell+1}}{\underbrace{E - E_R}_{\text{linear term}}}$$

$\nearrow$ known explicitely

Partial cross section :

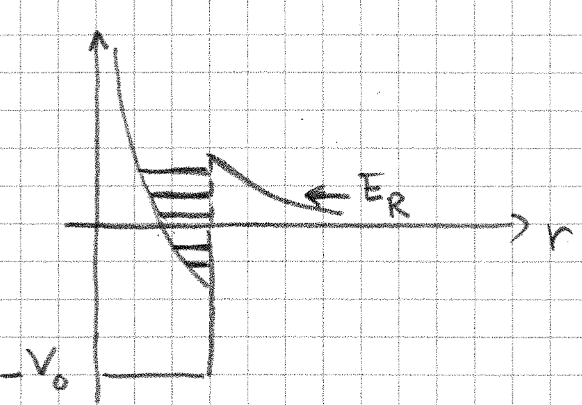
$$\sigma_\ell = \frac{4\pi(2\ell+1)}{k^2} \sin^2\delta_\ell \quad , \quad \sin^2 = \frac{\tan^2}{1+\tan^2}$$

$$\sigma_\ell = \frac{4\pi(2\ell+1)}{k^2} \; \frac{\gamma_\ell^2 (ka)^{4\ell+2}}{(E-E_R)^2 + \gamma_\ell^2 (ka)^{4\ell+2}}$$ Breit - Wigner formula



full width at half maximum
$\Delta E_\ell = 2\,|\gamma_\ell|\,(ka)^{2\ell+1}$

- sharp resonance, k·a is small
- other $\sigma_{\ell'}$ negligible (do not fulfill resonance condition)
- large part of the ℓ-wave tunnels through centrifugal barrier
- quasi-bound state, metastable, lifetime $\tau$ : $\Delta E_\ell \sim \frac{\hbar}{\tau}$, ℓ-wave emitted again → large $\sigma_\ell$



ℓ = 0 , s-wave scattering

Low-energy limit : $\tan\delta_0 = -k a_s$

$$a_s = a\left(1 - \frac{\tan(k_0 a)}{k_0 a}\right)$$ scattering length

$\Rightarrow \sigma_0 = \frac{4\pi}{k^2} \sin^2 \delta_0 \xrightarrow{k\to 0} 4\pi a_s^2 + O(k^2)$

Analysis of the exact expression for $\tan \delta_0$ yields

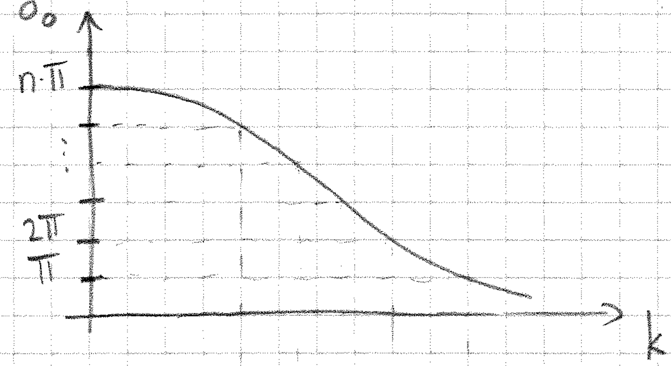
$$0 = \lim_{k\to 0} \tan \delta_0(k) = \lim_{k\to\infty} \tan \delta_0(k)$$

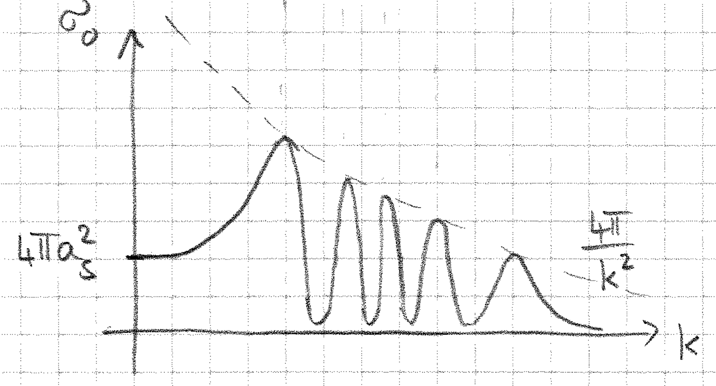
$\delta_\ell$ was introduced in $e^{2i\delta_\ell}$ → undetermined by $n\cdot\pi$

Convention: $\delta_0(\infty) = 0$ , $\delta_0(k)$ continuous

$\Rightarrow \delta_0(0) = n\cdot\pi$ , $n$ = # bound states in the potential well of depth $V_0$

$\Rightarrow$





$n$ resonances

## 7.4.4 Born Approximation for Scattering Phases

We had:

$$u_\ell'' + \left(k^2 - \frac{2m}{\hbar^2} V(r) - \frac{\ell(\ell+1)}{r^2}\right) u_\ell = 0$$

$u_\ell(0) = 0$

$$u_\ell \xrightarrow{r\to\infty} \frac{1}{k} i^\ell (2\ell+1) e^{i\delta_\ell} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right) \xrightarrow{\text{extract}} \delta_\ell$$

Let $u_\ell^{(0)}$ be the above solution for $V=0$:

$$u_\ell^{(0)} = i^\ell \, (2\ell+1) \, r \, j_\ell(kr)$$

Using the differential equations it can be shown

$$\int_0^\infty dr \left( \underset{\uparrow}{u_\ell''} \, \underset{\downarrow}{u_\ell^{(0)}} - \underset{\downarrow}{u_\ell} \, \underset{\uparrow}{u_\ell^{(0)''}} \right) = \frac{2m}{\hbar^2} \int_0^\infty dr \, V \, u_\ell \, u_\ell^{(0)}$$

partial integration

$$= \left( u_\ell' u_\ell^{(0)} - u_\ell u_\ell^{(0)'} \right) \Big|_0^\infty - 0$$

$$= \lim_{r\to\infty} \left( u_\ell' u_\ell^{(0)} - u_\ell u_\ell^{(0)'} \right)$$

$$= -k \left( \frac{1}{k} i^\ell (2\ell+1) \right)^2 e^{i\delta_\ell} \sin\delta_\ell$$

$$\Rightarrow \quad i^\ell (2\ell+1) \, e^{i\delta_\ell} \sin\delta_\ell = -\frac{2m}{\hbar^2} \int_0^\infty dr \, V \, kr \, j_\ell(kr) \, u_\ell$$

- exact relation (integral representation)

- not an explicit solution: $u_\ell$ on the right-hand side!

Born approximation: replace

$u_\ell \to u_\ell^{(0)}$ on the right-hand side

valid when:

- scattering $\propto V$ is a small effect

- $\delta_\ell(k)$ is small

Not in the resonance region, but for $k\to\infty$. There:

$$\delta_\ell \overset{k\to\infty}{\approx} -\frac{2m}{\hbar^2} \frac{1}{k} \int_0^\infty dr \, V(r) \left[ \underbrace{kr \, j_\ell(kr)}_{\approx \sin(kr) \text{ when } kr \gg \ell} \right]^2$$

# 7.5 Solution via Green Function

## 7.5.1 Schrödinger Equation as an Integral Equation

Stationary Schrödinger equation for scattering solution:

$$\left(\Delta_x + k^2\right) \varphi(\vec{x}) = v(\vec{x})\, \varphi(\vec{x}) \quad , \quad \Delta_x = \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2}$$

$$k^2 = \frac{2m}{\hbar^2} E \quad , \quad v(\vec{x}) = \frac{2m}{\hbar^2} V(\vec{x})$$

Green function:

$$\left(\Delta_x + k^2\right) G(\vec{x}-\vec{y}) = \delta^{(3)}(\vec{x}-\vec{y})$$

Then, the solution $\varphi(\vec{x})$ fulfills the integral equation

$$\varphi(\vec{x}) = \varphi_0(\vec{x}) + \int d^3y \; G(\vec{x}-\vec{y})\, v(\vec{y})\, \varphi(\vec{y}) \qquad (*)$$

where $\left(\Delta_x + k^2\right) \varphi_0(\vec{x}) = 0$

* $G(\vec{x}-\vec{y})$ is an integral kernel, distribution like $\delta^{(3)}(\vec{x}-\vec{y})$

* Boundary conditions must be imposed: $\varphi_0 + \varphi_s$ for $|\vec{x}| \to \infty$

Born series:

Ansatz: $\varphi = \sum_{n=0}^{\infty} \varphi_n$ , $\varphi_0$: homogeneous solution $\left(\Delta_x + k^2\right)\varphi_0 =$

insert in (*)

$$\Longrightarrow \quad \varphi_n = \int d^3y \; G(\vec{x}-\vec{y})\, v(\vec{y})\, \varphi_{n-1}(\vec{y}) \quad , \quad n \geq 1$$

power series in $v$, compare coeffs.

Mostly: $\varphi \cong \varphi_0 + \varphi_1$

$f(\theta,\phi)$ is determined from $\varphi_1$.

## 7.5.2 Green Function

Solution of $\left(\Delta^2 + k^2\right) G = \delta$ is not unique $\to$ boundary conditions are needed

We take: $\varphi_0 = e^{ikx_3}$ = incoming wave

$$\Rightarrow \int d^3y \; G(\vec{x}-\vec{y}) \, v(\vec{y}) \, \varphi(\vec{y}) \xrightarrow{|\vec{x}| \to \infty} \text{outgoing spherical wave}$$

If we assume: $v(\vec{y}) = 0$ for $|\vec{y}| > R_0$, then it must hold

$$G(\vec{x}) \xrightarrow{|\vec{x}| \to \infty} \text{outgoing spherical wave.}$$

Construction of G:

cf. electrostatics, there $\Delta_{\vec{x}} \frac{-1}{4\pi} \frac{1}{|\vec{x}-\vec{y}|} = \delta^{(3)}(\vec{x}-\vec{y})$

Coulomb potential of a point charge, i.e. the case $k^2 = 0$.

Method for general k: Fourier:

$$\left. \begin{aligned} G(\vec{x}) &= \int \frac{d^3p}{(2\pi)^3} \, \tilde{G}(\vec{p}) \, e^{i\vec{p}\cdot\vec{x}} \\ \delta^{(3)}(\vec{x}) &= \int \frac{d^3p}{(2\pi)^3} \, e^{i\vec{p}\cdot\vec{x}} \\ (\Delta_x + k^2) \, G(\vec{x}) &= \int \frac{d^3p}{(2\pi)^3} \, (-\vec{p}^{\,2} + k^2) \, \tilde{G}(\vec{p}) \, e^{i\vec{p}\cdot\vec{x}} \end{aligned} \right\} \Rightarrow$$

$$\tilde{G}(\vec{p}) = \frac{1}{-\vec{p}^{\,2} + k^2}$$

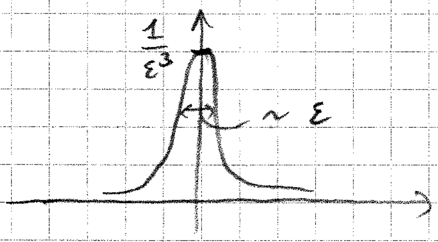
Where is the non-uniqueness? $\tilde{G}$ is singular for $\vec{p}^{\,2} = k^2$, the inverse transformation $G(\vec{x}) = \int \frac{d^3p}{(2\pi)^3} \tilde{G}(\vec{p}) \, e^{i\vec{p}\cdot\vec{x}}$ is ill-defined.

We define

$$G_\varepsilon(\vec{x}) = \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\vec{p}\cdot\vec{x}}}{-\vec{p}^{\,2} + (k+i\varepsilon)^2} \qquad (k \to k + i\varepsilon)$$

denominator $\neq 0$, $G_\varepsilon(\vec{x})$ exists as a normal function, like

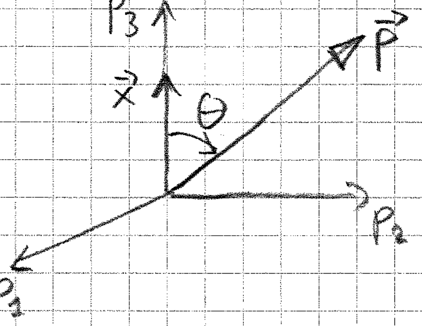
$$\lim_{\varepsilon \to 0+} \underbrace{\frac{1}{\varepsilon^3} \frac{e^{-\frac{|\vec{x}|^2}{2\varepsilon^2}}}{(2\pi)^{3/2}}}_{= \delta_\varepsilon^{(3)}(\vec{x})} = \delta^{(3)}(\vec{x})$$



We will see that $\lim_{\varepsilon\to 0+} G_\varepsilon \neq \lim_{\varepsilon\to 0-} G_\varepsilon$ $\Leftrightarrow$ ambiguity

Computation of $G_\varepsilon(\vec{x})$:

polar coordinates, $p_3$ along $\vec{x}$:



$\vec{p}\cdot\vec{x} = p\,|\vec{x}|\cos\theta \,, \quad p = |\vec{p}|$

$$G_\varepsilon(\vec{x}) = \frac{1}{(2\pi)^3}\int_0^\infty dp\,p^2 \int_{-1}^{1} d(\cos\theta)\int_0^{2\pi} d\phi \; \frac{e^{ip|\vec{x}|\cos\theta}}{-p^2+(k+i\varepsilon)^2}$$

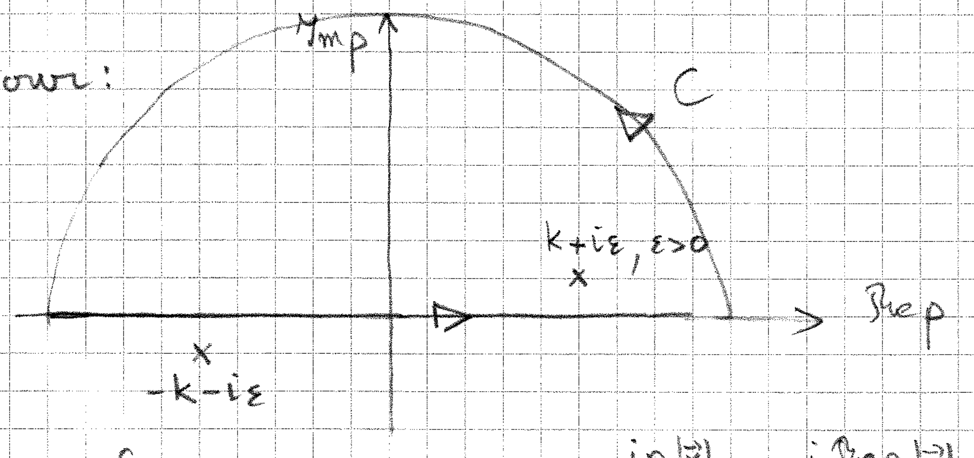
$$= \frac{1}{4\pi^2}\int_0^\infty dp\,\frac{p^2}{-p^2+(k+i\varepsilon)^2}\left[\frac{e^{ip|\vec{x}|u}}{ip|\vec{x}|}\right]_{u=-1}^{u=+1}$$

$$= \frac{1}{2\pi^2}\int_0^\infty dp\,\underbrace{\frac{\sin(p|\vec{x}|)}{|\vec{x}|}}\;\underbrace{\frac{p}{-p^2+(k+i\varepsilon)^2}}$$

odd functions of $p$

$$= \frac{1}{4\pi^2 i|\vec{x}|}\int_{-\infty}^{\infty} dp\; e^{ip|\vec{x}|}\;\frac{-p}{(p-k-i\varepsilon)(p+k+i\varepsilon)}$$

closed contour:



$$\int_{-\infty}^{\infty} dp\ldots = \oint_C dp\ldots \quad \text{since} \quad e^{ip|\vec{x}|} = e^{i\,\mathrm{Re}\,p|\vec{x}|}\cdot e^{-\mathrm{Im}\,p|\vec{x}|} \xrightarrow{|p|\to\infty} 0$$

on the circle with $\mathrm{Im}\,p > 0$

$\varepsilon > 0$ : $\quad = 2\pi i$ residuum at $p = k+i\varepsilon$

$\varepsilon < 0$ : $\quad = 2\pi i$ residuum at $p = -k-i\varepsilon$

pole $p=k+i\varepsilon$ , residuum $= \frac{1}{4\pi^2 i\,|\vec{x}|}\, e^{ik|\vec{x}| - \varepsilon|\vec{x}|} \left(-\frac{1}{2}\right)$

$(\varepsilon > 0)$

$= \frac{-1}{8\pi^2 i\,|\vec{x}|}\, e^{ik|\vec{x}|} + O(\varepsilon)$

pole $p=-k-i\varepsilon$ , residuum $= \frac{1}{4\pi^2 i\,|\vec{x}|}\, e^{-ik|\vec{x}| + \varepsilon|\vec{x}|} \left(-\frac{1}{2}\right)$

$(\varepsilon < 0)$

$= \frac{-1}{8\pi^2 i\,|\vec{x}|}\, e^{-ik|\vec{x}|} + O(\varepsilon)$

$$\Rightarrow \quad G_\pm(\vec{x}) = \lim_{\varepsilon \to 0\pm} G_\varepsilon(\vec{x}) = \underbrace{\frac{-1}{4\pi|\vec{x}|}}_{\text{Coulomb !}} e^{\pm ik|\vec{x}|}$$

$G_\pm$ correspond to outgoing(+)/incoming(−) spherical waves

$\Rightarrow \quad G_+(\vec{x}) = \frac{-1}{4\pi|\vec{x}|}\, e^{ik|\vec{x}|}$ for scattering

## 7.5.3 Born Approximation

$$\varphi(\vec{x}) = \varphi_0(\vec{x}) + \int d^3y\, G_+(\vec{x}-\vec{y})\, v(\vec{y})\, \varphi(\vec{y})$$

For $|\vec{x}| \to \infty$: $|\vec{x}-\vec{y}| = \sqrt{|\vec{x}|^2 + |\vec{y}|^2 - 2\vec{x}\cdot\vec{y}} \approx |\vec{x}| \left(1 - \frac{2\vec{x}\cdot\vec{y}}{|\vec{x}|^2}\right)^{1/2} \approx |\vec{x}| - \vec{y}\cdot\hat{x}$ , $\hat{x} = \frac{\vec{x}}{|\vec{x}|}$

$$\int_{|\vec{y}| \le R_0} d^3y\, \frac{-1}{4\pi|\vec{x}|}\, e^{ik|\vec{x}-\vec{y}|}\, v(\vec{y})\varphi(\vec{y}) \approx \frac{-e^{ik|\vec{x}|}}{4\pi|\vec{x}|} \int d^3y\, e^{-ik\vec{y}\cdot\hat{x}}\, v(\vec{y})\varphi(\vec{y})$$

Comparison with $\frac{e^{ikr}}{r} f(\theta,\phi)$ yields

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2} \int d^3y\, e^{-ik\vec{y}\cdot\hat{x}}\, V(\vec{y})\, \varphi(\vec{y})$$

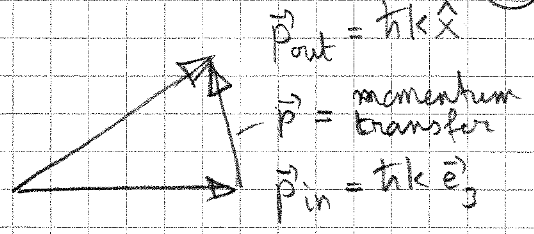
Lowest order of the Born approximation:

$$\varphi(\vec{y}) \approx \varphi_0(\vec{y}) = e^{ik\vec{y}\cdot\vec{e}_3}$$

$$\Rightarrow \quad f(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2} \int d^3y\, V(\vec{y})\, e^{-ik\vec{y}\cdot(\vec{x}-\vec{e}_3)}$$

In this approximation: Fourier transformation

$$f \sim \tilde{V}\left(\vec{p} = k\left(\hat{x} - \vec{e}_3\right)\hbar\right)$$



direction $\hat{x} \leftrightarrow (\theta, \phi)$, incoming wave parallel to $\vec{e}_3$,
no symmetry $V(|\vec{y}|)$ assumed $\Rightarrow f(\theta, \phi)$ depends on $\theta$ and $\phi$

Validity?
it should be $|\varphi_1| \leq |\varphi_0| = 1$ for large $|\vec{x}|$
Analysis (→ Nolting) shows that the approximation is plausible for large energy $kR_0 \gg 1$ and $V = V(|\vec{y}|)$ when

$$\left| \int_0^\infty dr\, V(r) \right| \ll \frac{\hbar^2 k}{m}$$

## 7.5.4 Rutherford Scattering Formula

First: Yukawa potential

$$V(\vec{x}) = V_0 \frac{e^{-\alpha|\vec{x}|}}{|\vec{x}|} \qquad (\alpha > 0)$$

Range $R_0 = \frac{1}{\alpha}$ (Coulomb limit: $\alpha \to 0$)

Scattering amplitude in first (lowest) order Born approximation

$$f(\theta) = -\frac{mV_0}{2\pi\hbar^2} \int d^3y\, \frac{e^{-\alpha|\vec{y}|}}{|\vec{y}|}\, e^{-i\vec{K}\cdot\vec{y}}$$

where $\vec{K} = k\left(\hat{x} - \vec{e}_3\right) = k\left(\sin\theta \cdot c, \sin\theta \cdot s, \cos\theta - 1\right)$

$c = \cos\phi$, $s = \sin\phi$

$$\hbar\vec{K} = \underset{\hbar k \hat{x}}{\underset{\shortparallel}{\vec{p}_{out}}} - \underset{\hbar k \vec{e}_3}{\underset{\shortparallel}{\vec{p}_{in}}}$$

Evaluate in polar coordinates (→ exercise):

$$\Rightarrow \quad f(\theta) = -\frac{2mV_0}{\hbar^2}\frac{1}{\alpha^2+\vec{K}^2}$$

$$\vec{K}^2 = k^2\left(\hat{x}-\vec{e}_3\right)^2 = k^2\left(2-2\hat{x}_3\right) = k^2\,2\left(1-\cos\theta\right) = 4k^2\sin^2\frac{\theta}{2}$$

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{4m^2V_0^2}{\hbar^4}\frac{1}{\left(\alpha^2+4k^2\sin^2\frac{\theta}{2}\right)^2}$$

$$\sigma_{tot} = \int d\Omega\,\frac{d\sigma}{d\Omega} = \frac{4m^2V_0^2}{\hbar^4}\frac{4\pi}{\alpha^2\left(\alpha^2+4k^2\right)}$$

Coulomb limit : $\alpha \searrow 0$ , $V_0 = \frac{q_1 q_2}{4\pi\varepsilon_0}$

exact Coulomb scattering amplitude:

$$f_c(\theta) = -\frac{\gamma}{4k\sin^2\frac{\theta}{2}}\,e^{\left(2i\sigma_0 - i\gamma\ln\left(\sin^2\frac{\theta}{2}\right)\right)}$$

$$\gamma = \frac{V_0 m}{\hbar^2 k}$$

differs from Born amplitude only by a phase factor, although Born approximation assumes a finite range ($\to$ more complicated treatment is needed).

$$\frac{d\sigma}{d\Omega} = \frac{V_0}{E^2}\frac{1}{16\sin^4\frac{\theta}{2}} \qquad (\text{Rutherford})$$

$\sigma_{tot} = \infty$ : in Coulomb potential there is a small deflection even for arbitrary large impact parameter b
→ unphysical, since charge is always screened at very large distances

# 7.6 Formalism of Scattering Theory

up to now: stationary scattering problem in position space → more general formalism

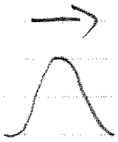
$$H = H_0 + V(\vec{x})$$

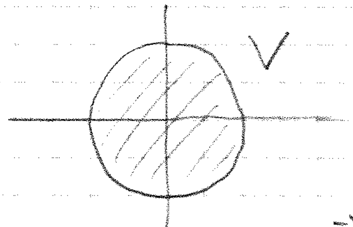
$V \xrightarrow{|\vec{x}|\to\infty} 0$ fast "enough" to be able to use asymptotically the eigenstates of $H_0$

## 7.6.1 Wave Operator (Møller Operator)

$$i\hbar \frac{d}{dt} |\varphi_-(t)\rangle = H_0 |\varphi_-(t)\rangle$$

represents free incoming state in the limit $t \to -\infty$ ,





for example : $\langle \vec{p} | \varphi_-(t)\rangle = e^{-\frac{i}{\hbar}\frac{\vec{p}^{\,2}}{2m}t} \; \tilde{\varphi}(\vec{p})$

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

represents the full exact solution with

$$\lim_{t\to-\infty} \Big| |\psi(t)\rangle - |\varphi_-(t)\rangle \Big| = 0$$

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{i}{\hbar}(t-\tau)H} \; |\psi(\tau)\rangle \\ &= \lim_{\tau\to-\infty} e^{-\frac{i}{\hbar}(t-\tau)H} \; |\varphi_-(\tau)\rangle \\ &= \lim_{\tau\to-\infty} \underbrace{e^{-\frac{i}{\hbar}(t-\tau)H}}_{U(t,\tau)} \; \underbrace{e^{+\frac{i}{\hbar}(t-\tau)H_0}}_{U_0(\tau,t)} \; |\varphi_-(t)\rangle \end{aligned}$$

$$|\psi(t)\rangle = \Omega_{in} \, |\varphi_-(t)\rangle$$

$$\Omega_{in} := \lim_{\tau \to -\infty} e^{-\frac{i}{\hbar}(t-\tau)H} \, e^{\frac{i}{\hbar}(t-\tau)H_0}$$

$$= \lim_{\tau \to -\infty} e^{+\frac{i}{\hbar}\tau H} \, e^{-\frac{i}{\hbar}\tau H_0}$$

$\Omega_{in}$ (free "incoming" solution) = (full scattering solution)

Analogously: free "outgoing" solution $|\varphi_+(t)\rangle$ :

$$|\psi(t)\rangle = \Omega_{out} \, |\varphi_+(t)\rangle$$

$$\Omega_{out} = \lim_{\tau \to +\infty} e^{\frac{i}{\hbar}\tau H} \, e^{-\frac{i}{\hbar}\tau H_0}$$

Convergence of operator for $\tau \to \pm\infty$ difficult to show, theorems, depend on $V$

Physical expectation: for a given $|\varphi_-(t)\rangle$ there exists $|\varphi_+(t)\rangle$ such that

$$\Omega_{in} \, |\varphi_-(t)\rangle = \Omega_{out} \, |\varphi_+(t)\rangle$$

$$\Omega_{in} \, \mathcal{H} = \Omega_{out} \, \mathcal{H} = \mathcal{H}_S = \text{space of scattering states}$$

$\mathcal{H}_B$ : space of bound states : it holds

$\mathcal{H}_B \perp \mathcal{H}_S$

Heuristic "proof":

$H \, |n\rangle = E_n \, |n\rangle$ , $E_n < 0$

$$e^{+\frac{i}{\hbar}E_n t} \langle n| \, \Omega_{in} \, |\varphi_-(t)\rangle = \underset{\nearrow}{\langle n|} \, \underbrace{e^{+\frac{i}{\hbar}Ht} \, \Omega_{in} \, |\varphi_-(t)\rangle} \xrightarrow{t \to -\infty} 0$$

localized incoming packet for $t \to -\infty$

rigorous proof for suitable potentials.

## 7.6.2 S-Matrix, T-Matrix

Probability to find a specific outgoing state $|\varphi_+(t)\rangle$ given a incoming state $|\varphi_-(t)\rangle$

$$W = \left| \langle \varphi_+(t) | \Omega^+_{out} \Omega_{in} | \varphi_-(t) \rangle \right|^2$$

W is independent of t, since

$$i\hbar \frac{d}{dt} \underbrace{\Omega_{in} |\varphi_-(t)\rangle}_{= |\psi(t)\rangle} = H \Omega_{in} |\varphi_-(t)\rangle$$

$$i\hbar \frac{d}{dt} \underbrace{\langle \varphi_+(t) | \Omega^+_{out}}_{= \langle \psi(t)|} = - \langle \varphi_+(t) | \Omega^+_{out} H \quad .$$

$|\varphi_\pm\rangle := |\varphi_\pm(t=0)\rangle \leftrightarrow$ Heisenberg states

$$W = \left| \langle \varphi_+ | S | \varphi_- \rangle \right|^2$$

$S = \Omega^+_{out} \Omega_{in}$ : S-matrix, scattering matrix

$S S^+ = \mathbb{1} = S^+ S$ (since $\Omega_x \Omega_x^+ = \mathbb{1} = \Omega^+_x \Omega_x$, $x = in, out$)

$$S = \lim_{\substack{\tau_+ \to \infty \\ \tau_- \to -\infty}} e^{\frac{i}{\hbar}\tau_+ H_0} e^{-\frac{i}{\hbar}(\tau_+ - \tau_-) H} e^{-\frac{i}{\hbar}\tau_- H_0}$$

$$= \lim_{\substack{\tau_+ \to \infty \\ \tau_- \to -\infty}} U_I(\tau_+, \tau_-)$$

↳ interaction picture

Limit of sharp energy:

$|\varphi\rangle = \int d^3p \, \tilde{\varphi}(\vec{p}) \, |\vec{p}\rangle \rightarrow$ discussion for $|\vec{p}\rangle$

$\langle \vec{p} | \vec{p}' \rangle = \delta^{(3)}(\vec{p} - \vec{p}')$ ; $H_0 |\vec{p}\rangle = E_{\vec{p}} |\vec{p}\rangle$ ; $E_{\vec{p}} = \frac{\vec{p}^{\,2}}{2m}$

$$|\vec{p}\ \text{in}\rangle = \Omega_{in}\, |\vec{p}\rangle$$

Proposition: $H\, |\vec{p}\ \text{in}\rangle = E_{\vec{p}}\, |\vec{p}\ \text{in}\rangle$

$\downarrow$ full Hamiltonian!

Proof:

$$e^{\frac{i}{\hbar}\tau H}\, e^{-\frac{i}{\hbar}\tau H_0}\, |\vec{p}\rangle \xrightarrow{\tau \to -\infty} |\vec{p}\ \text{in}\rangle$$ should converge

$$\Rightarrow i\hbar \frac{d}{d\tau} \left( \qquad \right) \xrightarrow{\tau \to -\infty} 0$$

$$= -H\, |\vec{p}\ \text{in}\rangle + \Omega_{in} H_0\, |\vec{p}\rangle$$

$$= \left( E_{\vec{p}} - H \right) |\vec{p}\ \text{in}\rangle \quad \square$$

$$\langle \vec{p}\ \text{in} | \vec{p}\,'\ \text{in}\rangle = \delta^{(3)}(\vec{p} - \vec{p}\,')$$

Likewise: $|\vec{p}\ \text{out}\rangle = \Omega_{out}\, |\vec{p}\rangle$

$$\langle \vec{p}\,' | S | \vec{p}\rangle = \langle \vec{p}\,' | \Omega_{out}^{\dagger}\, \Omega_{in} | \vec{p}\rangle$$

$$= \langle \vec{p}\,'\ \text{out} | \vec{p}\ \text{in}\rangle$$

$$=: \underset{\substack{\uparrow \\ \text{contribution for } V=0}}{\delta^{(3)}(\vec{p}\,' - \vec{p})} - 2\pi i\, \underset{\substack{\nearrow \\ \text{eigenstates of } H \\ \text{orthogonal when } E_{\vec{p}\,'} \neq E_{\vec{p}}}}{\delta(E_{\vec{p}\,'} - E_{\vec{p}})}\, \underset{\substack{\nwarrow \\ T\text{-matrix,} \\ \text{defined herewith}}}{T(\vec{p}\,', \vec{p})}$$

It can be shown:

$$\vec{p} = (0, 0, p)$$

$$\vec{p}\,' = p\, (\sin\theta \cos\varphi,\ \sin\theta \sin\varphi,\ \cos\theta)$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = (2\pi)^4\, (m\hbar)^2\, \left| T(\vec{p}\,', \vec{p}) \right|^2$$

# 7.6.3 Lippmann-Schwinger Equations

$$\Omega_{out} = \int_0^\infty dt \, \frac{d}{dt} \, e^{\frac{i}{\hbar}Ht} \, e^{-\frac{i}{\hbar}H_0 t} + \mathbb{1}$$

$$= \mathbb{1} + \frac{i}{\hbar}\int_0^\infty dt \, e^{\frac{i}{\hbar}Ht} \, \underbrace{V}_{=H-H_0} \, e^{-\frac{i}{\hbar}H_0 t}$$

$$\Omega_{out}|\varphi\rangle = |\varphi\rangle + \frac{i}{\hbar}\int_0^\infty dt \int d^3p \, \tilde{\varphi}(\vec{p}) \, e^{\frac{i}{\hbar}Ht} \, V \underset{\overset{\uparrow}{e^{-\frac{i}{\hbar}E_{\vec{p}} t}}}{e^{-\frac{i}{\hbar}H_0 t}} |\vec{p}\rangle$$

$$= |\varphi\rangle - \lim_{\varepsilon \to 0} \int d^3p \, \tilde{\varphi}(\vec{p}) \, (H - E_{\vec{p}} + i\varepsilon)^{-1} \, V \, |\vec{p}\rangle$$

$$-\frac{i}{\hbar}\int_0^\infty dt \, e^{\frac{i}{\hbar}(H - E_{\vec{p}} + i\varepsilon)t} = (H - E_{\vec{p}} + i\varepsilon)^{-1}$$

$\varepsilon > 0$ : damps the integrand for $t \to \infty$
needed to interchange $\int dt \Leftrightarrow \int d^3p$ , i.e. to act on $|\vec{p}\rangle$

$$|\vec{p} \text{ out}\rangle = |\vec{p}\rangle - (H - E_{\vec{p}} + i\varepsilon)^{-1} \, V \, |\vec{p}\rangle$$

$$|\vec{p} \text{ in}\rangle = |\vec{p}\rangle - (H - E_{\vec{p}} \underset{\overset{\uparrow}{!\ \text{convergence for } t \to -\infty}}{- i\varepsilon})^{-1} \, V \, |\vec{p}\rangle$$

$$|\vec{p} \text{ out}\rangle = \Big(\mathbb{1} - \underbrace{(H - E_{\vec{p}} + i\varepsilon)^{-1}}_{=(H-z)^{-1}} V \Big) |\vec{p}\rangle$$

Invert the relation:

$$\left(\mathbb{1} + (H_0 - z)^{-1} V\right)\left(\mathbb{1} - (H-z)^{-1} V\right) =$$

$$= \mathbb{1} + (H_0 - z)^{-1} V - (H-z)^{-1} V - (H_0 - z)^{-1} \underbrace{\overbrace{(H - H_0)}^{V}}_{=(H-z)-(H_0-z)} (H-z)^{-1} V$$

$$= \mathbb{1}$$

$$\Rightarrow |\vec{p}\rangle = \left( \mathbb{1} + (H_0 - E_{\vec{p}} + i\varepsilon)^{-1} V \right) |\vec{p}\ \mathrm{out}\rangle$$

$$|\vec{p}\rangle = |\vec{p}\ \mathrm{out}\rangle + (H_0 - E_{\vec{p}} + i\varepsilon)^{-1} V |\vec{p}\ \mathrm{out}\rangle$$

$$|\vec{p}\rangle = |\vec{p}\ \mathrm{in}\rangle + (H_0 - E_{\vec{p}} - i\varepsilon)^{-1} V |\vec{p}\ \mathrm{in}\rangle$$

In position space: identity

$$\left( -\frac{\hbar^2}{2m} \Delta_x - \frac{\vec{p}^{\,2}}{2m} \pm i\varepsilon \right) \langle \vec{x} | (H_0 - E_{\vec{p}} \pm i\varepsilon)^{-1} | \vec{x}\,' \rangle = \delta^{(3)}(\vec{x} - \vec{x}\,')$$

From section 7.5.2 we know:

$$\left( \Delta + \underbrace{(k \pm i\varepsilon)^2}_{= k^2 \pm 2i\varepsilon k} \right) G_\pm(\vec{x}) = \delta^{(3)}(\vec{x})$$

Comparison $\Rightarrow$

$$\langle \vec{x} | (H_0 - E_{\vec{p}} \pm i\varepsilon)^{-1} | \vec{x}\,' \rangle = -\frac{2m}{\hbar^2} G_\mp (\vec{x} - \vec{x}\,')$$

$$= \frac{m}{2\pi\hbar^2 |\vec{x} - \vec{x}\,'|} e^{\mp \frac{i}{\hbar} |\vec{p}| |\vec{x} - \vec{x}\,'|}$$

## 7.6.4 Born Series

$$\langle \vec{p}\,' \mathrm{out} | \vec{p}\ \mathrm{in} \rangle = \delta^{(3)}(\vec{p}\,' - \vec{p}) + \left( \langle \vec{p}\,' \mathrm{out}| - \langle \vec{p}\,' \mathrm{in}| \right) |\vec{p}\ \mathrm{in}\rangle$$

$$= \delta^{(3)}(\vec{p} - \vec{p}\,') - \langle \vec{p}\,' | V \Big[ (H - E_{\vec{p}\,'} \underset{\substack{\uparrow \\ \langle \vec{p}\,' \mathrm{out}|}}{-} i\varepsilon)^{-1} - (H - E_{\vec{p}\,'} \underset{\substack{\uparrow \\ \langle \vec{p}\,' \mathrm{in}|}}{+} i\varepsilon)^{-1} \Big] |\vec{p}\ \mathrm{in}\rangle$$

$$H |\vec{p}\ \mathrm{in}\rangle = E_{\vec{p}} |\vec{p}\ \mathrm{in}\rangle$$

$$\lim_{\varepsilon \to 0} \left[ (u - i\varepsilon)^{-1} - (u + i\varepsilon)^{-1} \right] = 2\pi i\, \delta(u)$$

$$\Rightarrow [\quad\quad] \rightarrow 2\pi i\, \delta(E_{\vec{p}} - E_{\vec{p}\,'})$$

Comparison with the definition of the T-matrix $\Rightarrow$

$$T(\vec{p}, \vec{p}\,') = \langle \vec{p}\,' | V | \vec{p}\ \text{in} \rangle$$

$$= \langle \vec{p}\,' | V \left[ |\vec{p}\rangle - \underset{\overset{\uparrow}{!}}{(H_0} - E_{\vec{p}} - i\varepsilon)^{-1} V \, |\vec{p}\ \text{in}\rangle \right]$$

see top page (103)

Series is obtained by recursively replacing

$$|\vec{p}\ \text{in}\rangle \rightarrow |\vec{p}\rangle - \dots$$

Leading order:

$$T(\vec{p}, \vec{p}\,') \cong \langle \vec{p}\,' | V | \vec{p}\rangle = \tilde{V}(\vec{p}\,' - \vec{p})$$

$$= (2\pi\hbar)^{-3} \int d^3x \; e^{-\frac{i}{\hbar}(\vec{p}\,' - \vec{p})\cdot\vec{x}} \; V(\vec{x})$$

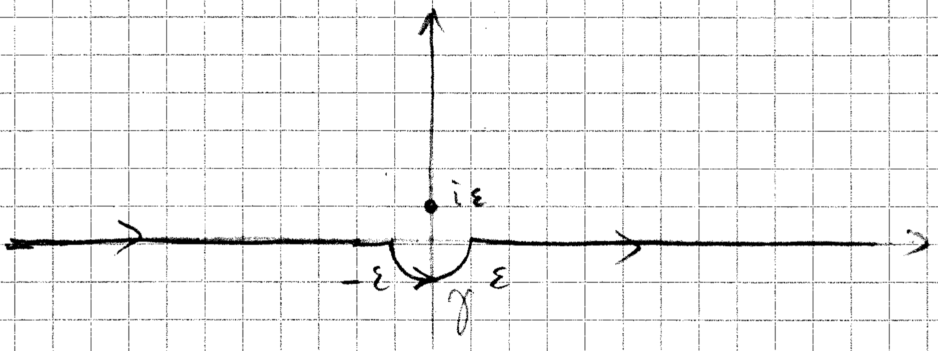
reproduce the result of section 7.5.3.

Proposition: $\lim\limits_{\varepsilon\to 0}\left[\frac{1}{u-i\varepsilon}-\frac{1}{u+i\varepsilon}\right] = 2\pi i\ \delta(u)$

Proof: we show:

$$\int_{-\infty}^{\infty} du\ f(u)\left[\frac{1}{u-i\varepsilon}-\frac{1}{u+i\varepsilon}\right] \xrightarrow{\varepsilon\to 0} 2\pi i\cdot f(0)$$

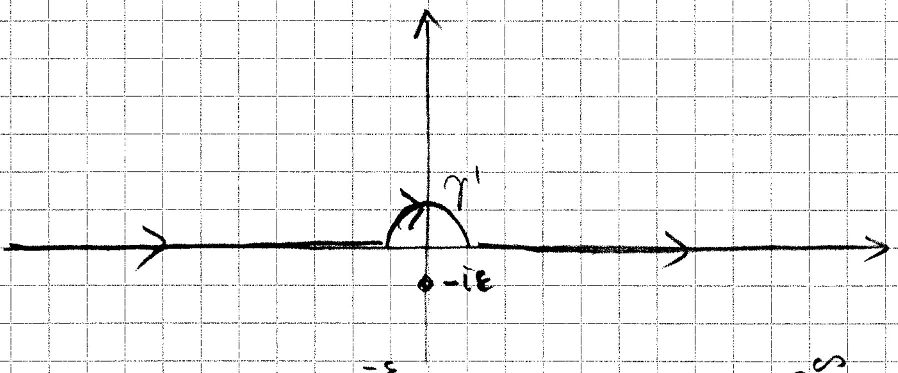
$\frac{1}{u-i\varepsilon}$:



$$\int_{-\infty}^{\infty} du\ f(u)\ \frac{1}{u-i\varepsilon} = \int_{-\infty}^{-\varepsilon} + \int_{\gamma} + \int_{\varepsilon}^{+\infty}$$

$$\int_{\gamma} du\ f(u)\ \frac{1}{u-i\varepsilon} \xrightarrow{\varepsilon\to 0} +\ i\cdot(\text{residuum } u=0)\,\pi = i\pi\ f(0)$$

$\frac{1}{u+i\varepsilon}$:



$$\int_{-\infty}^{\infty} du\ f(u)\ \frac{1}{u+i\varepsilon} = \int_{-\infty}^{-\varepsilon} + \int_{\gamma'} + \int_{\varepsilon}^{\infty}$$

$$\int_{\gamma'} du\ f(u)\ \frac{1}{u+i\varepsilon} \xrightarrow{\varepsilon\to 0} \underset{\substack{\uparrow\\ \text{orientation}}}{-}\ i\cdot(\text{residuum } u=0)\,\pi = -i\pi f(0)$$

$$\Rightarrow \int_{-\infty}^{\infty} du\ f(u)\left[\frac{1}{u-i\varepsilon}-\frac{1}{u+i\varepsilon}\right] = \int_{\gamma} - \int_{\gamma'} = 2\pi i\ f(0) \quad \boxed{E}$$

# 8. Relativistic Quantum Mechanics

## 8.1 Classical Relativistic Mechanics

Non-relativistic mechanics and quantum mechanics (Schrödinger-, Pauli-equation, ...) hold only when

$$|\vec{v}| = \frac{|\vec{p}|}{m} \ll c \approx 3 \times 10^8 \frac{m}{sec}$$

only then: $E = \frac{p^2}{2m}$

and $\hat{H} = \frac{\hat{\vec{p}}^2}{2m}$ ...

Otherwise:

$$p^\mu = \Big( \underset{\substack{\uparrow \\ \text{time-}}}{\frac{E}{c}}, \underset{\substack{\nwarrow \\ \text{space-components}}}{\vec{p}} \Big) \quad : \text{four-vector}, \; \mu = 0,1,2,3$$

$$p^2 = p^\mu p^\nu g_{\mu\nu} = \frac{E^2}{c^2} - \vec{p}^2 = m^2 c^2 \quad : \text{Lorentz-scalar (see below)}$$

$$g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \quad \text{diagonal matrix}$$

$$\vec{p} = \frac{m\vec{v}}{\sqrt{1-\beta^2}} \quad \Leftarrow \text{consistency with non-relativistic limit, see Jackson}$$

$$E = \sqrt{m^2 c^4 + c^2 \vec{p}^2} = \frac{mc^2}{\sqrt{1-\beta^2}} \quad , \quad \beta^2 = \frac{\vec{v}^2}{c^2} < 1$$

When $\beta \ll 1$:

$$E = mc^2 \left( 1 + \frac{1}{2}\beta^2 + \frac{3}{8}\beta^4 + O(\beta^6) \right) = \underset{\substack{\nearrow \\ \text{rest-energy}}}{mc^2} + \underset{\substack{\uparrow \\ \text{non-relat. term}}}{\frac{m}{2}\vec{v}^2} + \dots$$

$x^\mu = (ct, \vec{x})$ space-time vector

Lorentz-transformation: $x^\mu \to x'^\mu = \Lambda^\mu{}_\nu\, x^\nu$
leaves scalar product of 4-vectors invariant:

$$x'\cdot y' = x\cdot y \Leftrightarrow g_{\mu\nu}\,\Lambda^\mu{}_\kappa\,\Lambda^\nu{}_\lambda = g_{\kappa\lambda} = \begin{pmatrix}1 & & & 0\\ & -1 & & \\ & & -1 & \\ 0 & & & -1\end{pmatrix}$$

$(x\cdot y \equiv g_{\mu\nu}\,x^\mu y^\nu)$

"generalized rotations", pseudoorthogonal
= Lorentz-group, contains:

* rotations:

$$x'^0 = x^0$$

$x'^i = R^i{}_k\, x^k$, $i,k = 1,2,3$, $R^i{}_k$: rotation matrix as before

* boosts, for example:

$$p'^1 = p^1$$
$$p'^2 = p^2$$
$$\begin{pmatrix}p'^0\\ p'^3\end{pmatrix} = \begin{pmatrix}\cosh\alpha & \sinh\alpha\\ \sinh\alpha & \cosh\alpha\end{pmatrix}\begin{pmatrix}p^0\\ p^3\end{pmatrix};\quad \alpha\in\mathbb{R}$$

$p'^2 \equiv p'\cdot p' = p^2$ $\quad[\cosh^2\alpha - \sinh^2\alpha = 1]$

$$p = mc\begin{pmatrix}1\\0\\0\\0\end{pmatrix} \xrightarrow{\text{boost}} p' = mc\begin{pmatrix}\cosh\alpha\\0\\0\\\sinh\alpha\end{pmatrix}$$

↑ particle at rest ↓ particle (or observer) moving

Equation of motion: (holds independently of the reference frame)

$$\frac{dx^\mu}{d\tau} = \frac{1}{m}p^\mu \Rightarrow \begin{array}{l} dx^0 = c\,dt = \frac{p^0}{m}\,d\tau \\ d\vec{x} = \frac{\vec{p}}{m}\,d\tau \end{array} \Rightarrow \frac{d\vec{x}}{dt} = c\,\frac{\vec{p}}{p^0}$$

In moving frame: $\frac{d\vec{x}\,'}{dt'} = c\,\frac{\vec{p}\,'}{p'^0} = \underbrace{c\tanh\alpha}_{=v<c}\,\vec{e}_3$

$\left[d\tau = \frac{mc}{p^0}\,dt = \sqrt{1-\beta^2}\,dt\right.$ : proper time, Lorentz invariant $\left.\right]$

General infinitesimal Lorentz-transformation:

$$\Lambda^\mu{}_\kappa = \delta^\mu{}_\kappa + \omega^\mu{}_\kappa \qquad (\omega^2 \cong 0)$$

$$g_{\mu\nu}\Lambda^\mu{}_\kappa \Lambda^\nu{}_\lambda = g_{\kappa\lambda} \Rightarrow g_{\mu\nu}\left(\omega^\mu{}_\kappa \delta^\nu{}_\lambda + \delta^\mu{}_\kappa \omega^\nu{}_\lambda\right) \overset{!}{=} 0$$

$$\omega_{\nu\kappa}\delta^\nu{}_\lambda + \delta^\mu{}_\kappa \omega_{\mu\lambda} = \omega_{\lambda\kappa} + \omega_{\kappa\lambda} \overset{!}{=} 0$$

$\Rightarrow$ $\omega_{\mu\nu} = g_{\mu\lambda}\omega^\lambda{}_\nu$ must be anti-symmetric!

$\rightarrow$ $\omega_{\mu\nu}$ has $\frac{1}{2}\cdot 4\cdot 3 = 6$ free parameters

* rotations:

$$\left(\omega^\bullet{}_\bullet\right) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & & & \\ 0 & & \varphi\vec{n}\cdot\vec{T} & \\ 0 & & & \end{pmatrix}$$

$T^i$: generators of infinitesimal rotations in $\mathbb{R}^3$:

$$\left(\varphi\,\vec{n}\cdot\vec{T}\,\vec{x}\right)_k = \varphi\left(\vec{n}\times\vec{x}\right)_k \quad , \quad \left(T^i\right)_{kl} = \varepsilon_{kil}$$

$$\omega_{nl} = g_{nk}\,\omega^k{}_l = -\left(\varphi\,\vec{n}\cdot\vec{T}\right)_{nl} \quad \text{anti-symmetric}$$

* boosts: $\sinh\alpha \approx \alpha$, $\cosh\alpha \approx 1$

$$\left(\omega^\bullet{}_\bullet\right) = \begin{pmatrix} 0 & \alpha \\ \alpha & 0 \end{pmatrix} \qquad (\text{only } \nu = 0,3 \text{ shown})$$

$$\left(\omega_{\bullet\bullet}\right) = \begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} \qquad \text{anti-symmetric}$$

Gradient:

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu \quad \Rightarrow \quad \frac{\partial x'^\mu}{\partial x^\nu} = \Lambda^\mu{}_\nu$$

$$\partial_\mu = \left(\frac{\partial}{\partial(ct)}, \vec{\nabla}\right) = \frac{\partial}{\partial x^\mu}$$

$$\Rightarrow \quad \partial_\mu = \frac{\partial x'^\nu}{\partial x^\mu}\frac{\partial}{\partial x'^\nu} \qquad (\text{chain rule})$$

$\partial_\mu = \Lambda^\nu{}_\mu \, \partial'_\nu$ → covariant transformation rule

$x^\mu$ has a contravariant transformation rule $x'^\mu = \Lambda^\mu{}_\nu x^\nu$

$$\partial'_\mu = \frac{\partial x^\nu}{\partial x'^\mu} \partial_\nu = \underbrace{\Lambda_\mu{}^\nu}_{\text{new, introduced here}} \partial_\nu$$

$(\Lambda^{\cdot}{}_{\cdot})^T$, $(\Lambda_{\cdot}{}^{\cdot})$ are inverse to each other

$$\Lambda^\kappa{}_\mu \, \Lambda_\kappa{}^\nu = \delta_\mu{}^\nu \, .$$

Since $\Lambda$ is pseudoorthogonal the inversion is easy, ≈ transpose

Definition: $g_{\mu\kappa} g^{\kappa\nu} = \delta_\mu{}^\nu \Rightarrow g^{\cdot\cdot} = \begin{pmatrix} +1 & & & 0 \\ & -1 & & \\ & & -1 & \\ 0 & & & -1 \end{pmatrix}$

Definition of Lorentz-transf.: $g_{\kappa\lambda} \Lambda^\kappa{}_\mu \Lambda^\lambda{}_\sigma = g_{\mu\sigma}$

$$\Leftrightarrow \quad g_{\kappa\lambda} \Lambda^\kappa{}_\mu \Lambda^\lambda{}_\sigma g^{\sigma\nu} = \delta_\mu{}^\nu$$

$$\Rightarrow \Lambda_\kappa{}^\nu = g_{\kappa\lambda} \Lambda^\lambda{}_\sigma g^{\sigma\nu}$$

## 8.2 Preliminary Considerations

### 8.2.1 Invariance of Wave Equations

Schrödinger- and Pauli-equations are not Lorentz-invariant:

$$i\hbar \underset{\substack{\uparrow \\ \text{1st order}}}{\frac{\partial \psi}{\partial t}} = -\frac{\hbar^2}{2m} \underset{\substack{\uparrow \\ \text{2nd order}}}{\vec{\nabla}^2} \psi$$

, asymmetric space & time

$\psi(\vec{x}, t) = \psi(x^\mu)$ solution → $\psi(x')$, $x'^\mu = \Lambda^\mu{}_\nu x^\nu$ is in general not a solution

It was different for Maxwell equations:

Maxwell equations => discovery of Lorentz-invariance

=> look for a new wave equation

- $\frac{\partial}{\partial t}$, $\vec{\nabla}$ both first *or* both second order
  in particular for second order: interpretation? need $\psi$ and $\frac{\partial \psi}{\partial t}$ as initial conditions
- Lorentz-invariant!
- yieds Schrödinger- or Pauli-equation in non-relativistic limit

## 8.2.2 Difficulty with One-partice Quantum Mechanics

So far the particle number was conserved:

$\rho(\vec{x}) = \psi^*(\vec{x})\psi(\vec{x})$ ~ probability to find the particle at $\vec{x}$

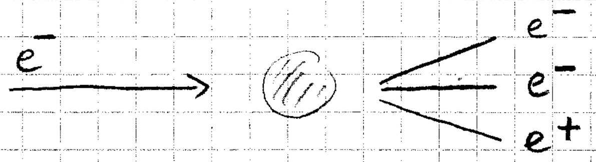
$\int d^3x \, \rho(\vec{x})$ = fixed (for example $= 1$)

$\frac{d}{dt} \int d^3x \, \rho(\vec{x}) = 0 \Leftarrow$ Schrödinger equation

$\psi(t, \vec{x}_1, \vec{x}_2)$ : two particles (for example 2 eletrons in He atom)

relativistic: $E = mc^2$ for a particle at rest

=> creation, annihilation possible when $E_{kin} > mc^2$



Problem of principles with $\psi(t, \vec{x}) \xrightarrow{?} \psi(t, \vec{x}_1, \vec{x}_2, \vec{x}_3)$

Solution: Quantum Field Theory:

$$\mathcal{H} = \mathcal{H}_{\text{vacuum}} \oplus \mathcal{H}_{\text{one-particle}} \oplus \underset{\substack{\downarrow \\ \mathcal{H}_{\text{one-particle}} \otimes \mathcal{H}_{\text{one-particle}}}}{\mathcal{H}_{\text{two-particles}}} \oplus \dots$$

Fock-space, transitions between different "sectors" are possible

but: small relativistic corrections, *before* particle production plays a role can be described by a modified wave equation:

$E < n \cdot mc^2$

like for example $E = mc^2 + \frac{p^2}{2m} - \underset{\substack{\uparrow \\ \text{relat. correction}}}{\frac{p^4}{8m^3c^2}} + \dots$

but in general get inconsistency when trying to formulate (fully) relativistic one-particle theory

## 8.3 Klein Gordon Equation

$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla}\right)$ covariant 4-vector operator

Scalar: $g^{\mu\nu}\partial_\mu\partial_\nu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta = \partial^2 = \Box$

d'Alembert ↔ wave equation of electrodynamics

We try to preserve the correspondences

$i\hbar\frac{\partial}{\partial t}$ ↔ energy

$\frac{\hbar}{i}\vec{\nabla}$ ↔ momentum

$\Rightarrow \quad -\hbar^2c^2\partial^2 \leftrightarrow E^2 - c^2\vec{p}^{\,2} = m^2c^4$

Trial:

$$\left(-\hbar^2\frac{\partial^2}{\partial t^2} + \hbar^2c^2\Delta\right)\psi = (mc^2)^2\psi \qquad (\Delta \equiv \vec{\nabla}^2)$$

$\Leftrightarrow \quad -\partial^2\psi = \left(\frac{mc}{\hbar}\right)^2\psi$ Klein Gordon equation (K.G.)

Solution: plain wave:

$$\psi = e^{-\frac{i}{\hbar}(Et - \vec{p}\cdot\vec{x})} = e^{-\frac{i}{\hbar}p^\mu x_\mu}$$

$$\left.\begin{aligned} &\text{Schrödinger equation} \Rightarrow E = \frac{\vec{p}^{\,2}}{2m} \\ &\text{Klein Gordon equation} \Rightarrow E^2 = \vec{p}^{\,2}c^2 + m^2c^4 \end{aligned}\right\} \text{for free particles}$$

$E = \pm \sqrt{\vec{p}^2 c^2 + m^2 c^4}$ : negative energy ?

Interpretation :

current , probability density :

$$\partial^\mu \left( \psi^* \overleftrightarrow{\partial}_\mu \psi \right) = \psi^* \partial^2 \psi - (\partial^2 \psi)^* \psi \overset{K.G.}{=} 0$$

[ definitions : $\partial^\mu = g^{\mu\nu} \partial_\nu = \left( \frac{1}{c} \frac{\partial}{\partial t} , -\vec{\nabla} \right)$

$f \overleftrightarrow{\partial}_\mu g = f (\partial_\mu g) - (\partial_\mu f) g$ ]

$$(c\rho , \vec{j}) = j^\mu := \frac{i\hbar}{2m} \psi^* \overleftrightarrow{\partial}^\mu \psi$$

$$\Rightarrow 0 = \partial_\mu j^\mu = \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j}$$

$\vec{j} = \frac{\hbar}{2mi} \psi^* \overleftrightarrow{\nabla} \psi$ like Schrödinger

$\rho = \frac{i\hbar}{2mc^2} \psi^* \frac{\overleftrightarrow{\partial}}{\partial t} \psi \neq \psi^* \psi$ , in general not $\geq 0$ !

However when $\psi = e^{-\frac{i}{\hbar} E t} \varphi(\vec{x})$

$$\Rightarrow \rho = \frac{E}{mc^2} \varphi^* \varphi$$

positive (negative) for positive (negative) energy !

- reinterpretation as charge density $\rho \rightarrow q \cdot \rho$,
  $E < 0 \rightarrow$ antiparticle , charge $= -q$
- small relativistic corrections : waves with only
  $E > 0$ components
- coupling to electromagnetic field

$$\left. \begin{aligned} \frac{\partial}{\partial t} &\rightarrow \frac{\partial}{\partial t} + \frac{iq}{\hbar} \phi \\ \vec{\nabla} &\rightarrow \vec{\nabla} - \frac{iq}{\hbar} \vec{A} \end{aligned} \right\} \text{minimal substitution}$$

$$\partial^\mu \longrightarrow \partial^\mu + \frac{iq}{\hbar} A^\mu \quad ; \quad A^\mu = \left( \frac{\phi}{c}, \vec{A} \right)$$

because of gauge invariance. $q =$ charge.

$$-\partial^2 \psi = \left(\frac{mc}{\hbar}\right)^2 \psi \longrightarrow -\left(\partial^\mu + \frac{iq}{\hbar} A^\mu\right)\left(\partial_\mu + \frac{iq}{\hbar} A_\mu\right)\psi = \left(\frac{mc}{\hbar}\right)^2 \psi$$

K.G. equation in electromagnetic potential

If $\psi$ is solution for charge $q$
$\rightarrow \psi^*$ is solution for charge $-q$

- eigenstates in Coulomb potential can be computed exactly
- $E_{n,l}$ : $l$-degeneracy of hydrogen atom is lifted but does not reproduce measurements
- better: relativistic Dirac equation
- Klein Gordon: spin 0 - mesons, for example $\pi^+, \pi^-$
- negative energy → Quantum Field Theory, antiparticles

# 8.4 Dirac Equation

## 8.4.1 Pauli Equation Revisited

Idea: first order differential equation

$$i\hbar \frac{\partial \psi}{\partial t} \rightarrow i\hbar \partial_\mu \psi$$

→ with what can index $\mu$ of $\partial_\mu$ be contracted, compare $\partial_\mu \partial^\mu$, to obtain a covariant equation?

→ Spin, Pauli:

$$\psi(\vec{x}) = \begin{pmatrix} \psi_+(\vec{x}) \\ \psi_-(\vec{x}) \end{pmatrix} \quad , \quad \text{spin } \frac{1}{2}$$

(active) rotation

$$\psi(\vec{x}) \longrightarrow \psi'(\vec{x}) = e^{-\frac{i}{\hbar}\alpha\vec{n}\cdot\vec{S}}\,\psi(R^{-1}\vec{x})$$

$\alpha$: angle, $\vec{n}$: axis, $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

$$\vec{\sigma} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{Pauli matrices}$$

infinitesimal: $\delta\psi = -\frac{i}{\hbar}\,\delta\,\vec{n}\cdot\vec{J}\,\psi$

$\vec{J} = \vec{L} + \vec{S}$ , $\vec{L} = \hat{\vec{x}} \times \hat{\vec{p}}$

$\vec{L}, \vec{S}$ vector operators

Pauli equation: $i\hbar\frac{\partial}{\partial t}\psi = \left(\frac{1}{2m}\left[\vec{\sigma}\cdot\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)\right]^2 + q\phi\right)$

The operator $\vec{\sigma}\cdot\vec{\nabla}$ appears. It is a scalar:

$$[J_k, \vec{\sigma}\cdot\vec{\nabla}] = 0 \quad \text{, therefore}$$

$$\vec{\sigma}\cdot\vec{\nabla}\, e^{\frac{i}{\hbar}\alpha\vec{n}\cdot\vec{J}}\psi = e^{\frac{i}{\hbar}\alpha\vec{n}\cdot\vec{J}}\,\vec{\sigma}\cdot\vec{\nabla}\psi$$

Proof: $[J_k, \sigma_i\nabla_i] = [L_k + S_k, \sigma_i\nabla_i]$

$$= \sigma_i[L_k, \nabla_i] + [S_k, \sigma_i]\nabla_i$$

$$[L_k, \nabla_i] = \frac{\hbar}{i}\varepsilon_{klm}[\hat{x}_l\nabla_m, \nabla_i] = \frac{\hbar}{i}\varepsilon_{klm}[\hat{x}_l, \nabla_i]\nabla_m$$

$$= \frac{\hbar}{i}\varepsilon_{klm}(-\delta_{li})\nabla_m = i\hbar\,\varepsilon_{kim}\nabla_m$$

$$[S_k, \sigma_i] = \frac{\hbar}{2}[\sigma_k, \sigma_i] = i\hbar\,\varepsilon_{kim}\sigma_m$$

$$\Rightarrow [J_k, \vec{\sigma}\cdot\vec{\nabla}] = i\hbar\,\underset{\substack{\uparrow \\ \text{anti-symmetric}}}{\varepsilon_{kim}}\big(\underbrace{\sigma_i\nabla_m + \sigma_m\nabla_i}_{\substack{\uparrow \\ \text{symmetric}}}\big) = 0 \qquad i \leftrightarrow m \qquad \square$$

$\vec{\sigma}, \vec{\nabla}$ are both vector operators → scalar product.

## 8.4.2 Lorentz-invariant Differential Equation of first order

We want to generalize :

rotation group → Lorentz-group
3d → 4d

$\psi$ : several components

| | | |
|---|---|---|
| $\vec{\sigma}$ | $\longrightarrow$ | $\gamma^\mu$ matrices such that |
| $\vec{\sigma}\cdot\vec{\nabla}$ | $\longrightarrow$ | $\gamma^\mu \partial_\mu$ |
| scalar operator under rotations | | scalar operator under Lorentz-transformations : that is, $\gamma^\mu$ is a 4-vector-operator |

$$x^\mu \longrightarrow x'^\mu = \Lambda^\mu{}_\nu x^\nu \underset{\substack{\uparrow \\ \text{infinitesimal}}}{\cong} x^\mu + \omega^\mu{}_\nu x^\nu \; ; \; \omega^2 \cong 0 \; ; \; \omega_{\mu\nu} = -\omega_{\nu\mu}$$

Finite Lorentz-transformation:

$$\lim_{n\to\infty}\left(1+\frac{\omega}{n}\right)^n = e^\omega$$

$$\psi'(x) = e^{-\frac{i}{\hbar}\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}\,\psi(\Lambda^{-1}x)$$

$$\psi'(x) \cong \left(1-\frac{i}{2\hbar}\omega_{\mu\nu}J^{\mu\nu}\right)\psi(x) \quad \text{infinitesimal}$$

$$J^{\mu\nu} = S^{\mu\nu} + L^{\mu\nu}$$

$$L^{\mu\nu} = +i\hbar\left(x^\mu\partial^\nu - x^\nu\partial^\mu\right)$$

$$\left(1-\frac{i}{2\hbar}\omega_{\mu\nu}L^{\mu\nu}\right)\psi(x) = \left(1+\omega_{\mu\nu}x^\mu\partial^\nu\right)\psi(x)$$

$$= \left(1-\omega^\mu{}_\nu x^\nu\partial_\mu\right)\psi(x) \cong \psi\left(x^\mu-\omega^\mu{}_\nu x^\nu\right) = \psi(\Lambda^{-1}x)$$

$$\Rightarrow \psi'(x) \cong \psi(\Lambda^{-1}x) - \frac{i}{2\hbar}\omega_{\mu\nu}S^{\mu\nu}\psi(x) \cong \left(1-\frac{i}{2\hbar}\omega_{\mu\nu}S^{\mu\nu}\right)\psi(\Lambda^{-1}x)$$

infinitesimal

$\gamma^\mu \partial_\mu$ is a Lorentz-scalar when

$$[\mathcal{J}^{\kappa\lambda}, \gamma^\mu \partial_\mu] = 0$$

in addition it must be: $\gamma^\mu$ is a 4-vector, in particular it transforms in the exact same way as $\partial^\mu$

$$\frac{i}{\hbar}\left[\frac{1}{2}\omega_{\kappa\lambda}\mathcal{J}^{\kappa\lambda}, \partial^\mu\right] = -\left[\omega_{\kappa\lambda} x^\kappa \partial^\lambda, \partial^\mu\right]$$

$$= -\omega_{\kappa\lambda}\underbrace{[x^\kappa, \partial^\mu]}\partial^\lambda = \omega^\mu{}_\lambda \partial^\lambda$$

$$= g^{\mu\nu}\left[x^\kappa, \frac{\partial}{\partial x^\nu}\right] = -g^{\mu\kappa}$$

$$\frac{i}{\hbar}\left[\frac{1}{2}\omega_{\kappa\lambda} S^{\kappa\lambda}, \gamma^\mu\right] \overset{!}{=} \omega^\mu{}_\lambda \gamma^\lambda$$

Solution: Pauli: $\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$

$\rightarrow \{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$

Proposition: $S^{\kappa\lambda} = \frac{i\hbar}{4}[\gamma^\kappa, \gamma^\lambda]$ is solution

Proof: $\frac{i}{\hbar}\left[\frac{1}{2}\omega_{\kappa\lambda} S^{\kappa\lambda}, \gamma^\mu\right] = -\frac{1}{4}\left[\omega_{\kappa\lambda}\gamma^\kappa\gamma^\lambda, \gamma^\mu\right]$

$$= -\frac{1}{4}\omega_{\kappa\lambda}\left(\gamma^\kappa\{\gamma^\lambda, \gamma^\mu\} - \{\gamma^\mu, \gamma^\kappa\}\gamma^\lambda\right)$$

$\uparrow$

$[AB, C] = A\{B, C\} - \{C, A\}B$

$$= -\frac{1}{4}\omega_{\kappa\lambda}\left(\gamma^\kappa 2g^{\lambda\mu} - 2g^{\mu\kappa}\gamma^\lambda\right)$$

$$= -\frac{1}{2}\left(\omega_\kappa{}^\mu \gamma^\kappa - \omega^\mu{}_\lambda \gamma^\lambda\right)$$

$$= \omega^\mu{}_\lambda \gamma^\lambda$$

$\ulcorner\ \omega_\kappa{}^\mu = g^{\mu\lambda}\omega_{\kappa\lambda} = -g^{\mu\lambda}\omega_{\lambda\kappa} = -\omega^\mu{}_\kappa\ \lrcorner$ ∎

Under the assumption that the matrices $\gamma^\mu$ exist, the equation

$$i\hbar\,\gamma^\mu \partial_\mu \psi(x) = mc\,\psi(x) \qquad \text{(Dirac equation)}$$

is a Lorentz-covariant equation, that is

$\psi(x)$ solution $\Rightarrow$ $\psi'(x)$ solution,

$$\psi'(x) = e^{\frac{1}{8}\omega_{\mu\nu}[\gamma^\mu,\gamma^\nu]}\,\psi(\Lambda^{-1}x)$$

$\uparrow$ generalized spin

$$\Rightarrow \left(i\hbar\gamma^\mu\partial_\mu + mc\right)\left(i\hbar\gamma^\mu\partial_\mu - mc\right)\psi = 0$$

$$\left[\hbar^2\left(\gamma^\mu\partial_\mu\right)^2 + m^2c^2\right]\psi = 0$$

$$\hookrightarrow \gamma^\mu\gamma^\nu\partial_\mu\partial_\nu = \frac{1}{2}\{\gamma^\mu,\gamma^\nu\}\partial_\mu\partial_\nu = \partial^2$$

$$\left(\hbar^2\partial^2 + m^2c^2\right)\psi = 0 \Leftrightarrow$$ Klein Gordon equation for each component

$$\psi = u\,e^{-\frac{i}{\hbar}p\cdot x} \quad : \quad -E^2 + c^2\vec{p}^{\,2} + m^2c^4 = 0$$

## 8.4.3 The Dirac Matrices $\gamma^\mu$

$$\left.\begin{aligned} \{\gamma^\mu,\gamma^\nu\} &= 2g^{\mu\nu} \\ \{\sigma^i,\sigma^j\} &= 2\delta_{ij} \end{aligned}\right\} \text{ pairwise anticommuting}$$

$$\sigma = \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)$$

There are no four anticommuting 2x2 matrices

- smallest representation is 4-dimensional:

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ \underbrace{0}_{2} & \underbrace{-1}_{2} \end{pmatrix} \begin{matrix} \}2 \\ \}2 \end{matrix} \qquad \gamma^k = \begin{pmatrix} 0 & \sigma_k \\ \underbrace{-\sigma_k}_{2} & \underbrace{0}_{2} \end{pmatrix} \begin{matrix} \}2 \\ \}2 \end{matrix}$$

- other 4x4 representations are unitary equivalent

$$\{\tilde{\gamma}^\mu, \tilde{\gamma}^\nu\} = 2g^{\mu\nu} \Rightarrow \tilde{\gamma}^\mu = U\gamma^\mu U^+ \; , \quad UU^+ = 1 = U^+U$$

- $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$

Rotation: $x'^0 = x^0$

$$x'^i = x^i + \omega^i{}_j x^j = x^i + \varphi\, (\vec{n}\times\vec{x})^i$$

$$\Rightarrow \omega_{ik} = -\omega^i{}_k = \varphi\, n^j \varepsilon_{jik} \; , \quad \omega_{0i} = \omega_{i0} = 0$$

$$\psi'(x^0, \vec{x}) = e^{\frac{1}{8}\omega_{ij}[\gamma^i,\gamma^j]}\, \psi(x^0, R^{-1}\vec{x})$$

$$\frac{1}{8}\omega_{ij}[\gamma^i,\gamma^j] = \frac{\varphi}{4} n^k \varepsilon_{kij}\gamma^i\gamma^j$$

$$\frac{1}{2}\varepsilon_{kij}\gamma^i\gamma^j =: -i\Sigma_k$$

for example $\frac{1}{2}\varepsilon_{1ij}\gamma^i\gamma^j = \gamma^2\gamma^3 = \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_3 \\ -\sigma_3 & 0 \end{pmatrix} = \begin{pmatrix} -i\sigma_1 & 0 \\ 0 & -i\sigma_1 \end{pmatrix}$

$\Rightarrow \Sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}$ → Pauli doubled

$$\psi' = e^{-i\frac{\varphi}{2}n^k\Sigma_k}\,\psi$$

$\Rightarrow \psi_{Dirac} = \begin{pmatrix} \psi_{Pauli,\,a} \\ \psi_{Pauli,\,b} \end{pmatrix}$ as far as the transformation under rotation is concerned, doubled Pauli-spinor

### 8.4.4 Hamiltonian Form of the Dirac Equation, free solution

$$c\gamma^0 / \quad i\hbar\left(\gamma^0\frac{\partial}{\partial x^0} + \gamma^k\nabla_k\right)\psi = mc\,\psi$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t}\psi = c\frac{\hbar}{i}\vec{\alpha}\cdot\vec{\nabla}\psi + mc^2\beta\psi$$

with $\alpha^k = \gamma^0\gamma^k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}$ , $\beta = \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ .

Hamilton operator: $H = c\frac{\hbar}{i}\vec{\alpha}\cdot\vec{\nabla} + mc^2\beta$

A) Solutions for particles at rest $(\vec{p} = 0)$

$\psi = u\, e^{-\frac{i}{\hbar}E\cdot t} \quad \Rightarrow \quad (E - mc^2\beta)\psi = 0$

$$\begin{pmatrix} E-mc^2 & & & \\ & E-mc^2 & & \\ & & E+mc^2 & \\ & & & E+mc^2 \end{pmatrix} u = 0$$

$$\Rightarrow \quad u^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} , \quad u^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{with } E = mc^2$$

$$u^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} , \quad u^{(4)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \text{with } E = -mc^2$$

Since $[\beta, \Sigma_3] = 0$ (diagonal matrices) , $\Sigma_3$ (spin) can be simultaneously diagonalized.

$$\frac{\hbar}{2}\Sigma_3\, u^{(k)} = \left\{ \begin{matrix} +\hbar/2 \\ -\hbar/2 \end{matrix} \right\} u^{(k)} \quad \text{for} \quad \left\{ \begin{matrix} k = 1,3 \\ k = 2,4 \end{matrix} \right.$$

| | k=1 | 2 | 3 | 4 |
|---|---|---|---|---|
| energy | + | + | − | − |
| spin | + | − | + | − |

$E = -mc^2 \longrightarrow$ positron at rest in Quantum Field Theory

B) now: momentum $\vec{p} = (0,0,p)$ imparted by boost

$$\underbrace{\begin{pmatrix} \hat{c} & \hat{s} \\ \hat{s} & \hat{c} \end{pmatrix}}_{= \Lambda^{\mu}{}_{\nu}\,,\ \mu,\nu \in \{0,3\}} \begin{pmatrix} \pm mc \\ 0 \end{pmatrix} = \pm\, mc \begin{pmatrix} \hat{c} \\ \hat{s} \end{pmatrix} \overset{!}{=} \begin{pmatrix} E'/c \\ p \end{pmatrix}$$

$\hat{c} = \cosh\varphi$ , $\hat{s} = \sinh\varphi$ ; with $E_p = +\sqrt{m^2c^4 + p^2c^2}$ :

$k = 1,2$ : $E' = +E_p$ , $\tanh\varphi = \frac{pc}{E_p}$

$k = 3,4$ : $E' = -E_p$ , $\tanh\varphi = -\frac{pc}{E_p}$

$$\psi^{(k)} = u^{(k)}(p)\, e^{-\frac{i}{\hbar}(E' t - p x^3)}$$

$$u^{(k)}(p) = e^{\frac{1}{8}\omega_{\mu\nu}[\gamma^{\mu},\gamma^{\nu}]}\ u^{(k)}(0)$$

Boost with "angle" $\varphi$ in 3-direction = sequence of infinitesimal boosts with "angle" $\delta$ and spin transformation

$$u \longrightarrow \left(1 + \frac{\omega_{\mu\nu}}{8}[\gamma^{\mu},\gamma^{\nu}]\right) u = \left(1 + \frac{\omega_{03}}{2}\gamma^0\gamma^3\right) u$$

$$\approx e^{\frac{\delta}{2}\gamma^0\gamma^3}\, u \qquad (\omega_{03} = +\delta)$$

finite boost: $u \longrightarrow e^{\frac{\varphi}{2}\gamma^0\gamma^3}\, u = e^{\frac{\varphi}{2}\alpha^3}\, u$

$$e^{\frac{\varphi}{2}\alpha^3} = \begin{pmatrix} \hat{c}_{1/2} & 0 & \hat{s}_{1/2} & 0 \\ 0 & \hat{c}_{1/2} & 0 & -\hat{s}_{1/2} \\ \hat{s}_{1/2} & 0 & \hat{c}_{1/2} & 0 \\ 0 & -\hat{s}_{1/2} & 0 & \hat{c}_{1/2} \end{pmatrix} , \quad \hat{c}_{1/2} = \cosh\frac{\varphi}{2} , \quad \hat{s}_{1/2} = \sinh\frac{\varphi}{2} .$$

$\Rightarrow$ the boosted spinors of the 4 free solutions are:

$$u^{(1)}(p) = A \begin{pmatrix} 1 \\ 0 \\ r \\ 0 \end{pmatrix} \quad , \quad u^{(2)}(p) = A \begin{pmatrix} 0 \\ 1 \\ 0 \\ -r \end{pmatrix} \quad , \quad A = \text{normalization}$$

$$k = 1,2 : \quad \tanh\varphi = \frac{pc}{E_p} \Rightarrow \tanh\frac{\varphi}{2} = \frac{\sinh\varphi}{\cosh\varphi + 1} = \frac{pc}{E_p + mc^2} =: r$$

$$k = 3,4 : \quad \tanh\varphi = \frac{-pc}{E_p} \Rightarrow \tanh\frac{\varphi}{2} = -r \Rightarrow$$

$$u^{(3)}(p) = A \begin{pmatrix} -r \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad u^{(4)}(p) = A \begin{pmatrix} 0 \\ r \\ 0 \\ 1 \end{pmatrix}$$

$$u^{(k)}(p)^{+} u^{(\ell)}(p) = |A|^2 (1 + r^2)\, \delta_{k\ell}$$

normalize $\Rightarrow A = (1+r^2)^{-1/2} = \left( \frac{2E_p}{E_p + mc^2} \right)^{-1/2}$

# 8.5 Non-relativistic Limit of the Dirac Equation

## 8.5.1 Leading Order

Free solution for $E > 0$ $(k = 1,2)$:

$$\left|u^{(k)}_{3,4}\right| = r \left|u^{(k)}_{1,2}\right| \quad , \quad r = \frac{pc}{E_p + mc^2} \underset{\text{relat.}}{\overset{\text{non-}}{\sim}} \frac{mvc}{2mc^2} = O\left(\frac{v}{c}\right)$$

large "upper", small "lower" components

More in general: stationary solution in the electromagnetic potential

$$E \psi = \left[ -e\phi + c\vec{\alpha}\left(\frac{\hbar}{i}\vec{\nabla} + e\vec{A}\right) + mc^2 \beta \right] \psi$$

with $A^\mu = \left(\frac{\phi}{c}, \vec{A}\right)$ , $q = -e$ (electron).

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \quad ; \quad \varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \quad ; \quad \chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad ; \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

$$\Rightarrow \quad E\varphi = \left(-e\phi + mc^2\right)\varphi + c\vec{\sigma}\left(\frac{\hbar}{i}\vec{\nabla} + e\vec{A}\right)\chi$$

$$E\chi = \left(-e\phi - mc^2\right)\chi + c\vec{\sigma}\underbrace{\left(\frac{\hbar}{i}\vec{\nabla} + e\vec{A}\right)}_{=:\vec{\pi} = \vec{p} + e\vec{A}}\varphi$$

Non-relativistic, $E > 0$ : $E = mc^2 + E'$

$$0 \leq E' \ll mc^2$$

$$|e\phi| \ll mc^2$$

2nd equation $\Rightarrow$ $\chi = \frac{1}{2mc^2 + E' + e\phi} c\vec{\sigma}\cdot\vec{\pi}\varphi \approx \frac{c\vec{\sigma}\cdot\vec{\pi}}{2mc^2}\varphi$

$$|\chi| \ll |\varphi|$$

1st equation $\Rightarrow$ $$E'\varphi \approx -e\phi\varphi + c\vec{\sigma}\cdot\vec{\pi}\,\underbrace{\frac{\vec{\sigma}\cdot\vec{\pi}}{2mc}\varphi}_{\approx\chi}$$

$$= \left(-e\phi + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m}\right)\varphi$$

$\Leftrightarrow$ Pauli equation

$$(\vec{\sigma}\cdot\vec{\pi})^2 = \sigma_k\sigma_\ell\,\pi_k\pi_\ell = \vec{\pi}^2 + i\,\sigma_m\,\varepsilon_{k\ell m}\,\pi_k\pi_\ell = \vec{\pi}^2 + i\,\vec{\sigma}\cdot(\vec{\pi}\times\vec{\pi})$$

$$\vec{\pi}\times\vec{\pi} = \left(\frac{\hbar}{i}\vec{\nabla}+e\vec{A}\right)\times\left(\frac{\hbar}{i}\vec{\nabla}+e\vec{A}\right) = \frac{e\hbar}{i}\,\vec{\nabla}\times\vec{A} = \frac{e\hbar}{i}\,\vec{B}$$

$$\Rightarrow\; E'\varphi = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}+e\vec{A}\right)^2\varphi - e\phi\varphi + \underbrace{\frac{e\hbar}{2m}}_{=\mu_B}\,\vec{B}\cdot\vec{\sigma}\,\varphi$$

$$E'\varphi = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}+e\vec{A}\right)^2\varphi - e\phi\varphi + 2\,\frac{\mu_B}{\hbar}\,\vec{B}\cdot\vec{S}\,\varphi$$

$\Rightarrow$ magnetic moment associated with spin with Landé factor $g = 2$ (so far empirically determined, orbital angular momentum $\leftrightarrow$ $g = 1$) from the Dirac equation!

### 8.5.2 Expansion in $\frac{v}{c}$

Special case: $\vec{A} = 0$, $-e\phi = V(|\vec{x}|)$

again: $E = +mc^2 + E'$

$$(E' - V)\,\varphi = c\,\vec{\sigma}\cdot\hat{\vec{p}}\,\chi$$

$$(E' - V + 2mc^2)\,\chi = c\,\vec{\sigma}\cdot\hat{\vec{p}}\,\varphi$$

$$\Rightarrow \left[E' - V - c^2\,\vec{\sigma}\cdot\hat{\vec{p}}\,\left(E' - V + 2mc^2\right)^{-1}\vec{\sigma}\cdot\hat{\vec{p}}\right]\varphi = 0$$

still exact, not an eigenvalue equation for $E'$, instead

$$A(E')\,\varphi = 0$$

Operator $$A(E') = E' - V - \frac{1}{2m}\,\vec{\sigma}\cdot\hat{\vec{p}}\left(1 + \frac{E'-V}{2mc^2}\right)^{-1}\vec{\sigma}\cdot\hat{\vec{p}}$$

Expansion in $\frac{1}{c^2}$ respectively $\frac{v^2}{c^2}$, where $v$ = typical velocity: up to and including $O\left(\frac{1}{c^2}\right)$:

$$A = E' - V - \frac{\hat{\vec{p}}^2}{2m} + \frac{1}{4m^2c^2}\,\vec{\sigma}\cdot\hat{\vec{p}}\,(E'-V)\,\vec{\sigma}\cdot\hat{\vec{p}} + O\left(\frac{1}{c^4}\right)$$

$$= E'\left(1+\frac{\hat{\vec{p}}^2}{4m^2c^2}\right) - \frac{\hat{\vec{p}}^2}{2m} - V - \frac{1}{4m^2c^2}\,\vec{\sigma}\cdot\hat{\vec{p}}\,V\,\vec{\sigma}\cdot\hat{\vec{p}}$$

$$=: E'\,H_1 - H_2$$

$$H_1 = 1 + \frac{\hat{\vec{p}}^2}{4m^2c^2} \quad ; \quad H_2 = \frac{\hat{\vec{p}}^2}{2m} + V + \frac{1}{4m^2c^2}\,\vec{\sigma}\cdot\hat{\vec{p}}\,V\,\vec{\sigma}\cdot\hat{\vec{p}} \quad ; \quad H_i^\dagger = H_i$$

$$A\varphi = 0 \iff E' H_1 \varphi = H_2 \varphi$$

generalited eigenvalue problem

$$\Rightarrow E' H_1^{1/2}\varphi = \underbrace{H_1^{-1/2} H_2 H_1^{-1/2}}_{=:\,H'}\ \underbrace{H_1^{1/2}\varphi}_{\text{eigenvector}}$$

$E'$ ⟺ eigenvalues of $H'$ (effective theory!)

$$H_1^{\pm 1/2} = 1 \pm \frac{\hat{\vec{p}}^2}{8m^2c^2} + O\left(\frac{1}{c^4}\right)$$

$$\left(1 - \frac{\hat{\vec{p}}^2}{8m^2c^2}\right)\frac{\hat{\vec{p}}^2}{2m}\left(1 - \frac{\hat{\vec{p}}^2}{8m^2c^2}\right) = \frac{\hat{\vec{p}}^2}{2m} - \frac{(\hat{\vec{p}}^2)^2}{8m^3c^2} + O\left(\frac{1}{c^4}\right)$$

$$\left(\quad '' \quad\right) V \left(\qquad\right) = V - \frac{1}{8m^2c^2}\left\{V, \hat{\vec{p}}^2\right\} + O\left(\frac{1}{c^4}\right)$$

$$\vec{\sigma}\cdot\hat{\vec{p}}\,V\,\vec{\sigma}\cdot\hat{\vec{p}} = \frac{1}{2}\left(\hat{\vec{p}}^2 V - \vec{\sigma}\cdot\hat{\vec{p}}\left[\vec{\sigma}\cdot\hat{\vec{p}}, V\right] + V\hat{\vec{p}}^2 - \left[V, \vec{\sigma}\cdot\hat{\vec{p}}\right]\vec{\sigma}\cdot\hat{\vec{p}}\right)$$

$$= \frac{1}{2}\left(\left\{V, \hat{\vec{p}}^2\right\} - \left[\vec{\sigma}\cdot\hat{\vec{p}}, \left[\vec{\sigma}\cdot\hat{\vec{p}}, V\right]\right]\right)$$

$$\Rightarrow H' = \frac{\hat{\vec{p}}^2}{2m} - \frac{(\hat{\vec{p}}^2)^2}{8m^3c^2} + V - \frac{1}{8m^2c^2}\left[\vec{\sigma}\cdot\hat{\vec{p}}, \left[\vec{\sigma}\cdot\hat{\vec{p}}, V\right]\right] + O\left(\frac{1}{c^4}\right)$$

$$[\vec{\sigma}\cdot\hat{\vec{p}}, V] = \frac{\hbar}{i} (\vec{\nabla} V)\cdot\vec{\sigma}$$

$$[\vec{\sigma}\cdot\hat{\vec{p}}, (\vec{\nabla} V)\cdot\vec{\sigma}] = \sigma_k [\hat{p}_k, (\vec{\nabla} V)\cdot\vec{\sigma}] + [\sigma_k, (\vec{\nabla} V)\cdot\vec{\sigma}]\, \hat{p}_k$$

$$= \frac{\hbar}{i} \Delta V + i 2 \varepsilon_{klm} \sigma_m (\nabla_l V)\, \hat{p}_k$$

$$= \frac{\hbar}{i} \Delta V - 2i\, (\vec{\nabla} V \times \hat{\vec{p}})\cdot\vec{\sigma}$$

$$\Big( [AB, C] = A[B,C] + [A,C]B \, ;$$

$$\sigma_k [\hat{p}_k, (\nabla_l V)]\sigma_l = \frac{\hbar}{i}(\nabla_k \nabla_l V)\, \sigma_k \sigma_l = \frac{\hbar}{i}(\nabla_k \nabla_l V)\frac{1}{2}\{\sigma_k, \sigma_l\} = \frac{\hbar}{i}\Delta V \Big)$$

$$H' \cong \frac{\hat{\vec{p}}^2}{2m} - \frac{(\hat{\vec{p}}^2)^2}{8m^3c^2} + V + \frac{\hbar^2}{8m^2c^2}\Delta V + \frac{\hbar}{4m^2c^2}(\vec{\nabla} V \times \hat{\vec{p}})\cdot\vec{\sigma}$$

relativistic energy-momentum relation ↗ (for the $\frac{(\hat{\vec{p}}^2)^2}{8m^3c^2}$ term)

Darwin ↑

$$V = V(|\vec{x}|) \quad , \quad \vec{\nabla} V = V' \frac{\hat{\vec{x}}}{|\hat{\vec{x}}|}$$

last term $= \dfrac{\hbar V'}{4m^2c^2|\hat{\vec{x}}|}(\hat{\vec{x}} \times \hat{\vec{p}})\cdot\vec{\sigma}$

$= \dfrac{V'}{2m^2c^2|\hat{\vec{x}}|}\, \vec{L}\cdot\vec{S}$ spin-orbit coupling

$\vec{L}\cdot\vec{S}$ commutes with $\vec{J} = \vec{L} + \vec{S}$ ; not with $\vec{L}, \vec{S}$ individually

→ compare Clebsch-Gordan

# 8.6 The Relativistic Coulomb Problem

Relativistic Coulomb problem can be solved exactly, see book of G. Münster.

Stationary solution in the potential $A^\mu = \left(\frac{\phi}{c}, \vec{A} = 0\right)$ with

$$-e\phi(|\vec{x}|) = -\frac{\gamma}{|\vec{x}|} = V(|\vec{x}|) \quad , \quad q = -e \ (\text{electron}) , \quad \gamma = \frac{Ze^2}{4\pi\varepsilon_0}$$

$$E\psi = \left(V + c\vec{\alpha}\cdot\hat{\vec{p}} + mc^2\beta\right)\psi$$

$$\rightarrow \quad E_{nj} = mc^2\left[1 + \frac{Z^2\alpha^2}{(n-\varepsilon_j)^2}\right]^{-1/2}$$

with $\varepsilon_j = j + \frac{1}{2} - \sqrt{\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2} = \mathcal{O}(c^{-2})$

$j$ = total angular momentum : $\vec{J} = \vec{L} + \vec{S} = \hat{\vec{x}} \times \hat{\vec{p}} + \frac{\hbar}{2}\vec{\Sigma}$

$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \cong \frac{1}{137}$ fine-structure constant

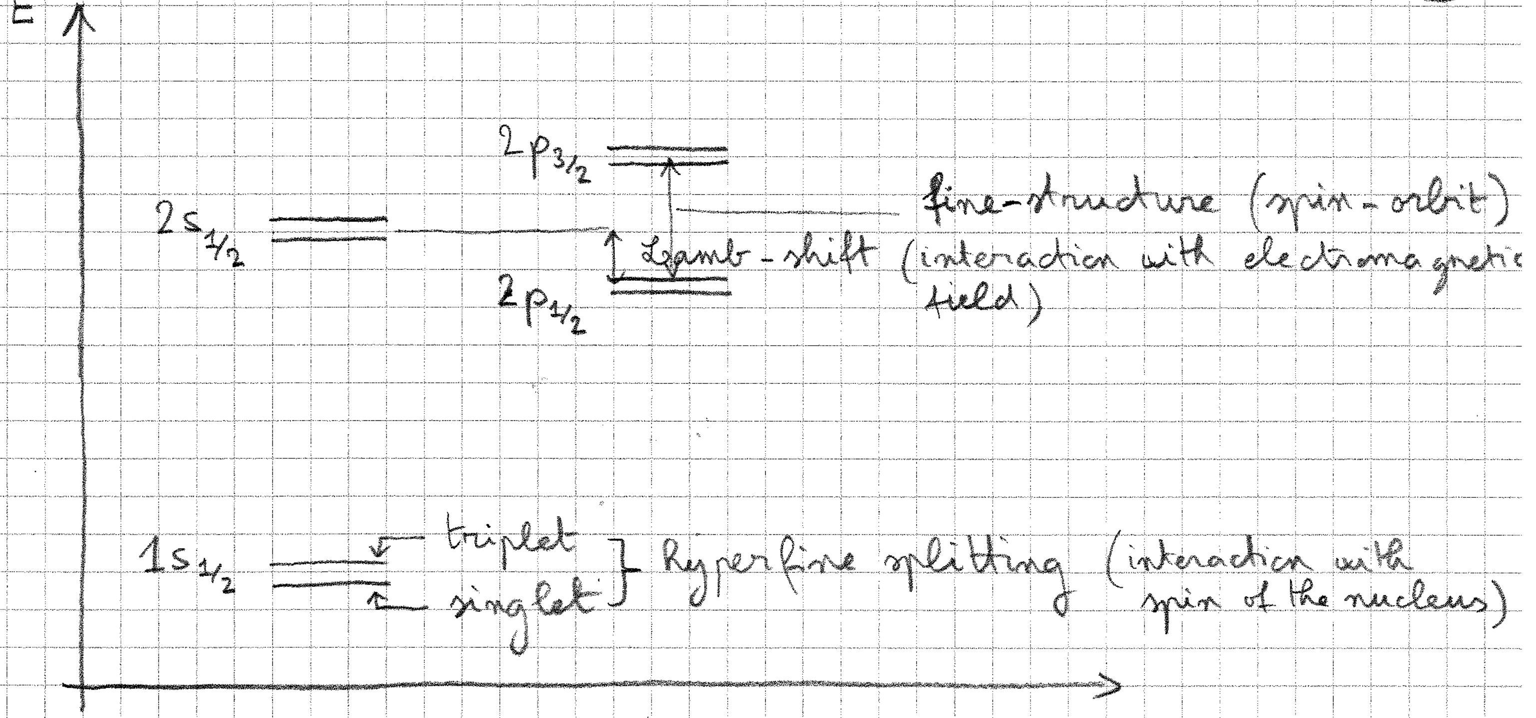
$n = 1, 2, \ldots$

$j = \frac{1}{2}, \frac{3}{2}, \ldots, n - \frac{1}{2}$

each with $\underset{\substack{\downarrow \\ \text{from } l = j \pm \frac{1}{2}}}{2} \times (2j+1)$ solutions except $j = n - \frac{1}{2}$, there only $1 \underset{\substack{\uparrow \\ l \leq n-1}}{\times} (2j+1)$, therefore only $j = l + \frac{1}{2}$ is possible

Energy level diagram : (notation: $n\,l_j$)

| | | | | |
|---|---|---|---|---|
| $n=1$ | $j=\frac{1}{2}$ | $1s_{\frac{1}{2}}$ | | |
| $n=2$ | $j=\frac{1}{2}$ | $2s_{\frac{1}{2}}$ | $2p_{\frac{1}{2}}$ | (degenerate) |
| | $j=\frac{3}{2}$ | | $2p_{\frac{3}{2}}$ | |



(diagram is not to scale)

Expand:

$$\varepsilon_j = \left(j+\frac{1}{2}\right)\left(1-\sqrt{1-\left(\frac{Z\alpha}{j+\frac{1}{2}}\right)^2}\right) = \frac{1}{2}\,\frac{Z^2\alpha^2}{j+\frac{1}{2}} + \mathcal{O}(\alpha^4)$$

$$E_{nj} = mc^2\left[1-\frac{1}{2}\,\frac{Z^2\alpha^2}{n^2}\left(1+2\,\frac{\varepsilon_j}{n}\right)+\frac{1}{2}\cdot\frac{3}{4}\,\frac{Z^4\alpha^4}{n^4}+\mathcal{O}(\alpha^6)\right]$$

$$= mc^2\left[1-\frac{1}{2}\left(\frac{Z\alpha}{n}\right)^2+\left(\frac{Z\alpha}{n}\right)^4\left(\frac{3}{8}-\frac{n}{2j+1}\right)+\mathcal{O}(\alpha^6)\right]$$

$$\frac{1}{2}mc^2\alpha^2 = \frac{1}{2}mc^2\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{\hbar^2c^2} = \frac{\hbar^2}{2m\left(\frac{4\pi\varepsilon_0}{e^2}\,\frac{\hbar^2}{m}\right)^2} = \frac{\hbar^2}{2ma_B^2} = E_R$$

= Rydberg energy

$mc^2\,\frac{\alpha^4}{n^4}\left(\frac{3}{8}-\frac{n}{2j+1}\right)$ is $=\mathcal{O}(c^{-2})$ w.r.t. $E_R$

For $Z \to 137$ the non-relativistic approximation becomes problematic because of large velocities of the electron.

# 9. Many Particle Systems

Atoms, nuclei, solid states

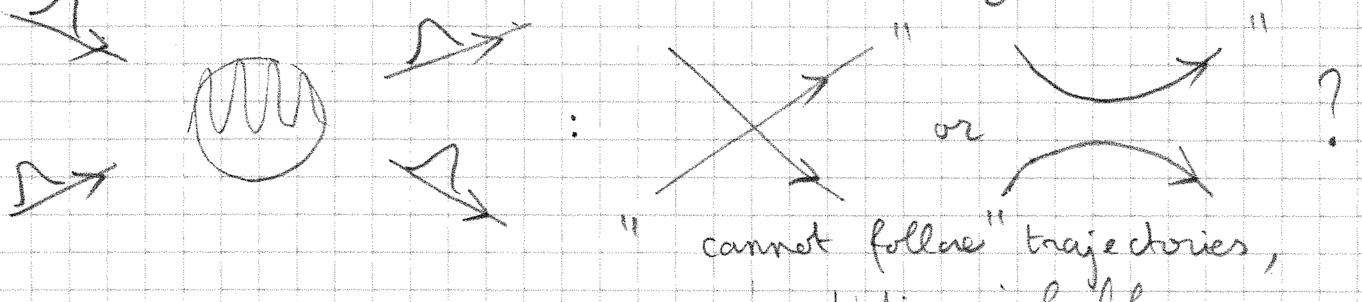
## 9.1 Identical Particles

For example N $e^-$ in the atom, same mass, spin, etc.

Classical physics:

- number the particles (somehow)
- determine $\vec{x}_i(0)$, $\vec{p}_i(0)$
- solve $\rightarrow \vec{x}_i(t)$, $i = 1, \ldots, N$
- identity of the particles is preserved through continuous trajectories
- different numbering at $t=0$ $\Leftrightarrow$ later different numbering

Quantum mechanics, for example scattering of two particles:



" cannot follow" trajectories, undistinguishable

$$|\Psi(t)\rangle = \int d^3x_1\, d^3x_2\ |\vec{x}_1\rangle |\vec{x}_2\rangle\ \varphi(\vec{x}_1, \vec{x}_2, t)$$

Further problem:

$\mathcal{H}$ is spanned by basis states $\{ |\vec{x}_1 \vec{x}_2\rangle = |\vec{x}_1\rangle |\vec{x}_2\rangle \}$

Describe two identical $e^-$

$$\langle \vec{x}_1\, \vec{x}_2 | \vec{x}_1'\, \vec{x}_2' \rangle = \delta^{(3)}(\vec{x}_1 - \vec{x}_1')\ \delta^{(3)}(\vec{x}_2 - \vec{x}_2')$$

Measurement / preparation:

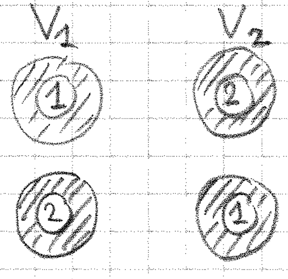
$e^-$ in $V_1$ and $e^-$ in $V_2$ (simultaneously),
$V_1 \cap V_2 = \phi$ disjoint

Wave function $\varphi_i \neq 0$ only in $V_i$

State:

$$|A\rangle = \int d^3x \int d^3y \;\varphi_1(\vec{x})\,\varphi_2(\vec{y})\;|\vec{x}\,\vec{y}\rangle \quad \text{or}$$

$$|B\rangle = \int d^3x \int d^3y \;\varphi_2(\vec{x})\,\varphi_1(\vec{y})\;|\vec{x}\,\vec{y}\rangle \quad ?$$



Since $V_1 \cap V_2 = \phi$ it holds $\langle A|B\rangle = 0$
→ different rays in the 2-particle Hilbert space

Experience tells: undistinguishable particles → no other observable exist, which distinguishes $|A\rangle$, $|B\rangle$

→ $n!$ states with $n$ identical particles

QM principles? inconsistency?

## 9.2 Permutations, Bosons, Fermions

Problem ⟺ Exchange of (arbitrary but unavoidable) particle indices (cf. choice of coordinates, necessary but physics independent → structural consequences like Galilei / Lorentz invariance)

Permutations $\pi \in S_n$: $(1, 2, \dots, n) \longrightarrow (\pi(1), \pi(2), \dots, \pi(n))$,
$\pi(j) \in \{1, \dots, n\}$
$\pi$ is invertible → $1, \dots, n$ appear only once in the range $\{\pi(j)\}$
→ $|S_n| = n!$ different permutations

Transposition $\Pi_{ij}$ $(i \neq j)$

$$\Pi_{ij}(k) = \begin{cases} j & \text{if } k=i \\ i & \text{if } k=j \\ k & \text{otherwise} \end{cases}$$

$$\Pi = \Pi_{i_1 j_1} \circ \Pi_{i_2 j_2} \circ \dots \Pi_{i_N j_N}$$

- $\Pi$ can always be decomposed as composition of permutations
- not unique
- $(-1)^N$ is uniquely determined by $\Pi$, $= \mathrm{sig}(\Pi)$

$S_n$ is a group

in general $\Pi \circ \Pi' \neq \Pi' \circ \Pi$ (not abelian)

Induced unitary representation $P$ in the Product-Hilbert-space:

$$\mathcal{H} = \underbrace{\mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_1}_{n \text{ factors}}$$

$$|\varphi\rangle = \sum_{i_1,\dots,i_n} \varphi_{i_1 \dots i_n} \underbrace{|i_1\rangle |i_2\rangle \dots |i_n\rangle}_{=|i_1 \dots i_n\rangle}$$

or

$$|\varphi\rangle = \int d^3x_1 \dots d^3x_n \, \varphi(\vec{x}_1, \dots, \vec{x}_n) \, |\vec{x}_1\rangle |\vec{x}_2\rangle \dots |\vec{x}_n\rangle$$

$$\langle i_1 \dots i_n | P(\Pi) | \varphi \rangle = \langle i_{\Pi^{-1}(1)} \dots i_{\Pi^{-1}(n)} | \varphi \rangle$$

$P(\Pi)$ is a unitary representation of $S_n$

( cf. for example rotations $\langle \vec{x} | \mathcal{U}(R) | \varphi \rangle = \langle R^{-1} \vec{x} | \varphi \rangle$ )

Transposition: $P(\Pi_{ij}) = P_{ij}$

$$\langle k_1 \dots \underset{\uparrow}{k_i} \dots \underset{\uparrow}{k_j} \dots k_n | P_{ij} | \varphi \rangle = \langle k_1 \dots \underset{\uparrow}{k_j} \dots \underset{\uparrow}{k_i} \dots k_n | \varphi \rangle$$

$P_{ij} \; |k_1\rangle \cdots |k_i\rangle \cdots |k_j\rangle \cdots |k_n\rangle = |k_1\rangle \cdots |k_j\rangle \cdots |k_i\rangle \cdots |k_n\rangle$

$P_{12} \; |\vec{x}_1 \vec{x}_2\rangle = |\vec{x}_2 \vec{x}_1\rangle$

→ previous example : $P_{12} \; |A\rangle = |B\rangle$

Postulate of symmetrization:

Physical states of $n$ identical particles are invariant under permutations: $P(\pi)\,|\varphi\rangle = \lambda\, |\varphi\rangle \;, \; \lambda \in \mathbb{C}$

- it is enough to consider $P_{ij}$
- it holds $(P_{ij})^2 = 1$
- $P_{ij}\, |\varphi\rangle = \pm |\varphi\rangle$

$$\Rightarrow P(\pi)\,|\varphi\rangle = \left\{ \begin{matrix} 1 \\ \mathrm{sig}(\pi) \end{matrix} \right\} |\varphi\rangle$$

Case "+": bosons

Case "−": fermions (Pauli principle)

For the localization of two particles in $V_1 \cap V_2 = \phi$ this implies not $|A\rangle$, not $|B\rangle$ but insted

$|\varphi_+\rangle = |A\rangle + |B\rangle \;\rightarrow\; P_{12}\, |\varphi_+\rangle = |\varphi_+\rangle$ or

$|\varphi_-\rangle = |A\rangle - |B\rangle \;\rightarrow\; P_{12}\, |\varphi_-\rangle = -|\varphi_-\rangle$

$e^-$ are fermions, therefore $|\varphi_-\rangle$ !

Relativistic Quantum Field Theory ⇒ (spin-statistics
half-integer spin ⟺ fermions theorem, Pauli,
integer spin ⟺ bosons 1940 )

spin $\frac{1}{2}$ : e, p, n, quarks, neutrinos,

spin 1 : $\gamma$, Z, W-bosons, gluons ; spin 0 : Higgs

Nuclei, Atoms can be fermion or boson → behavior is essentially different

Permutations acts on all the quantum numbers:

$P_{12} |\vec{x}_1 \varepsilon_1 ; \vec{x}_2 \varepsilon_2\rangle = |\vec{x}_2 \varepsilon_2 ; \vec{x}_1 \varepsilon_1\rangle \quad (\varepsilon_i = \pm)$

physical state of two $e^-$ : $|\vec{x}_1 \varepsilon_1 ; \vec{x}_2 \varepsilon_2\rangle - |\vec{x}_2 \varepsilon_2 ; \vec{x}_1 \varepsilon_1\rangle$

## 9.3 (Anti) symmetric Space of States

In $\mathcal{H} = \underbrace{\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}_{n \text{ factor}}$ the (anti) symmetric states form

a subspace $|\varphi_\pm\rangle \in \mathcal{H}_\pm \subset \mathcal{H}$ , $P_{ij} |\varphi_\pm\rangle = \pm |\varphi_\pm\rangle$

$\mathcal{H}_\pm$ : physical Hilbert space of bosons (+) or fermions (−)

Matrix elements of observables:

$$\langle \varphi_\pm | \underbrace{A | \chi_\pm\rangle}$$

$A|\chi_\pm\rangle$ is again projected onto $\mathcal{H}_\pm$ through scalar product

⟹ symmetrization postulate for observables:

only observables A are admissible (as physical observables) for which $A : \mathcal{H}_+ \to \mathcal{H}_+$ or $\mathcal{H}_- \to \mathcal{H}_-$

⟹ A is fully determined through matrix elements

$$\langle \varphi_\pm | A | \chi_\pm\rangle = \langle \varphi_\pm | P_{ij}^+ A P_{ij} | \varphi_\pm\rangle$$

$$\Longrightarrow A = P_{ij}^+ A P_{ij} = P_{ij} A P_{ij} \iff [A, P_{ij}] = 0$$

This does not hold for example for $\hat{x} \otimes 1$ :

$$(\hat{\vec{x}} \otimes 1)\left(|\vec{y}_1 \vec{y}_2\rangle - |\vec{y}_2 \vec{y}_1\rangle\right) = \vec{y}_1 \, |\vec{y}_1 \vec{y}_2\rangle - \vec{y}_2 \, |\vec{y}_2 \vec{y}_1\rangle$$

$$P_{12} \, (\hat{\vec{x}} \otimes 1) \, P_{12} \, \left( |\vec{y}_1 \vec{y}_2\rangle - |\vec{y}_2 \vec{y}_1\rangle \right) = \qquad \updownarrow \text{ different}$$

$$- P_{12} \left( \vec{y}_1 \, |\vec{y}_1 \vec{y}_2\rangle - \vec{y}_2 \, |\vec{y}_2 \vec{y}_1\rangle \right) = \vec{y}_2 \, |\vec{y}_1 \vec{y}_2\rangle - \vec{y}_1 \, |\vec{y}_2 \vec{y}_1\rangle$$

but as we can see the following holds:

$$\underset{\substack{\uparrow \\ \text{exchange}}}{P_{12}} \, (\hat{\vec{x}} \underset{\substack{\uparrow \\ \text{measure 1st factor}}}{\otimes} 1) \, \underset{\substack{\uparrow \\ \text{exchange}}}{P_{12}} = \underset{\substack{\uparrow \\ \text{measure 2nd factor}}}{1 \otimes \hat{\vec{x}}}$$

$\Rightarrow$ $\hat{\vec{x}} \otimes 1 + 1 \otimes \hat{\vec{x}}$ is an admissible observable

plus sign for $\mathcal{H}_-$ as well as for $\mathcal{H}_+$

$\Rightarrow$ observable is symmetric in the particle indices for indistinguishable particles

Projectors $\mathcal{H} \to \mathcal{H}_\pm$

$$S^+ = \frac{1}{n!} \sum_{\pi \in S_n} P(\pi)$$

$$S^- = \frac{1}{n!} \sum_{\pi \in S_n} \operatorname{sig}(\pi) \, P(\pi)$$

Properties of projectors:

$$(S^\pm)^+ = S^\pm \, , \quad (S^\pm)^2 = S^\pm$$

$$S^+ S^- = S^- S^+ = 0 \, , \quad \mathcal{H}_+ \perp \mathcal{H}_-$$

Easy to show: $P_{ij} \, S^\pm |\varphi\rangle = \pm \, S^\pm |\varphi\rangle$

In general it does not hold $S^+ + S^- = 1_{\mathcal{H}}$ (holds only for $n = 2$)

→ there exist also subspaces of $\mathcal{H}$, which are neither symmetric nor antisymmetric → unphysical

Basis of $\mathcal{H}_\pm$ :

$$S^\pm |\vec{x}_1 \vec{x}_2\rangle = \frac{1}{2}\left(|\vec{x}_1 \vec{x}_2\rangle \pm |\vec{x}_2 \vec{x}_1\rangle\right)$$

$$|\varphi_\pm\rangle = \int d^3x_1\, d^3x_2\, \varphi(\vec{x}_1, \vec{x}_2)\, \frac{1}{2}\left(|\vec{x}_1 \vec{x}_2\rangle \pm |\vec{x}_2 \vec{x}_1\rangle\right)$$

⇒ only (anti) symmetric part of the wave fuction contributes
→ choose (anti) symmetric wave functions $\varphi$

Discrete basis $|i_1 \cdots i_n\rangle = |i_1\rangle |i_2\rangle \cdots |i_n\rangle$

$S^\pm |i_1 \cdots i_n\rangle$ only depends on which $\{i_1 \cdots i_n\}$ appear but not on their ordering

Occupation-number basis :

1-particle state $|0\rangle$ : appears $N_0$ times
1-particle state $|1\rangle$ : appears $N_1$ times
⋮
etc

appearing in $\{i_1 \cdots i_n\}$ with $\underbrace{\sum_j}_{\text{sum over all 1-particle states forming basis of } \mathcal{H}_1} N_j = n$ = number of particles

$\mathcal{H}_+$ : all $|N_0 N_1 N_2 \cdots\rangle$ are linear independent, build a basis

$\mathcal{H}_-$ : like above, but only $N_j = 0, 1$ admissible because

$S^- |i_1 \cdots i_n\rangle = 0$ when the same index appears twice, for example $i_1 = i_2$

Pauli exclusion principle:
each 1-particle state can be occupied by at most one $e^-$

Do we need to antisymmetrize between all $e^-$ in the universe?

$$|\varphi\rangle = \underset{\text{Earth}}{\underset{\uparrow}{|\varphi_E\rangle}} \underset{\text{Moon}}{\underset{\uparrow}{|\varphi_M\rangle}} \quad \in \quad \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_1$$

$\langle \varphi_E | \varphi_M \rangle = 0$ no overlap

$$|\varphi_-\rangle = \frac{1}{\sqrt{2}} \left( |\varphi_E\rangle |\varphi_M\rangle - |\varphi_M\rangle |\varphi_E\rangle \right)$$

Symmetric (= admissible) observable:

$$P_\Delta = \int_\Delta d^3x \left( |\vec{x}\rangle\langle\vec{x}| \otimes 1 + 1 \otimes |\vec{x}\rangle\langle\vec{x}| \right)$$

$\langle \varphi_- | P_\Delta | \varphi_- \rangle$ = probability for $e^-$ in volume $\Delta$ near the Earth

$$= \frac{1}{2} \int_\Delta d^3x \left\{ 2 \left| \langle \vec{x} | \varphi_E \rangle \right|^2 \langle \varphi_M | \varphi_M \rangle + 2 \underset{\approx 0}{\left| \langle \vec{x} | \varphi_M \rangle \right|^2} \langle \varphi_E | \varphi_E \rangle \right\}$$

$$= \int_\Delta d^3x \left| \langle \vec{x} | \varphi_E \rangle \right|^2$$

same result as for separate Earth / Moon systems

## 9.4 Atoms with Many Electrons

nucleus with charge $Z$, number $Z$ of $e^-$ with spin $\frac{1}{2}$

$$H = \sum_{i=1}^{Z} H_i + \sum_{i<j} V_{ij}$$

$$H_i = \frac{\hat{\vec{p}}_i^{\,2}}{2m} - \frac{Ze^2}{4\pi\varepsilon_0} \frac{1}{|\hat{\vec{x}}_i|}$$

$$V_{ij} = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\hat{\vec{x}}_i - \hat{\vec{x}}_j|}$$

H is symmetric, $[H, P(\pi)] = 0$

looking for: bound states in $\mathcal{H}_-$

very complicated! → Approximations.

Principle: first set $V_{ij} \rightarrow 0$.
Each $H_i$: 1-particle operator with eigenstates $|n \ell m m_s\rangle$,

$$E_n = -\frac{Z^2 E_R}{n^2}$$

in $\mathcal{H}_-$ occupation numbers $N_{n\ell m m_s} = 1$ for the lowest Z energy eigenstates

$\rightarrow$ ground state $E = -2E_1 - 8E_2 \dots$

No degeneracy when shells are fully occupied:
$Z = 2, 2+8, 2+8+18, \dots$

Better approximation: Central field approximation

$$H \approx \sum_{i=1}^{Z} \left( H_i + \overline{V}(|\hat{\vec{x}}_i|) \right)$$

$\overline{V}$ shall approximate $\sum_{i<j} V_{ij}$

Heuristically:

$$\overline{V}(|\vec{x}_i|) \cong \begin{cases} 0 & \text{for } |\vec{x}_i| \to 0 \quad (\text{nucleus dominates}) \\ +\dfrac{(Z-1)e^2}{4\pi\varepsilon_0 |\vec{x}_i|} & \text{for } |\vec{x}_i| \to \infty \quad \left(\text{when added to } \dfrac{-Ze^2}{4\pi\varepsilon_0 |\vec{x}_i|} :\right. \\ & \left.\text{nucleus charge is screened } Z \to 1 \right) \end{cases}$$

Specification of $\overline{V}$ such that $\sum_{i<j} V_{ij} - \sum_i \overline{V}(|\vec{x}_i|)$ is a small perturbation

Eigenstates with nucleus and $\overline{V}$

$$|n\ell m m_s\rangle \;, \quad E_{n\underset{\uparrow}{\ell}}$$

accidental degeneracy for $\frac{1}{r}$-potential is lifted

$E_{n\ell}$ can be occupied with at most $2\cdot(2\ell+1)$ $e^-$.

For the sequence of occupation there are heuristic and empirical rules:

| | # $e^-$ | sum $e^-$ | |
|---|---|---|---|
| 1s ($\ell=0, n=1$) | 2 | 2 | He |
| 2s ($\ell=0, n=2$), 2p ($\ell=1, n=2$) | 8 | 10 | Ne |
| 3s, 3p | 8 | 18 | Ar |
| 4s, 3d, 4p | 18 | 36 | Kr |
| 5s, 4d, 5p | 18 | 54 | Xe |
| 6s, 4f, 5d, 6p | 32 | 86 | Rn |

Each row in the above table which starts with s-$e^-$ is called a shell. Shells are particularly stable.

## 9.5 Hartree-Fock Approximation

Look for ground state as the optimal antisymmetrized product ("Slater determinant") of 1-particle states; determine their wave function!

Ansatz: $|\varphi\rangle = \sqrt{Z!}\; S^- \, |\varphi_1\rangle |\varphi_2\rangle \cdots |\varphi_Z\rangle$

with $\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$

Minimize $E = \dfrac{\langle\varphi|H|\varphi\rangle}{\langle\varphi|\varphi\rangle}$ through the choice of $|\varphi_i\rangle$ above.

$\Rightarrow$ Hartree-Fock equation for $\{ |\varphi_i\rangle, \; i = 1, \dots, Z \}$

This is an approximation. Because of $V_{ij}$ the exact state is not a product state!

Result:

Basis $|\vec{x}\sigma\rangle$, $\sigma = \pm$ of 1-particle states

$$|\varphi_i\rangle = \sum_\sigma \int d^3x \; \varphi_{i\sigma}(\vec{x}) \; |\vec{x}\sigma\rangle$$

Hartree-Fock equation

$$\left( -\frac{\hbar^2}{2m}\Delta - \frac{Ze^2}{4\pi\varepsilon_0 |\vec{x}|} + W_i(\vec{x}) \right) \varphi_{i\sigma}(\vec{x})$$

$$- \sum_{\sigma'} \int d^3y \; A_{i\sigma\sigma'}(\vec{x},\vec{y}) \, \varphi_{i\sigma'}(\vec{y}) = \varepsilon_i \, \varphi_{i\sigma}(\vec{x})$$

with $$W_i(\vec{x}) = \sum_{j\neq i} \sum_{\sigma} \int d^3y \; \frac{|\varphi_{j\sigma}(\vec{y})|^2}{4\pi\varepsilon_0 |\vec{x}-\vec{y}|}$$

$$A_{i\sigma\sigma'}(\vec{x},\vec{y}) = \sum_{j\neq i} \frac{\varphi_{j\sigma}(\vec{x}) \, \varphi^*_{j\sigma'}(\vec{y})}{4\pi\varepsilon_0 |\vec{x}-\vec{y}|}$$

Solve by iteration:

$\{\varphi_{i\sigma}\} \rightarrow$ compute $W_i$, $A_{i\sigma\sigma'} \rightarrow$ eigenvalue equation for each $\varphi_{i\sigma}(\vec{x}) \longrightarrow$ new $W_i$, $A_{i\sigma\sigma'} \rightarrow$ etc. Convergence

$W_i$: average repulsion

$A_{i\sigma\sigma'}$: exchange term $\leftrightarrow$ Fermi statistics,
Pauli principle

Proof of Hartree-Fock equation:

norm:

$$\langle \varphi|\varphi\rangle = Z!\ \langle\varphi_1|\langle\varphi_2|\cdots\langle\varphi_n|\ \frac{1}{Z!}\sum_{\pi} \mathrm{sig}(\pi)\ |\varphi_{\pi(1)}\rangle\cdots|\varphi_{\pi(Z)}\rangle$$

$$= \sum_{\pi} \mathrm{sig}(\pi)\ \langle\varphi_1|\varphi_{\pi(1)}\rangle\cdots\langle\varphi_Z|\varphi_{\pi(Z)}\rangle = 1$$

where we used: - $(S^-)^+ = S^- = (S^-)^2$

- only contribution from $\pi$ = identity

Computation of $\langle\varphi|H|\varphi\rangle = E$ :

H is symmetric $\Rightarrow [S^-, H] = 0$

same applies to $\sum H_i$ , $\sum_{i<j} V_{ij}$ individually

$$\sum_i \langle\varphi|H|\varphi\rangle = \sum_i \sum_{\pi} \mathrm{sig}(\pi)\ \langle\varphi_1|\cdots\langle\varphi_Z|\,H_i\,|\varphi_{\pi(1)}\rangle\cdots|\varphi_{\pi(Z)}\rangle$$

$$= \sum_{i=1}^{Z} \langle\varphi_i|H_i|\varphi_i\rangle \quad (\langle\varphi_i|\varphi_j\rangle = \delta_{ij} \to \text{only } \pi = \text{identity contributes})$$

$$\sum_{i<j}\langle\varphi|V_{ij}|\varphi\rangle = \sum_{i<j}\sum_{\pi} \mathrm{sig}(\pi)\ \langle\varphi_i|\langle\varphi_j|\,V_{ij}\,|\varphi_{\pi(i)}\rangle|\varphi_{\pi(j)}\rangle \prod_{k\neq i,j}\langle\varphi_k|\varphi_{\pi(k)}\rangle$$

$$= \sum_{i<j}\Big(\langle\varphi_i|\langle\varphi_j|\,V_{ij}\,|\varphi_i\rangle|\varphi_j\rangle - \langle\varphi_i|\langle\varphi_j|\,V_{ij}\,|\varphi_j\rangle|\varphi_i\rangle\Big)$$

- contributions from $\pi$ = identity and $\pi = \pi_{ij}$ (transposition) with $\mathrm{sig}(\pi_{ij}) = -1$
- exchange term → important effects from Fermi statistics

Minimization of E: consider variations $|\varphi_i\rangle \longrightarrow |\varphi_i\rangle + |\delta_i\rangle$

and require: $\delta E = 0$, constraint: $\langle\varphi_i|\varphi_j\rangle = \delta_{ij}$ !

In order to fulfill the constraint introduce Lagrange multipliers $\varepsilon_{ij} = \varepsilon_{ji}^*$ and add to the energy functional

$$E - \underbrace{\sum_{i,j} \varepsilon_{ij} \left( \langle \varphi_i | \varphi_j \rangle - \delta_{ij} \right)}_{\text{real}}$$

→ stationary under $|\delta_i\rangle$ (unconstrained!) and

$\delta \varepsilon_{ij} \Rightarrow$ constraint conditions

$$0 = \sum_i 2\,\mathrm{Re}\,\langle \delta_i | H_i | \varphi_i \rangle \qquad \left[ \leftarrow \left( \langle \varphi_i | + \langle \delta_i | \right) H_i \left( |\varphi_i\rangle + |\delta_i\rangle \right) \right]$$

$$+ \sum_{i<j} 2\,\mathrm{Re} \Big\{ \langle \delta_i | \langle \varphi_j | \, V_{ij} \left( |\varphi_i\rangle |\varphi_j\rangle - |\varphi_j\rangle |\varphi_i\rangle \right)$$
$$+ \langle \varphi_i | \langle \delta_j | \;\; '' \;\; \left( \qquad '' \qquad \right) \Big\} \qquad (*)$$

$$- \sum_{i,j} 2\,\mathrm{Re} \left( \varepsilon_{ij} \langle \delta_i | \varphi_j \rangle \right)$$

[ $(*)$: $\langle \delta_i | \langle \varphi_j | V_{ij} | \varphi_i \rangle |\varphi_j\rangle + \langle \varphi_i | \langle \varphi_j | V_{ij} | \delta_i \rangle | \varphi_j \rangle =$

$\mathrm{Re} \left\{ \langle \delta_i | \langle \varphi_j | V_{ij} | \varphi_i \rangle | \varphi_j \rangle \right\}$

similarly for exchange term and $|\delta_j\rangle$ ]

$$\sum_{i<j} \left( \langle \delta_i | \langle \varphi_j | X_{ij} \rangle + \langle \varphi_i | \langle \delta_j | X_{ij} \rangle \right)$$

$$= \sum_{i<j} \langle \delta_i | \langle \varphi_j | X_{ij} \rangle + \sum_{i>j} \underbrace{\langle \varphi_j | \langle \delta_i | X_{ji} \rangle}_{= \langle \delta_i | \langle \varphi_j | X_{ij} \rangle}$$

because the observable $V_{ij}$ is symmetric

$$= \sum_i \sum_{j \neq i} \langle \delta_i | \langle \varphi_j | X_{ij} \rangle$$

$\langle \delta_i|$ is arbitrary $\Longrightarrow$

$$0 = H_i|\varphi_i\rangle + \sum_{j\neq i}\left(\underbrace{\langle\varphi_j|V_{ij}|\varphi_j\rangle}_{\text{operator !}}|\varphi_i\rangle - \langle\varphi_j|V_{ij}|\varphi_i\rangle\,|\varphi_j\rangle\right)$$

$\langle\varphi_j|\cdots|\varphi_j\rangle$ : second tensor product factors

The solution is covariant under unitary transformation

$$|\tilde\varphi_i\rangle = \sum_j U_{ij}|\varphi_j\rangle \qquad U_{ij}:\ Z\times Z\ ,\ \text{unitary}$$

$\{|\varphi_i\rangle\}$ solution $\Longrightarrow$ $\{|\tilde\varphi_i\rangle\}$ also solution with

$$\tilde\varepsilon_{ij} = \sum_{kl} U_{ik}\,\varepsilon_{kl}\,U^+_{kl}$$

Choose $U$ such that $\tilde\varepsilon_{ij} = \varepsilon_i\,\delta_{ij}$

$$|\tilde\varphi\rangle = S^-\,|\tilde\varphi_1\rangle\cdots|\tilde\varphi_Z\rangle$$

$$= \frac{1}{Z!}\sum_{\pi}\operatorname{sig}\pi\sum_{j_1,\dots,j_Z} U_{\pi(1)j_1}\cdots U_{\pi(Z)j_Z}\,|\varphi_{j_1}\rangle\cdots|\varphi_{j_Z}\rangle$$

$$= \frac{1}{Z!}\sum_{\pi,\pi'}\operatorname{sig}\pi\; U_{\pi(1)\pi'(1)}\cdots U_{\pi(Z)\pi'(Z)}\,|\varphi_{\pi'(1)}\rangle\cdots|\varphi_{\pi'(Z)}\rangle$$

$$= \det U\;S^-\,|\varphi_1\rangle\cdots|\varphi_Z\rangle = \det U\;|\varphi\rangle$$

$\Rightarrow$ same ray in $\mathcal{H}_-$