

Advanced Quantum Mechanics

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Status: 8.2.2017

This document uses TikZ-Feynman (arXiv:1601.05437)

Contents

0	Overview	4
0.1	Recap of classical Quantum Mechanics	4
0.2	Symmetries in QM	4
0.3	Propagators, path-integrals, scattering	5
0.4	QM with multiple particles	5
0.5	Relativistic QM	5
1	QM Recap	7
1.1	Stochastics	7
1.2	Hilbert spaces, operators	8
1.3	Eigenvalues, eigenvectors, spectrum	12
1.4	Principles of Quantum theory	15
1.5	Further tools	16
1.6	Generalized states	18
1.7	Coupling to the EM-field	20
2	Symmetries in Quantum Mechanics	22
2.1	Symmetries and unitary representations	22
2.2	Continuous symmetries	26
2.3	Rotational symmetry $SO(3)$	29
2.4	Spin $j = n + \frac{1}{2}, n \in \mathbb{N}_0$	34
2.5	General form of symmetries	36
3	Time evolution, propagators, path integrals	37
3.1	Review of basic motions	37
3.2	Propagators	41
3.3	The Feynman path integral	44
3.4	Perturbation theory with Feynman diagrams	48
4	Scattering Theory	53
4.1	S -matrix, scattering amplitudes	55
4.2	Lippman-Schwinger equation	57
4.3	Scattering amplitude and scattering cross section	59
5	Identical Particles	63
5.1	Introduction	63
5.2	n identical particles	65
5.3	Fermi- and Bose-Einstein statistics	67
5.4	Fermi and Boson gas	68
5.5	Fock space	70
6	Relativistic Quantum Mechanics	73
6.1	Short review of special relativity	73

6.2	Some representations of $\mathcal{P}(3, 1)$ and $O(3, 1)$	76
6.3	Klein-Gordon equation	78
6.4	Dirac equation	79
6.5	Connection to QFT	90

0 Overview

0.1 Recap of classical Quantum Mechanics

- Observables: Operators on Hilbert-spaces
 - also elements of an algebra a
 - in general: $[\hat{a}, \hat{b}] \neq 0$ (for two operators \hat{a} and \hat{b})
- Spectra: Each observable a comes with a spectrum

$$\text{spec}(a) \subset \mathbb{R} \quad (0.1)$$

- Interpretation: Spectrum of an observable a are all possible values of a

- States: Give probability measure

$$\psi \mapsto dP_{\psi}^{(a)} \quad (0.2)$$

- In classical physics all this is true, but

$$dP^{(A)} = a \cdot dP \quad (0.3)$$

where a is function in phase space and dP is probability measure on phase space

0.2 Symmetries in QM

Operations which leave probabilities invariant and respect time evolution are called **Symmetries**.

- unitary or anti-unitary operators (see Wigner's theorem)
- Representations (up to phase) of a symmetry group
- Consequences for spectra
- Continuous symmetries \leftrightarrow **Lie-algebra** of conserved quantities

$$V(t) = e^{k \cdot t} \quad (0.4)$$

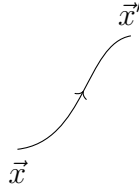
Operator V and k is element of a Lie-algebra

- Rotational- / Isospin-symmetry

0.3 Propagators, path-integrals, scattering

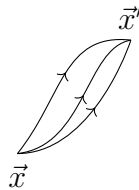
- Propagators have the form of:

$$U(\vec{x}, \vec{x}', t) = \langle \vec{x}' | U(t) | \vec{x} \rangle \quad (0.5)$$



- Can be written as path-integral

$$U(\vec{x}, \vec{x}', t) = \int_{\{\vec{x}: \vec{x}(0)=\vec{x}, \vec{x}(t)=\vec{x}'\}} D x(\cdot) e^{i\int \mathcal{L}(\vec{x}(\cdot))} \quad (0.6)$$



- Approximation: (Here sum over all different paths)
- Scattering: $\langle \vec{k} | U(-\infty, \infty) | \vec{k}' \rangle = ?$

0.4 QM with multiple particles

- Tensor product
- Particle exchange as symmetry
- Identical particles
- Infinite many particles: **Fock-space**: $\mathcal{F}^{(h)} = e^h = \mathbb{C} \oplus h \oplus h \otimes h \oplus \dots$

0.5 Relativistic QM

QM with **lorentz-group** as symmetry-group

- Representations of lorentz-groups
- Evolution equation for scalar particles:

$$\square \psi - \frac{m^2}{\hbar^2} \psi = 0 \quad (0.7)$$

(**Klein-Gordon-equation**)

- Evolution equation for massless spinors

$$\sigma^\mu \partial_\mu \psi_R = 0 ; \sigma^\mu \partial_\mu \psi_L = 0 \quad (0.8)$$

(**Veyl-equation**)

- Evolution-equation for massive spinors

$$\gamma^\mu \partial_\mu \psi + m \mathbb{1} \psi = 0 \quad (0.9)$$

(**Dirac-equation**)

- Majorana fermions

1 QM Recap

1.1 Stochastics

Most statements of QM are about probabilities.

Probability space: Space \mathcal{P} , probability measure dP

- $\int_{\mathcal{P}} dP = 1$
- $\int_{\mathcal{P}} \varphi dP \geq 0$ for $f \geq 0$

Observables: (math.: random variables) Functions of $f: \mathcal{P} \rightarrow \mathbb{C}$

Examples:

- Fair dice: $\mathcal{P} = \{1, 2, 3, 4, 5, 6\}$

$$\int_{\mathcal{P}} f dP = \frac{1}{6} \sum_{i=1}^6 f(i) \quad (1.1)$$

- Particle in a box: $\mathcal{P} = [0, L]^3$, uniform dP

$$\int_{\mathcal{P}} f dP = \frac{1}{L^3} \int_{[0,L]^3} f d^3x \quad (1.2)$$

Expectation value: Probability space (\mathcal{P}, dP) , observable f

$$\langle f \rangle := \int_{\mathcal{P}} f dP \quad (1.3)$$

Distribution of observable: (\mathcal{P}, dP) given, then $(f(\mathcal{P}), f(dP))$ is a new probability space

$$\langle g \rangle_{f(\mathcal{P})} = \int g \circ f dP \quad (1.4)$$

Covariance and other moments:

$$\text{Cov}(f, g) = \langle fg \rangle - \langle f \rangle \langle g \rangle \quad (1.5)$$

$$\text{Var}(f) = \text{Cov}(f, f) \quad (1.6)$$

Covariance measures failure of multiplicativity. Variance measures „spread“ the distribution of higher moments

$$\langle f^m \rangle, \langle (f - \langle f \rangle)^m \rangle, m = 3, 4, \dots \quad (1.7)$$

Law of large numbers:

x_1, x_2, \dots : Independent identically distributed observables.
 Let $\langle x_i \rangle = e$, then make new probability space:

$$\bar{x} : \lim_{n \rightarrow \infty} \frac{1}{n} (x_1 + x_2 + \dots + x_n) \quad (1.8)$$

It holds that $\bar{x} = e$ almost surely (whatever that evs).

Important lesson: Expectation value \cong average of repeated measurements.

Remarks:

- For classical physics:
 - \mathcal{P} : Phase space
 - dP : State of the system
- Random variables \equiv observables \rightarrow Can choose:

$$dP = f(p_0, p) dP \quad (1.9)$$

for some p_0

- Sometimes expectation values are probabilities

$$\langle \chi_{\mathcal{R}} \rangle = \int_{\mathcal{R}} dP = \text{Prob}(p \in \mathcal{R}) \quad (1.10)$$

$$\mathcal{R} \subseteq \mathcal{P}$$

1.2 Hilbert spaces, operators

Vector spaces are $\mathbb{F} \begin{cases} \mathbb{C} \\ \mathbb{R} \end{cases}$

Scalar product: $\langle \circ, \circ \rangle : v \times v \rightarrow \mathbb{F}$

- (conjugate) symmetric: $\langle x, y \rangle = \overline{\langle x, y \rangle}$
- Linearity: $\langle x, y + \lambda z \rangle = \langle x, y \rangle + \lambda \langle x, z \rangle$
- Positive definite: $\langle x, x \rangle \geq 0$, $\langle x, x \rangle = 0 \Rightarrow x = 0$

Norm: $\|v\| = \sqrt{\langle v, v \rangle}$

CS-inequality: $|\langle x, y \rangle| \leq \|x\| \cdot \|y\|$

Hilbert-space: \mathbb{F} -vector space, together with scalar product, complete in $\|\cdot\|$ -top

Examples:

- $\mathcal{L}^2(\mathbb{R}^3, d^3x)$, $\langle f, g \rangle = \int_{\mathbb{R}^3} \bar{f}(x)g(x) d^3x$
- $l^2(\mathbb{C}) = \begin{cases} \text{square summable} \\ \text{cases} \end{cases} = \langle (c_n), (d_n) \rangle = \sum_{k=1}^{\infty} \bar{c}_k d_k$
- \mathbb{C}^n , $\langle \underline{x}, \underline{y} \rangle = \sum_{k=1}^n \bar{x}_k y_k$

Hilbert spaces are classified by size of basis (aka. dimension). Same dimension evs that the Hilbert-spaces are isomorphic (Here \mathcal{L}^2 is isomorphic to l^2 but they are not isomorphic to \mathbb{C}^n)

Orthogonal-basis: Basis $\{b_i\}$ with $\langle b_i, b_j \rangle = \delta_{ij}$

Bra-Ket: with $v \in \mathcal{H}$ as $|v\rangle$ („Ket“) linear form (linear map to \mathbb{F} for fixed w

$$v \mapsto \langle w, v \rangle \quad (1.11)$$

denoted by $\langle w|$ („Bra“) then

$$\langle w| (v) \equiv \langle w| (|v\rangle) \equiv \langle w|v \equiv \langle w, v \rangle \quad (1.12)$$

Direct sum: Given some index set I , \mathbb{F} -vector spaces V_i , $i \in I$ then

$$\bigoplus_{i \in I} v_i = \{(v_i)_{i \in I} | v_i \in V_i, \text{ finitely many } v_i \text{ non-zero}\} \quad (1.13)$$

because \mathbb{F} -vector spaces. For $\dim(V_i) < \infty$, $|I| < \infty$ holds

$$\dim \left(\bigoplus_i V_i \right) = \sum_i \dim(V_i) \quad (1.14)$$

If V_i are Hilbert-spaces, \bigoplus becomes Hilbert space via

$$\langle (v_i), (w_i) \rangle_{\bigoplus} = \sum_i \langle v_i, w_i \rangle_{V_i} \quad (1.15)$$

Example: $\mathbb{C}^n \bigoplus \mathbb{C}^m = \mathbb{C}^{n+m}$

$$\begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} \quad \begin{pmatrix} d_1 \\ \vdots \\ d_m \end{pmatrix} \rightarrow \begin{pmatrix} c_1 \\ \vdots \\ c_n \\ d_1 \\ \vdots \\ d_m \end{pmatrix} \quad (1.16)$$

Operators: Linear maps between vector (Hilbert-) spaces.

Examples:

- $\mathbb{C}^n \rightarrow \mathbb{C}^m$, $f(\underline{x}) = \underline{Mx}$, $M \in M(m \times n, \mathbb{C})$
- Momentum operator

$$p_k \frac{\hbar}{i} \frac{\partial}{\partial x_k} \text{ on } \mathcal{H} = \mathcal{L}^2(\mathbb{R}^3, d^3x) \quad (1.17)$$

Expectation values: Operators \equiv observables in QM. For A operator on \mathcal{H} , $\psi \in \mathcal{H}$

$$\langle A \rangle_\psi = \frac{1}{\|\psi\|} \langle \psi, A\psi \rangle \quad (1.18)$$

is interpreted exactly the same as expectation value in stochastics. Also

$$\text{Var}_\psi(A) = \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2 \quad (1.19)$$

interpreted as width of distribution of observable A .

First: Nuisance unbounded operators

Bounded (continuous) operator: $A : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ bounded.

$$\Leftrightarrow \exists c > 0 \quad \|Av\|_2 \leq c\|v\|_1 \quad \forall v \in \mathcal{H}_1 \quad (1.20)$$

$$A \text{ bounded} \Leftrightarrow A \text{ continuous} \quad (1.21)$$

For ∞ -dim \mathcal{H}_1 and \mathcal{H}_2 all operators are bounded:

Surprising: For ∞ -dim. \mathcal{H} -spaces there are unbounded operators.

Problem: Unbounded operators can not be defined on entire \mathcal{H} -space. Operator A , with $\text{dom}(A)$, the *domain* of A .

Example: x^i , p_k , $i, k = 1, 2, 3$ unbounded on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$

Schwartz functions: $S(\mathbb{R}^3)$: smooth, decaying quicker than any polynomial, same derivatives

\rightarrow convenient dense domain for x^i , p_k

Adjoint operator: Idea: $\langle v, Aw \rangle := \langle A^\dagger v, w \rangle$.

More precisely: For $A : \mathcal{H}_1 \rightarrow \mathcal{H}_2$, $\text{dom}(A) \subset \mathcal{H}_1$, dense

- $\text{dom}(A^\dagger) = \{w \in \mathcal{H}_2 | \exists z(w) \in \mathcal{H}_1 : \langle w, Av \rangle = \langle z(w), v \rangle \forall v \in \text{dom}(A)\}$
- $A^\dagger := z(w)$

Important cases:

- $A^\dagger = A^{-1}$: Unitary operation
- $\text{dom}(A^\dagger) = \text{dom}(A)$, $A^\dagger|_{\text{dom}(A)} = A$: Symmetric operation
- $\text{dom}(A^\dagger) = \text{dom}(A)$: $A^\dagger = A$: Selfadjoint operation

Projectors: Given $v, w \in \mathcal{H}$, how to approximate w by v ?

$\lambda \in \mathbb{C}$ such that $\|\lambda v - w\| \stackrel{!}{=} \min \rightarrow$ unique solution for λ . $P_v(w) = \lambda v$ is called projection of w onto the subspace spanned by v

$$P_v(w) = \underbrace{\frac{\langle v, w \rangle}{\|v\|^2}}_{\lambda} v = \frac{1}{\|v\|^2} |v\rangle \langle v| w \quad (1.22)$$

Linear operation generalizes to projection onto subspace $h \subset \mathcal{H}$:

$$v \in h \text{ such that } \|v - w\| \stackrel{!}{=} \min \quad (1.23)$$

For $\{b_i\}$ ONB of h :

$$P_h(\circ) = \sum_i \langle b_i, \circ \rangle b_i = \sum_i |b_i\rangle \langle b_i| \quad (1.24)$$

One finds:

$$P_h^2 = \sum_{ij} |b_i\rangle \underbrace{\langle b_i | b_j \rangle}_{\delta_{ij}} \langle b_j| = \sum_i |b_i\rangle \langle b_i| = P_h \quad (1.25)$$

And also:

$$P_h^\dagger = P_h \quad (1.26)$$

$\Rightarrow P_h$ is uniform.

Projections correspond to yes/no questions („proposition“). Sometimes useful: If $\{b_i\}$ is ONB for entire \mathcal{H} , $\mathbb{1}_{\mathcal{H}} = P_{\mathcal{H}} = \sum_i |b_i\rangle \langle b_i|$. Can use this to write formally:

$$A = \mathbb{1}_{\mathcal{H}} A \mathbb{1}_{\mathcal{H}} = \sum_{kl} |b_k\rangle \langle b_k | A | b_l \rangle \langle b_l| = \sum_{kl} \langle b_k | A b_l \rangle |b_k\rangle \langle b_l| \quad (1.27)$$

Uncertainty relations: A, B on \mathcal{H} , $A^\dagger = A$, $B^\dagger = B$, $\psi \in \mathcal{H}$, $\|\psi\| = 1$

$$|\langle AB \rangle_\psi|^2 = |\langle A\psi | B\psi \rangle|^2 \leq \langle A^2 \rangle_\psi \langle B^2 \rangle_\psi \quad (1.28)$$

$$\operatorname{Re}(\langle AB \rangle_\psi) = \frac{1}{2} \langle AB + BA \rangle_\psi := \frac{1}{2} [A, B]_+ \quad (1.29)$$

$$\operatorname{Im}(\langle AB \rangle_\psi) = \frac{1}{2i} \langle [A, B] \rangle_\psi \quad (1.30)$$

$$\text{So } \langle A^2 \rangle_\psi \langle B^2 \rangle_\psi \geq \frac{1}{4} \left(\langle [A, B]_+ \rangle_\psi^2 - \langle [A, B] \rangle_\psi^2 \right) \geq \frac{1}{4} |\langle [A, B] \rangle_\psi|^2 \quad (1.31)$$

$$\text{Replace } A \mapsto A - \langle A \rangle_\psi, \quad B \mapsto B - \langle B \rangle_\psi \quad (1.32)$$

$$\Rightarrow \operatorname{Var}(A)_\psi \cdot \operatorname{Var}(B)_\psi \geq \frac{1}{4} |\langle [A, B] \rangle_\psi|^2 \quad (1.33)$$

1.3 Eigenvalues, eigenvectors, spectrum

Eigenvalue, eigenvector: A operation on \mathcal{H} . If $\psi \in \mathcal{H}$, $\lambda \in \mathbb{C}$ solve

$$A\psi = \lambda\psi \quad (1.34)$$

then λ is called „eigenvalue“ and ψ is called „eigenvector“.

- $\{\text{eigenvalues of } A\} =: \operatorname{spec}_{pp}(A)$
- $\mathcal{H}_\lambda = \{\psi \in \mathcal{H} | A\psi = \lambda\psi\}$

Properties: A operation on \mathcal{H} , λ eigenvalue of A , then

- $A = A^\dagger \Rightarrow \lambda \in \mathbb{R}$
- $A = A^{-1} \Rightarrow \lambda \in \mathbb{C}$
- $A^2 = A \Rightarrow \lambda \in \{0, 1\}$
- $A^2 = 1 \Rightarrow \lambda \in \{-1, +1\}$
- A invertible $\Rightarrow \lambda^{-1}$ eigenvalue of A^{-1}

For $A = A^\dagger$ or $A = A^{-1}$: $\mathcal{H}_\lambda \perp \mathcal{H}_{\lambda'}$ for $\lambda \neq \lambda'$

Assumption: A operator such that

$$\mathcal{H} = \bigoplus_{\lambda \in \operatorname{spec}_{pp}(A)} \mathcal{H}_\lambda \quad (1.35)$$

then there is ONB of eigenvectors

$$\left. \begin{array}{l} A|\lambda, i_\lambda\rangle = \lambda|\lambda, i_\lambda\rangle \\ \langle \lambda, i_\lambda | \lambda', i'_{\lambda'} \rangle = \delta_{\lambda\lambda'} \end{array} \right\} \lambda \in \operatorname{spec}_{pp}(A), \quad i_\lambda \in \{1, 2, \dots, \dim(\mathcal{H}_\lambda)\} \quad (1.36)$$

Now rewrite expectation value

$$\langle A \rangle_\psi = \frac{1}{\|\psi\|^2} \langle \psi | A \psi \rangle = \frac{1}{\|\psi\|^2} \sum_{\lambda, i_\lambda} \sum_{\lambda', i'_{\lambda'}} \langle \psi | \lambda, i_\lambda \rangle \underbrace{\langle \lambda, i_\lambda | A | \lambda', i'_{\lambda'} \rangle}_{\lambda \delta_{\lambda\lambda'} \delta_{i_\lambda i'_{\lambda'}}} = \quad (1.37)$$

$$\sum_{\lambda, i_\lambda} \lambda \frac{|\langle \psi | \lambda, i_\lambda \rangle|^2}{\|\psi\|^2} =: \sum_{\lambda \in \text{spec}_{pp}(A)} \lambda P_\psi(\lambda) \quad (1.38)$$

with

$$P_\psi(\lambda) = \sum_{i_\lambda} \frac{|\langle \psi | \lambda, i_\lambda \rangle|^2}{\|\psi\|^2} = \langle P_{\mathcal{H}_\lambda} \rangle_\psi \quad (1.39)$$

then $P_\psi(\lambda)$ is probability measure on $\text{spec}_{pp}(A)$ with $\text{spec}_{pp}(A) \geq 0$.

$$\sum_{\lambda} P_\psi(\lambda) = \left\langle \sum_{\lambda} P_{\mathcal{H}_\lambda} \right\rangle_\psi = \langle \mathbb{1}_{\mathcal{H}} \rangle_\psi = 1 \quad (1.40)$$

$$\frac{\|P_{\mathcal{H}_\lambda}\|}{\|\psi\|^2} = P_\psi(\lambda) \geq 0 \quad (1.41)$$

So after all it's the stochastic expectation value.

$$\langle A \rangle_\psi = \sum_{\lambda \in \text{spec}_{pp}(A)} \lambda P_\psi(\lambda) \quad (1.42)$$

Get rid of assumption \rightarrow generalize notion of spectrum.

Spectral calculus: For A fulfilling an (I.20) (whatever equ. this is...), f continuous bounded on $\text{spec}_{pp}(A)$ define $f(A)$ on \mathcal{H} :

$$f(A) |\lambda, i_\lambda\rangle := f(\lambda) |\lambda, i_\lambda\rangle \quad (1.43)$$

Remark: $\langle f(A) \rangle_\psi = \sum_{\lambda} f(\lambda) P_\psi(\lambda)$

So functions of A behave like classical random variables on same probability space.

Spectrum:

$$\text{res}(A) = \{\lambda \in \mathbb{C}, (A - \lambda \mathbb{1}) \text{ has bounded inverse}\} \quad (1.44)$$

$$\text{spec}(A) = \mathbb{C} \setminus \text{res}(A) \quad (1.45)$$

Obviously $\text{spec}_{pp}(A) \subseteq \text{spec}(A)$ but sometimes no equality!

Example: Position operator x^k with $k = 1, 2, 3, \dots$:

$\frac{1}{x^k - \lambda}$ bounded for $\lambda \in \mathbb{C} / \mathbb{R}$, unbounded for $\lambda \in \mathbb{R}$, so $\text{spec}(x^k) = \mathbb{R}$.

Spectral theorem: (for self-adjoint, bounded operators)

For A s.a. bounded operator on \mathcal{H} :

- measures $d\mu$ on \mathbb{R} (concentrated on $\text{spec}(A)$)
- unitary map U , $N \in \mathbb{N} \cup \infty$:

$$U : \mathcal{H} \rightarrow \bigoplus_{i=1}^N \mathcal{L}^2(\mathbb{R}, d\mu_i) \quad (1.46)$$

$$\text{such that } (UAU^{-1}) \bigoplus_{i=1}^N \psi_i(\lambda) = \bigoplus_{i=1}^N \lambda \psi_i(\lambda) \quad (1.47)$$

Remarks:

- for $\text{spec}(A) = \text{spec}_{pp}(A)$: $d\mu_i(\lambda) = \sum_{\alpha \in \text{spec}(A)} \delta(\lambda, \alpha) d\lambda$
 $U|\alpha, i_\alpha\rangle = \bigoplus_{j=1}^N \delta_{j, i_\alpha} \delta_{\lambda, \alpha}$
- x on $\mathcal{L}^2(\mathbb{R}, dx)$: $U = \mathbb{1}$, $N = 1$, $d\mu = dx$
- p on $\mathcal{L}^2(\mathbb{R}, dx)$: $U = \mathcal{F}$, $N = 1$, $d\mu = dx$
- x^k on $\mathcal{L}^2(\mathbb{R}^3 d^3x)$: $N = \infty$
 For definiteness : $k = 3, x^3 = t$
 Pick ONB $\{b_i(x, y)\}$ of $\mathcal{L}^2(\mathbb{R}^2, dx dy)$
 $\rightarrow \psi \in \mathcal{L}^2(\mathbb{R}^2, dx dy dz)$: $\psi(x, y, z) = \sum_i(x, y) \psi_i(z)$
 with $\psi_i(z) \int dx dy \bar{b}_i(x, y) \psi(x, b, z)$
 then $U\psi = \bigoplus_{i=1}^\infty \psi_i(z) \in \otimes_i \mathcal{L}^2(\mathbb{R}, dz)$

Spectral calculus: $A \rightarrow f(A)$, $\lambda \psi_i(\lambda) \rightarrow f(\lambda) \psi_i(\lambda)$

$$(Uf(A)U^{-1}) \bigoplus \psi_i(\lambda) = \bigoplus_i f(\lambda) \psi_i(\lambda) \quad (1.48)$$

Expectation values: A as above, $\psi \in \mathcal{H}$

$$\langle f(A) \rangle_\psi = \langle Uf(A)U^{-1} \rangle_{U\psi} \quad (1.49)$$

$$= \int_{\text{spec}(A)} f(\lambda) dP_\psi(\lambda) \quad (1.50)$$

with $dP_\psi(\lambda) = \sum_{i=1}^N |\psi_i\rangle^2(\lambda) \frac{1}{\|\psi\|^2} d\mu_i(\lambda)$

Remark: Example (1) continued $dP_\psi(x) = \frac{|\psi|^2(x)}{\|\psi\|^2} dx$

Control:

$$dP_\psi(z) = \sum_i \langle \psi | b_i \rangle_{\mathcal{L}^2(\mathbb{R}^2)} \cdot \langle b_i | \psi \rangle_{\mathcal{L}^2(\mathbb{R}^2)} \frac{1}{\|\psi\|^2}(z) dz \quad (1.51)$$

$$= \langle \psi | \psi \rangle_{\mathcal{L}^2(\mathbb{R}^2)}(z) \frac{1}{\|\psi\|^2} dz = \frac{1}{\|\psi\|^2} \left(\int dx \int dy |\psi|^2(x, y, z) dz \right) \quad (1.52)$$

Theorem: For $A = A^\dagger$, $B = B^\dagger$ with $[A, B] = 0$ there is unitary $U : \mathcal{H} \rightarrow \bigoplus_i \mathcal{L}^2(\mathbb{R}, d\mu_i)$ such that

$$(UAU^{-1}) \bigoplus_i \psi_i(\lambda) = \bigoplus_i f_A(\lambda) \psi_i(\lambda) \quad (1.53)$$

$$(UBU^{-1}) \bigoplus_i \psi_i(\lambda) = \bigoplus_i f_B(\lambda) \psi_i(\lambda) \quad (1.54)$$

$$(1.55)$$

If $[A, B] \neq 0$, it is impossible to find such a decomposition.

1.4 Principles of Quantum theory

1. States: described by vectors in Hilbert-spaces.

Note: $v \in \mathcal{H}$ and $\lambda v, \lambda \in \mathbb{C} / \{0\}$ describe the same physical state!

2. Observables: represented by s.a. operators.

3. Predictions:

- Possible values of A in a measurement are given by $\text{spec}(A)$
- For a system in state ψ , probability distributions of measurements by $dP_\psi(\lambda)$

4. Time evolution: Linear Map $\mathcal{H} \rightarrow \mathcal{H}$, $v \mapsto Tv$. At least two cases:

- unitary time evolution:

$$Tv = U(t, t_0)v \text{ with } U(t, t_0)^\dagger = U^{-1}(t, t_0) \quad (1.56)$$

U is obtained a solution of

$$H(t)U(t, t_0) = i\hbar \frac{\partial}{\partial t} U(t, t_0), \quad U(t, t_0) = \mathbb{1} \quad (1.57)$$

- (strong) measurement: $Tv = Pv$ for some projector P :
For measuring „ $A \in \mathcal{M} \subset \text{spec}(A)$ “
 $P = \chi_\mu(A)$

Note: More general description of measurements exist („weak measurement“)

Remarks:

- Nontrivial part of (2.) is association

$$\underbrace{\theta}_{\text{classical}} \leftrightarrow \underbrace{\hat{\theta}}_{\text{quantum}} \quad (1.58)$$

„→“: strictly speaking guessing

„←“: well defined problem („classical problem“)

- physical states are in 1-1 correspondence to *rays*

$$\mathcal{H} \supset [\psi] = \{\lambda\psi | \lambda \in \mathbb{C} / \{0\}\} \quad (1.59)$$

1.5 Further tools

Relation between selfadjoint \leftrightarrow unitary : For $A = A^\dagger$
can show from (26) :

$$(f(A))^\dagger = \bar{f}(A) \quad (1.60)$$

$$f_1(A) \cdot f_2(A) = (f_1 \cdot f_2)(A) \quad (1.61)$$

Apply (31) to $f(A) = e^{ikA}$, $k \in \mathbb{R}$:

$$(e^{ikA})^\dagger = e^{-ekA} \quad (1.62)$$

and (32) for $f_1 = f$, $f_2 = \bar{f}$

$$e^{-ikA} e^{ikA} = \mathbb{1}_{\mathcal{H}}(A) = \mathbb{1}_{\mathcal{H}} \quad (1.63)$$

So e^{ikA} is unitary. For $U_k = e^{ikA}$

$$U_k \cdot U_{k'} = U_{k+k'} \text{ and } \lim_{\epsilon \rightarrow 0} U_{k+\epsilon} \psi = U_k \psi \quad (1.64)$$

Map $\mathbb{R} \ni k \mapsto U_k$ unitary, $U_0 = \mathbb{1}$ with (1.64): *One parameter unitary group* (1PUG)

Stone's theorem : Every 1PUG U_k is of the form

$$U_k = e^{ikA} \quad (1.65)$$

for some s.a. operator A . Can find A by differentiating

$$\left. \frac{1}{i} \frac{d}{dk} \right|_{k=0} U_k \psi = A\psi \quad (1.66)$$

A is called *generator* of U_k

Examples

- Time independent Hamiltonian H

$$U_t := e^{-\frac{itH}{\hbar}} \quad (1.67)$$

is 1PUG. Then:

$$i\hbar \frac{d}{dt} U_t = H U_t \quad (1.68)$$

$$(1.69)$$

$\Rightarrow U_t \equiv U(t, 0)$ is the time evolution operator.

- Translation:

$$\left(T_{\vec{\delta}\psi} \right) (\vec{x}) := \psi(\vec{x} - \vec{\delta}) \quad (1.70)$$

Then:

$$T_{\vec{\delta}_1} T_{\vec{\delta}_2} = T_{\vec{\delta}_1 + \vec{\delta}_2}, \quad \langle T_{\vec{\delta}} \psi | \Phi \rangle = \langle \psi | T_{-\vec{\delta}} \Phi \rangle \quad (1.71)$$

So $T_{\vec{\delta}}$ is unitary group (3 separate 1PUG). Can also check continuity. Generator:

$$\left. \frac{1}{i} \frac{d}{d\delta^j} T_{\vec{\delta}} \psi(x) \right|_{\vec{\delta}=0} = \frac{1}{i} (-1) \frac{dx^j}{\psi}(\vec{x}) = -\frac{1}{\hbar} p_j \psi(\vec{x}) \quad (1.72)$$

Thus:

$$T_{\vec{\delta}} = \exp \left(-\frac{i}{\hbar} \vec{\delta} \cdot \vec{p} \right) \quad (1.73)$$

Tensor product: For two vector spaces V and W : $V \otimes W$.

Consists of formal linear combinations

$$x = \sum_i \lambda_i (v_i, w_i) \quad \lambda_i \in \mathbb{F}, \quad v_i \in V, w_i \in W \quad (1.74)$$

subject to rules:

- $(v_1 + v_2, w) = (v_1, w) + (v_2, w)$
- $(v, w_1 + w_2) = (v, w_1) + (v, w_2)$
- $\lambda(v, w) = (\lambda v, w) = (v, \lambda w), \quad \lambda \in \mathbb{F}$

also write $(v, w) \equiv v \otimes w$. If $\dim V, W < \infty$:

$$\dim(V \otimes W) = \dim(V) \cdot \dim(W) \quad (1.75)$$

For basis $\{v_i\}$ of V , $\{w_i\}$ of W then $\{v_i \otimes w_k\}$ is basis of $V \otimes W$.

If V, W are Hilbert-spaces then we can make $V \otimes W$ a Hilbert-space via

$$\langle v_1 \otimes w_1 | v_2 \otimes w_2 \rangle_{\otimes} = \langle v_1 | v_2 \rangle_V \cdot \langle w_1 | w_2 \rangle_W \quad (1.76)$$

$$\left. \begin{array}{l} A \text{ operator on } V \\ B \text{ operator on } W \end{array} \right\} \rightarrow A \otimes B \text{ on } V \otimes W \text{ by } A \otimes B(v \otimes w) := (Av) \otimes (Bw) \quad (1.77)$$

Example:

- System 1: $\{v_i\}$ ONB of V with $H_1 v_i = E_i^1 v_i$
 System 2: $\{w_j\}$ ONB of W with $H_2 w_j = E_j^2 w_j$
 Combine into one system
 - non-interacting: $H = H_1 \otimes \mathbb{1}_W + \mathbb{1}_V \otimes H_2$ Hamiltonian of combined system
 - interacting: $H = H_1 \otimes \mathbb{1}_W + \mathbb{1}_V \otimes H_2 + H_I$
 H_I : interaction, $H_I = \sum_k A_k \otimes B_k \cdot \left(\text{Coulomb} \sim \frac{1}{|\vec{x}_1 \otimes \mathbb{1} - \mathbb{1} \otimes \vec{x}_2|} \right)$
- Two spinless particles (special case of above) (distinguishable)

$$\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3, d^3x) \otimes \mathcal{L}^2(\mathbb{R}^3, d^3x) \quad (1.78)$$

Useful fact:

$$\mathcal{L}^2(\mathbb{R}^m, d^m x) \otimes \mathcal{L}^2(\mathbb{R}^n, d^n x) \simeq \mathcal{L}^2(\mathbb{R}^{m+n}, d^{m+n} x) \quad (1.79)$$

Therefore can describe the two particle systems by wave-functions

$\psi_{\vec{x}_1, \vec{x}_2}$ on \mathbb{R}^6 . (Coulomb: $\sim \frac{1}{|\vec{x}_1 - \vec{x}_2|}$)

So note: Interpretation of „ \otimes “:

- Two systems with Hilbert-spaces V, W from joint system with states of combined system in $V \otimes W$.
 - Mathematical \oplus and \otimes work almost like the multiplication and addition of numbers or functions with \mathbb{F}, \emptyset as neutral elements. (ex: $V \otimes \mathbb{F} = V$)
- Electron with spin:

$$\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3, d^3x) \otimes \mathbb{C}^2 \quad (1.80)$$

Note that

$$\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3) \otimes (\mathbb{C} \oplus \mathbb{C}) \quad (1.81)$$

$$= \mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C} \oplus \mathcal{L}^2(\mathbb{R}^3) \quad (1.82)$$

$$= \mathcal{L}^2(\mathbb{R}^3) \otimes \mathcal{L}(\mathbb{R}^3) \quad (1.83)$$

Therefore can describe the electron by 2-component wave function

$$\psi_{\vec{x}} \equiv \begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \end{pmatrix} \quad (1.84)$$

1.6 Generalized states

Consider statistical mixture of quantum states

$$\mathcal{H} \ni \psi_i, \text{ with probability } p_i \quad (1.85)$$

Described by *density operator (or density matrix)*

$$\rho = \sum_j \frac{p_j}{\|\psi_j\|^2} |\psi_j\rangle\langle\psi_j| \quad (1.86)$$

Indeed for $\{b_i\}$ an ONB, A an observable

$$\langle A \rangle_\rho := \text{tr}(\rho A) := \sum_i \langle b_i | \rho A | b_i \rangle = \sum_j p_j \langle A \rangle_{\psi_j} \quad (1.87)$$

Must have $\sum \frac{p_j}{\|\psi_j\|}$ absolutely convergent, A bounded for it to make sense. Operators of form 1.86 have

$$\text{tr}(\rho) = 1, \rho > 0 \text{ and } \text{spec}(\rho) = \text{spec}_{pp}(\rho). \quad (1.88)$$

Vice versa, any operator satisfieng (1.88) can be written as (1.86).

Time evolution:

$$\rho(t) = U(t, t_0) \rho U(t, t_0)^{-1} \quad (1.89)$$

$$\rho'(t) = \frac{P\rho P}{\text{tr}(\rho P)} \quad (1.90)$$

Important special case:

$$\rho = \frac{1}{\|\Psi\|} |\Psi\rangle\langle\Psi| \quad (1.91)$$

Then ρ is equivalent in all aspects to $\Psi \in \mathcal{H}$. Often one calls states of form (1.91) “pure” and of form (1.86) “mixed”.

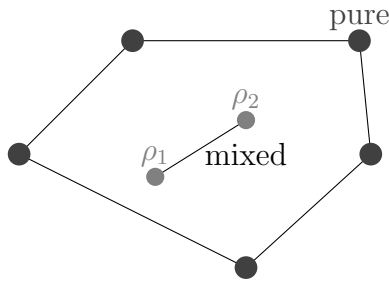


Figure 1: Sketch of pure and mixed states

However: For any ρ on \mathcal{H} there is \mathcal{H}' in which ρ has form (1.91). Better Definition: Consider:

$$\chi = c_1 \rho_1 + c_2 \rho_2 \text{ with } c_1, c_2 \geq 0 \text{ and } c_1 + c_2 = 1 \quad (1.92)$$

where ρ_1 and ρ_2 are density matrices. Then χ again is a density matrix. \Rightarrow space of states S is a convex space. Now given $\chi \in S$ if $\exists \rho_1, \rho_2 \in S \exists c_1, c_2 > 0$ according to (1.92) the state is “mixed” else the state is “pure” in a fundamental distinction.

Slight generalization:

Definition 1.1. Given a \mathbb{C} -Vectorspace A with $a, b \in A$ and $\lambda \in \mathbb{C}$. A $*$ -algebra has

1. Multiplication which is associative, and distributive: $(\lambda a)b = \lambda(ab)$
2. Map $*$, s.t. $a^{**} = a$, $(ab)^* = b^*a^*$ and $(\lambda a)^* = \bar{\lambda}a^*$

Example 1.1. Heisenberg algebra, generated by abstract objects $x, p, 1$ with:

$$[x, p] = i1, x^* = x, p^* = p, 1^* = 1, 1x = x \text{ and } 1p = p$$

State on $*$ -algebra: For A a $*$ -algebra with unit, lineat map $\omega : A \rightarrow \mathbb{C}$ with:

$$\omega(1) = 1, \omega(a^*) = \bar{\omega(a)}, \omega(a^*a) \geq 0 \forall a \in A$$

Definition 1.2. A representation of A is a linear map $\pi : A \rightarrow \mathcal{H}$ (Hilbert space) with

1. $\pi(ab) = \pi(a)\pi(b)$
2. $\pi(a)^* = \pi(a)^\dagger$

Theorem 1.2. (GNS construction) Given a state ω on an algebra A there is a representation π_ω on \mathcal{H}_ω and a $\Psi_\omega \in \mathcal{H}_\omega$ with $\omega(a) = \langle \pi_\omega(a)\Psi_\omega, \Psi_\omega \rangle$

1.7 Coupling to the EM-field

A particle with charge q in external EM field $\vec{E}(\vec{x}, t), \vec{B}(\vec{x}, t)$. Classically:

$$m\ddot{\vec{x}} = q\vec{E}(\vec{x}, t) + \frac{q}{c}\dot{\vec{x}} \times \vec{B}(\vec{x}, t)$$

For $\left\| \dot{\vec{x}} \right\| \ll c$ we get the Lagrange function

$$L = \frac{1}{2}m\dot{\vec{x}}^2 + \frac{q}{c}\dot{\vec{x}}\vec{A} - q\Phi \tag{1.93}$$

$$\text{with } \vec{B} = \nabla \times \vec{A}, \vec{E} = -\nabla\Phi - \frac{\partial \vec{A}}{\partial t} \tag{1.94}$$

And the gauge trafos:

$$\vec{A} \rightarrow \vec{A}' = \vec{A} + \nabla\Lambda \text{ and } \Phi \rightarrow \Phi' = \Phi - \frac{\dot{\Lambda}}{c} \tag{1.95}$$

Change L only by $\frac{d}{dt}\Lambda(\vec{x}(t), t)$.

Canonical formulation

$$\begin{aligned}\vec{p} &= \vec{p}_{\text{kin}} + \frac{q}{c}\vec{A}(\vec{x}, t) \quad (\vec{p}_{\text{kin}} = m\dot{\vec{x}}) \\ H &= \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\Phi\end{aligned}\quad (1.96)$$

Quantisation on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$ via $\hat{p} = \frac{\hbar}{i}\nabla$ and $\hat{x} = \vec{x}$.

Remark. • Kinematic momentum is non-commutative: $[p_j^{\text{kin}}, p_k^{\text{kin}}] = \frac{i\hbar q}{c} \sum_l \varepsilon_{jkl} B^l(\vec{x})$

- Aharonov-Bohm effect: Due to coupling to \vec{A} interference effect although $\vec{B} = 0$ in region accessible to particle.

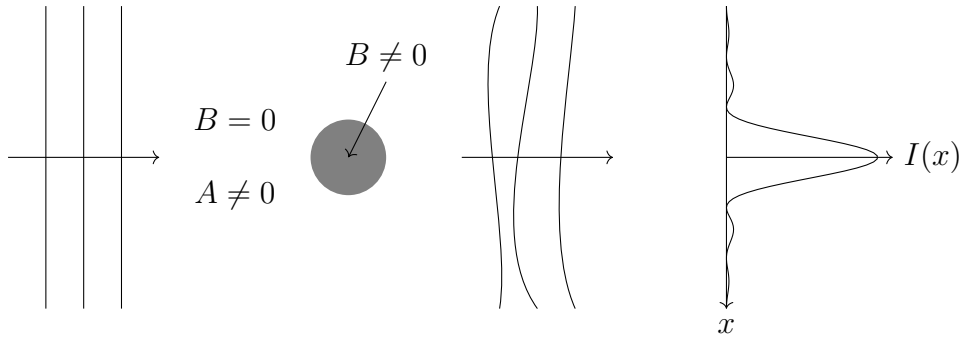


Figure 2: Aharonov Bohm effect

- Gauge transformations: if one changes \vec{A} one also needs to change the wave function

$$H\Psi = i\hbar\frac{\partial\Psi}{\partial t} \Leftrightarrow H'\Psi' = i\hbar\frac{\partial\Psi'}{\partial t}$$

with Λ the generator of the gauge trafo

$$H' = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}'\right)^2 + q\Phi' \quad \text{and} \quad \Psi'(\vec{x}, t) = \exp\left(\frac{iq\Lambda(\vec{x}, t)}{\hbar c}\right)\Psi(\vec{x}, t) \quad (1.97)$$

Only the expectation values are gauge invariant quantities (ex. $\vec{x}, \vec{p}_{\text{kin}}$)

Pauli equation

Charged particles with spin. This results in a magnetic moment

$$\vec{\mu} = \gamma\vec{S} = g\frac{q}{2m}\vec{S}. \quad (1.98)$$

Where γ is the gyro magnetic ratio and g the g -factor. The energy in the magnetic field is given as $U = -\frac{1}{c}\vec{\mu}\vec{B}$ and gives an additional term in H . Plugging this in the Schrödinger equation yields

$$\frac{1}{2m} \left[\left(\vec{p} - \frac{q}{c}\vec{A} \right)^2 - g\frac{q}{c}\vec{S}\vec{B} \right] \Psi + q\Phi\Psi = i\hbar\frac{\partial}{\partial t}\Psi. \quad (1.99)$$

This is also known as the Pauli equation. It will be shown that for an electron e^- one must have $g \approx 2$ as a consequence of the Lorentz-invariance.

2 Symmetries in Quantum Mechanics

Consideration of symmetries are a powerful tool.

- Continuous symmetry \leftrightarrow conservation laws
- Symmetries give degeneracies
- symmetries restrict (atomic) transitions
- way symmetries operate in QM connected to fundamental properties of matter (spin, boson/fermions)

2.1 Symmetries and unitary representations

Consider properties to come to precise definition!

1. Symmetries are operators on (or changes of description of) physical systems, hence in QM, symmetry g :

$$\pi_S(g) : \text{States} \rightarrow \text{states}, [v] \rightarrow \pi_S(g)([v]) \equiv [v'] \quad (2.1)$$

$$\pi_\sigma(g) : \text{Obs.} \rightarrow \text{obs.}, A \rightarrow \pi_\sigma(g)(A) = A' \quad (2.2)$$

2. Symmetries should leave predictions invariant!

$$|\langle v_1 | Av_2 \rangle|^2 = |\langle v'_1 | Av'_2 \rangle|^2 \text{ for } v'_i \in \pi_S(g)([v_i]) \quad (2.3)$$

3. Symmetries should respect time evolution:

$$\pi_\sigma(g)(U_t A U_t^{-1}) = U_t \pi_\sigma(g)(A) U_t^{-1} \quad (2.4)$$

where $U_t = U(t, t_0)$ is the time evolution operator.

4. Symmetries:

- can be concatenated: g_1, g_2 are symmetries so is $g_1 g_2$

- can not destroy information, so they must be invertible, and inverse should also be a symmetry
- trivial transition (do nothing) is a symmetry

If we make the (reasonable) assumption: concatenation of symmetries is associative, we can summarize: *Symmetries form a group*

Definition 2.1. A representation of a group G on a space S is an assignment $G \ni g \rightarrow \pi_S(g), \pi_S(g) : S \rightarrow S$ with

$$\pi_S(g_1) \circ \pi_S(g_2) = \pi_S(g_1 g_2) \quad (2.5)$$

$$\pi_S(\mathbb{1}) = \text{Id} \quad (2.6)$$

Then:

Definition 2.2. Symmetry of a QM system (\mathcal{H}, O, H) is a group G , with representations on S and σ that leave H invariant.

Remark. • From ((2.5), f) follows

$$\pi(g^{-1}) = \pi(g)^{-1} \quad (2.7)$$

- for a representation $\pi : G \rightarrow$ invertible lin. operator on V where V : a vector space:
(2.5) \Rightarrow (2.6)

Example 2.1. Translation:

- group: $G = (\mathbb{R}^3, +)$
- $\pi_S(\vec{\delta})[\Psi] = [T_{\vec{\delta}}\Psi]$
- one can also define: $\pi_\sigma(\vec{\delta})(A) \equiv T_{\vec{\delta}} A T_{\vec{\delta}}^{-1}$

Then, because of $T_{\vec{\delta}} T_{\vec{\delta}'} = T_{\vec{\delta} + \vec{\delta}'}$, π_S, π_σ fulfill (2.5). Moreover, for $H = \frac{\vec{p}^2}{2m}$ one can check $\pi_\sigma(\vec{\delta})(H) = H$. Finally one can check that (2.3) is fulfilled. Translations are symmetries of the free particle.

Definition 2.3. *Unitary representation of a group* is a representation where all $\pi(g)$ $g \in G$ are unitary operators.

Observation: π is unitary representation of G on \mathcal{H} of (\mathcal{H}, O, H) , with $\pi(g)H\pi(g)^{-1} = H$. Then get symmetry via

$$\pi_S(g)[v] \equiv [\pi(g)v] \text{ and } \pi_\sigma(g)(A) \equiv \pi(g)A\pi(g)^{-1} \quad (2.8)$$

Example 2.2. • Rotations: $SO(3) = \{M \in M(3 \times 3, \mathbb{R}), \det(M) = 1\}$ Multiplication: Matrix mult. Representation of $\mathcal{L}^2(\mathbb{R}, d^3x)$ via:

$$(\pi(R)\Psi)(\vec{x}) \equiv \Psi(R^{-1}\vec{x}) \quad (2.9)$$

check (2.5):

$$(\pi(R')\pi(R)\Psi)(\vec{x}) = \Psi(R^{-1}R'^{-1}\vec{x}) = (\pi(R'R)\Psi)(\vec{x})$$

Is it unitary?

$$\langle \varphi | \pi(R)\Psi \rangle = \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \Psi(\underbrace{R^{-1}\vec{x}}_{=\vec{x}'}) d^3x = \int_{\mathbb{R}^3} \bar{\varphi}(R\vec{x}') \Psi(\vec{x}') d^3x'$$

But: $\frac{\partial x^a}{\partial x'^a} = R_b^a$ with $\det(R) = 1$ thus: $\langle \varphi | \pi(R)\Psi \rangle = \langle \pi(R^{-1})\varphi | \Psi \rangle$, so

$$\pi(R)^\dagger = \pi(R^\dagger) = \pi(R)^{-1}.$$

- Parity: Spatial reflections at origin

$$P\vec{x} = -\mathbb{1}\vec{x} = -\vec{x} \quad (2.10)$$

Together with $\mathbb{1}$ form a group called S_2 . Unitary action on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$ via

$$(P\Psi)(\vec{x}) = \Psi(-\vec{x}) \quad (2.11)$$

- Particle exchange: Our particle \mathcal{H} -space $\mathcal{H}_1 = \mathcal{L}^2(\mathbb{R}^3, d^3x)$ N distinguishable particles:

$$\mathcal{H}_N = \underbrace{\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}_{N \text{ times}} \quad (2.12)$$

S_N : Group of permutations of N things. Unitary action on \mathcal{H}_N

$$\pi(\sigma)v_1 \otimes \cdots \otimes v_N = v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(N)} \quad (2.13)$$

Definition 2.4. (π, \mathcal{H}) representation of G , \mathcal{H}_1 proper subspace!

1. $\mathcal{H}_1 \subset \mathcal{H}$ invariant subspace $:\Leftrightarrow \pi(G)\mathcal{H}_1 \subseteq \mathcal{H}_1$
2. (\mathcal{H}, π) irreducible $:\Leftrightarrow \nexists$ nontrivial ($\neq \emptyset, \neq \mathcal{H}$) invariant subspace $\mathcal{H}_1 \subset \mathcal{H}$

Lemma 2.3. Complete reducibility: If we have

- unitary representation of G (π, \mathcal{H})
- $\mathcal{H}_1 \subset \mathcal{H}$ invariant
- $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_1^\perp$

then \mathcal{H}_1^\perp is invariant

Remark. irreducible unitary representations are the building blocks of general unitary representations.

Example 2.4. • $\mathcal{L}^2(\mathbb{R}^3, d^3x) \ni \Psi(\vec{x}) \equiv \Psi(|\vec{x}|)$ such Ψ span a 1-dim. sub-rep of rotation rep (2.9)

- Totally (anti-)symmetric states in \mathcal{H}_N (2.12) gives two different sub-reps. of (S_N, π) (2.13)
- Hydrogen $|nlm\rangle$: $\mathcal{H}_{ln} = \text{span}|n, l, m\rangle$: $m \in \{-l, -l+1, \dots, +l\}$ gives $2l+1$ dim subrep. more generally: for fixed j

$$\begin{aligned} |j, m\rangle m \in \{-j, -j+1, \dots, j\} \\ J^2|j, m\rangle \hbar^2 j(j+1)|j, m\rangle \\ J_3|j, m\rangle = \hbar m|j, m\rangle \end{aligned}$$

form an irred. rep. of the rotation group $SO(3)$.

Because $\pi(g)H\pi(g)^{-1} = H$, $\pi(g)$ leaves eigenspaces of H invariant.

Symmetries and eigenspaces:

$(\pi \mathcal{H})$ rep of G assume:

- $\pi(g)H\pi(g^{-1}) = H \forall g \in G$
- $\mathcal{H}_\lambda \subset \mathcal{H}$ eigenspan of H with eigenvalue λ

Then for $v \in \mathcal{H}_\lambda$

$$H\pi(g)v = \pi(g)H\pi(g)^{-1}\pi(g)v \quad (2.14)$$

$$= \pi(g)Hv = \lambda\pi(g)v \quad (2.15)$$

So \mathcal{H}_1 is invariant subspace. Two cases:

1. $(\pi|_{\mathcal{H}_\lambda}, \mathcal{H}_\lambda)$ is irreducible: Symmetry explains degeneracies.
2. $(\pi|_{\mathcal{H}_\lambda}, \mathcal{H}_\lambda)$ is reducible: accidental degeneracies

Example 2.5. Tut.: 3D H.O. Symmetric under rotations ($O(3)$)

This symmetry does not explain degeneracy.

Accidental or larger symmetry group?

$\rightarrow U(3)$ symmetry induced from $a_i \mapsto \sum_j U_{ij}a_j$, $i \in 1, 2, 3$
for $U \in U(3)$

Example 2.6. Isospin

Another example for postulating symmetries based on degeneracy. Proton and neutron (+ anti-particles)

- \sim same mass
- \sim same resonances
- \sim same strong interaction

Heisenberg + Wigner: Hamiltonian has *isospin* symmetry
 Ground state is 2-fold degenerate, spanned by

$$|p\rangle = |\uparrow\rangle \quad |n\rangle = |\downarrow\rangle \quad (I = \frac{1}{2}, I_3 = \pm\frac{1}{2}) \quad (2.16)$$

Can see with mesons, too:

$$|\pi^+\rangle, |\pi^0\rangle, |\pi^-\rangle \hat{=} |1, 1\rangle, |1, 0\rangle, |1, -1\rangle \quad (2.17)$$

for isospin states $|I, I_3\rangle$ analogous to $|j, j_2\rangle$ of angular momentum. Assumption of interaction Hamiltonian symmetric under this symmetry leads to prediction (Tut.).

Gal-hamm: Even bigger symmetry?

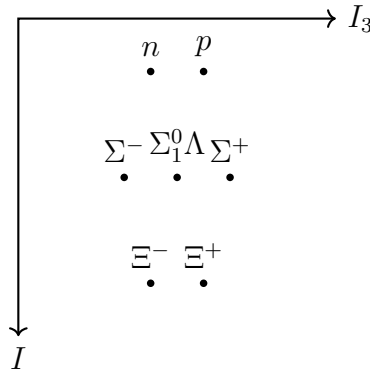


Figure 3: Isospin sketch

Multiplets correspond to irreducible representations of $SU(3)$
 \rightarrow (eventually) Quark model

2.2 Continuous symmetries

When symmetry group is smoothly parameterized, we speak of a continuous symmetry.

Example 2.7. Group of translations $(\mathbb{R}^3, +)$ acting via $T_{\vec{g}}$ on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$. Had seen:

$$T_{\vec{g}} = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{g}} \quad (2.18)$$

If $T_{\vec{g}}$ give rise to a symmetry, must leave

$$H = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{g}} H e^{+\frac{i}{\hbar}\vec{p}\cdot\vec{g}} \quad (2.19)$$

Differentiate with respect to δ^k at $\vec{g} = 0$: $k = 1, 2, 3$

$$0 = -\frac{i}{\hbar} p_k H + \frac{i}{\hbar} H p_k \Leftrightarrow [H, p_k] \quad (2.20)$$

So we have shown that \vec{p} is conserved. Holds more generally.

Principle 2.8. generators of continuous symmetries are conserved
 → make this more precise:

Matrix-Lie-Group Subgroups of $GL(n, \mathbf{F})$, that has smooth parametrization around $\mathbb{1}$, i.e., \exists map $\mathbb{R}^m \supset \mathcal{V} \mapsto G$ such that:

$$g : (t_1, \dots, t_m) \mapsto g(t_1, \dots, t_m) \in G \quad (2.21)$$

- 1-1 map between \mathcal{V} and neighbourhood $g(\mathcal{V})$ of $\mathbb{1}$
- smooth

Remark. • It follows that it has smooth parametrization everywhere

- $m =: \dim(G)$

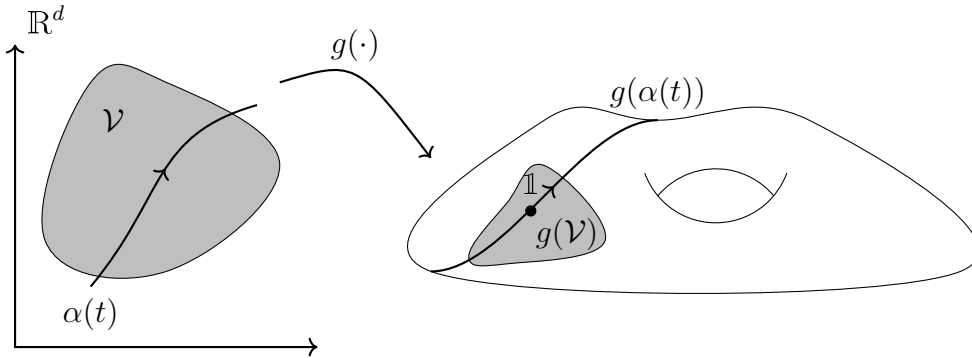


Figure 4: Lie-Group and Lie-Algebra

Each such group comes with a

Definition 2.5. *Matrix-Lie-Algebra:* Let

$$A = \left\{ \left. \frac{d}{dt} \right|_{t=0} g(\alpha(t)) \mid \alpha(t) \text{ curve through } \mathcal{V} \text{ with } g(\alpha(0)) = \mathbb{1} \right\} \quad (2.22)$$

- is a \mathbb{R} -vectorspace with basis $\left\{ \left. \frac{\partial}{\partial t} \right|_{\mathbb{1}} g(t_1, \dots, t_m) \right\}, i = 1, 2, \dots, m$
- becomes an algebra with product given by commutator:

$$a, b \in A \Rightarrow [a, b] \in A \quad (2.23)$$

For $h \in G$, $g(\alpha(t)) \equiv g(t)$ curve as above: $hg(t)h^{-1}$ again curve through $\mathbb{1}$ and

$$\left. \frac{\partial}{\partial t} \right|_{t=0} hg(t)h^{-1} = h\dot{g}(0)h^{-1} \in A \forall h \in G \quad (2.24)$$

Now I let $h(t)$ be a curve in G , and $h(0) = \mathbb{1}$ then

$$\left. \frac{d}{dt} \right|_{t=0} h(t)\dot{g}(0)h(t)^{-1} = [\dot{h}(0), \dot{g}(0)] \quad (2.25)$$

because (using $h(0) = \mathbb{1}$ we get) $0 = \left. \frac{d}{dt} \right|_{t=0} h(t)h(t)^{-1} = \dot{h}(0) + \dot{h}^{-1}(0)$. A is a vector space. So

$$\left. \frac{d}{dt} \right|_{t=0} \Lambda(t) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \Lambda(\epsilon) - \frac{1}{\epsilon} \dot{g}(0) \in A \text{ with } \Lambda(t) = h(t)\dot{g}(0)h(t)^{-1}$$

This algebra is called then Lie-Algebra of G .

The miracle: Can construct G from A up to global structure: For G *connected* matrix Lie Group

$$G = \{e^a, a \in A\} \quad (2.26)$$

and then product of G is completely encoded in $[\cdot, \cdot]$ on A :

$$e^a \cdot e^b = e^c \quad \text{with } e^a = \sum_{n=0}^{\infty} \frac{1}{n!} a^n \quad (2.27)$$

and

$$c = a + b + \frac{1}{2} [a, b] + \frac{1}{12} ([a, [a, b]] + [b, [b, a]]) + \text{higher orders} \quad (2.28)$$

(Baker, Campbell, Hausdorff)

Definition 2.6. Representations of a (matrix) Lie-algebra A are maps $\pi : A \rightarrow$ linear operators on V with $\pi([a, b]) = [\pi(a), \pi(b)]$

For a connected G : rep. Π of $G \rightarrow$ rep π of A .

$$\pi(\dot{g}(0)) := \left. \frac{d}{dt} \right|_{t=0} \Pi(g(t)) \quad (2.29)$$

For simply connected A we have \Leftarrow , too

$$\Pi(e^a) := e^{\pi(a)} \text{ with } a \in A \quad (2.30)$$

Now we can make the principles more precise.

Symmetries and conservation laws

Lie group A as symmetry group $\Rightarrow \pi(A)$ is a commutator algebra of conserved quantities:

$$0 = \frac{d}{dt} \Big|_{t=0} \Pi(e^{at}) H \Pi(e^{-at}) = \pi(a) t H - H \pi(a) t = [\pi(a), H]$$

Remark. If Π is unitary then π must be skew-adjoint $\pi(a)^\dagger = -\pi(a)$. Physicists call the self-adjoint $-i\pi(a)$ the generator.

2.3 Rotational symmetry $SO(3)$

Consider rotations around z :

$$g(t) = \begin{pmatrix} \cos(t) & \sin(t) & 0 \\ -\sin(t) & \cos(t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ which is a curve through } \mathbb{1}_{3 \times 3}.$$

With the Lie-algebra element $(a_3)_{ab} := (\dot{g}(0))_{ab} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{ab} = \epsilon_{3ab}$. We can do this analogous for x and y and get $(a_i)_{ab} = \epsilon_{iab}$. With this we can calculate

$$[a_i, a_j] = - \sum_k \epsilon_{ijk} a_k \quad (2.31)$$

In the representation on wave functions:

$$\begin{aligned} (\pi(a_3)\Psi)(\vec{x}) &= \frac{d}{dt} \Big|_{t=0} (\pi(g(t))\Psi)(\vec{x}) = \frac{d}{dt} \Big|_{t=0} \Psi \left(\begin{pmatrix} \cos t & -\sin t & 0 \\ \sin t & \cos t & 0 \\ 0 & 0 & 1 \end{pmatrix} \vec{x} \right) \\ &= \left(\frac{\partial \Psi}{\partial x^1} \right) (-x^2) + \left(\frac{\partial \Psi}{\partial x^2} \right) x^1 = \frac{i}{\hbar} (x^1 p_2 - x^2 p_1) \Psi = \frac{i}{\hbar} L^3 \Psi(\vec{x}) \end{aligned}$$

where $\vec{L} = \vec{x} \times \vec{p}$ is the *angular momentum*. In general we find

$$\pi(a_k) = \frac{i}{\hbar} L^k. \quad (2.32)$$

This is indeed a representation, as

$$[\pi(a_k), \pi(a_l)] = \frac{i}{\hbar} [L^k, L^l] = -\frac{1}{\hbar^2} \sum_m i \hbar \epsilon_{klm} L^m = \sum_m -\epsilon_{lkm} \pi(a_m) = \pi([a_k, a_l])$$

conforms to (2.31). Made use of the algebra of the angular momentum. The generators:

$$L^k = \frac{\hbar}{i} \pi(a_k) \text{ fulfill the well known} \quad (2.33)$$

$$[L^k, L^l] = i \hbar \sum_m \epsilon_{lkm} L^m \quad (2.34)$$

Remark. • The Lie algebra $SO(3)$ is given by the span of a_i with the commutator (2.31) as product.

- The Casimir of $SO(3)$: Let L^k as in (2.32) for some rep. π . We can form

$$\vec{L}^2 = \sum_i L^i L^i \text{ then } [L^a, \vec{L}^2] = \dots = 0 \quad (2.35)$$

Thus eigenspaces of \vec{L}^2 are invariant subspaces.

Irreducible representation of $SO(3)$

Theorem 2.9. Let (\mathcal{H}, π) be a irred. rep. of $SO(3)$, then there is a

$$j \in \frac{\mathbb{N}}{2} (= \left\{ 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \right\}) \text{ and ONB } |j, m\rangle, m \in \{-j, -j+1, \dots, j\} \quad (2.36)$$

$$\text{of } \mathcal{H} \text{ with } L^3 |j, m\rangle = \hbar m |j, m\rangle \text{ and } \vec{L}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle \quad (2.37)$$

Proof. • \vec{L}^2 must be proportional to $\mathbb{1}$, for π to be irreducible.

- \vec{L}^2 positive
Together: $\vec{L}^2 = \hbar^2 \lambda(\lambda+1) \mathbb{1}_{\mathcal{H}}$ with $\lambda \in \mathbb{R}_{0,+}$
- Ladder operators

$$L_{\pm} := L^1 \pm iL^2 \quad (2.38)$$

As $L^3 \Psi = \hbar m \Psi, m \in \mathbb{R}$, it follows that

$$L^3 L_{\pm} \Psi = \hbar(m \pm 1) \Psi \text{ and } \|L_{\pm} \Psi\|^2 = \hbar(j(j+1) - m(m \pm 1)) \|\Psi\|^2 \quad (2.39)$$

- Where the positivity of “ $\|\cdot\|$ ” gives (2.35) and (2.36)

□

This is the classification of all irred. reps of $SO(3)$. (Similar for a general Lie algebra)

Addition of angular momenta

For a general π , also $J^k = \frac{\hbar}{i} \pi(a_k)$. Given (π, \mathcal{H}) rep. of $SO(3)$:

1. Pick eigenstate $|j, m\rangle \in \mathcal{H}$ of \vec{J}^2 and J^3
2. Hit it with ladder operators to obtain basis of sub-rep. (irreducible) $(\mathcal{H}_j, \pi|_{\mathcal{H}_j})$
3. Repeat for $\mathcal{H}' = \mathcal{H}_j^{\perp}$

With this obtain the decomposition:

$$\mathcal{H} = \oplus_{j \in \mathbb{N}/2} \left(\oplus_{m=1}^j \mathcal{H}_j \right) \quad (2.40)$$

Now we do this for tensor products: $(\mathcal{H}_{(k)}, \pi_{(k)}) \rightarrow \mathcal{H} = \otimes_k \mathcal{H}_{(k)}$:

$$\vec{J}_{tot} := \sum_k \vec{J}_{(k)}, \vec{J}_{(k)} = \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{(k-1)\text{-times}} \vec{J}_{(k)} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \quad (2.41)$$

Since \otimes, \oplus are distributive, associative it suffices to consider:

$$\vec{J}_{tot} = \vec{J}^{(1)} + \vec{J}^{(2)} = \vec{J}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \vec{J}_2 \text{ with } \vec{J}_k := -i\hbar\pi_{jk}(\vec{a}) \text{ on } \mathcal{H}_k \quad (2.42)$$

$$\mathcal{H} = \mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}, \vec{J}_k := i\hbar\pi_{jk}(\vec{a}) \text{ on } \mathcal{H}_{j_k} \quad (2.43)$$

$$\vec{J}^{tot} := \vec{J}^{(1)} + \vec{J}^{(2)} = \vec{J}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \vec{J}_2 \quad (2.44)$$

\vec{J}^{tot} from representation of $\mathfrak{so}(3)$:

$$[J^{tot,a}, J^{tot,b}] = [J_1^a, J_1^b] \otimes \mathbb{1} + \mathbb{1} \otimes [J_2^a, J_2^b] \quad (2.45)$$

$$= i\hbar \sum_c \epsilon_{abc} (J_1^c \otimes \mathbb{1} + \mathbb{1} \otimes J_2^c) \quad (2.46)$$

$$= i\hbar \sum_c \epsilon_{abc} J^{tot,c} \quad (2.47)$$

This works the same way for any to representations of any Lie-algebra. Hence can decompose \mathcal{H} into irreducibles as in eq. (2.40). Let:

$$|m_1, m_2\rangle := |j_1, m_1\rangle \otimes |j_2, m_2\rangle \quad (2.48)$$

this is ONB of \mathcal{H} . Look for another ONB $|j, m\rangle$ such that

$$\left(\vec{J}^{tot} \right)^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle, \quad j^{tot,3} |j, m\rangle = m\hbar |j, m\rangle \quad (2.49)$$

Observe:

$$J_{tot}^3 |m_1, m_2\rangle = \hbar(m_1 + m_2) |m_1, m_2\rangle \quad (2.50)$$

Let:

- $m(j)$: # of j -irreducibles as in eq (2.40)
- $n'(m)$: degeneracy of $J^{tot,3}$ eigenvalue

Then

$$n'(m) = \sum_{j \geq |m|} k(j) \quad (2.51)$$

$$n'(m) - n'(m+1) = \left(\sum_{j \geq m} - \sum_{j \geq m+1} \right) n(j) = n(m) \quad (2.52)$$

Need to find $n'(m)$. For this, consider eq (2.50), make diagram:

$$n(m) = \begin{cases} 1 & \text{for } m \in \{j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2|\} \\ 0 & \text{otherwise} \end{cases} \quad (2.53)$$

Let:

$$\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} = \bigoplus_{k=|j_1-j_2|}^{j_1+j_2} \mathcal{H}_k \quad (2.54)$$

To find Basis change, start with $|m_1 = j_1, m_2 = j_2\rangle$ and use $J_-^{\text{tot},1} := J_-^{\text{tot},1} - iJ_-^{\text{tot},2}$ and so down to get $j_1 + j_2$ rep.

Remark. Useful formulars for ireps of so(3):

$$|j, m\rangle = \left[\frac{(j+m)!}{(2j)!(j-m)!} \right]^{\frac{1}{2}} (J_-)^{j-m} |j, j\rangle \quad (2.55)$$

$$= \left[\frac{(j-m)!}{(2j)!(j+m)!} \right]^{\frac{1}{2}} (J_+)^{j+m} |j, -j\rangle \quad (2.56)$$

In the $|j, m\rangle$ basis, the J 's are give by matrices:

$$(J^3)_{mm'} \equiv \langle j, m | J^3 | j, m' \rangle = \hbar m \delta_{mm'} \quad (2.57)$$

$$(J_{\pm})_{mm'} \equiv \langle j, m | J_{\pm} | j, m' \rangle = \hbar \sqrt{j(j+1) - mm'} \delta_{m,m' \pm 1} \quad (2.58)$$

This is the *standard form* of the j -irrep of $SO(3)$

Spherical harmonics: Consider $\mathcal{L}^2(S^2, m \, d\theta \, d\varphi) = \mathcal{H}$, ONB given by

$$\psi_l^m(\theta, \varphi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos \theta) e^{im\varphi} \quad (2.59)$$

with $l \in \mathbb{N}_0$, $m \in \{-l, -l+1, \dots, l\}$ ONB means:

$$\langle \psi_l^m | \psi_{l'}^{m'} \rangle = \int_0^\pi d\theta \int_0^{2\pi} \sin \theta \overline{\psi_l^m}(\theta, \varphi) \psi_{l'}^{m'}(\theta, \varphi) = \delta_{ll'} \delta_{mm'} \quad (2.60)$$

and they span \mathcal{H} . In spherical coordinates, orbital angular momentum

$$\vec{L} = \vec{x}\vec{p} = \hbar \begin{pmatrix} i \sin \varphi \partial_\theta + i \cos \varphi \cot(\theta) \partial_\varphi \\ \cos \varphi \partial_\theta - \sin \varphi \cot(\theta) \partial_\varphi \\ -i \partial_\varphi \end{pmatrix} \quad (2.61)$$

independent of r . Thus \vec{L} acts on \mathcal{H} , and one finds

$$\vec{L}^2 \psi_l^m = \hbar^2 l(l+1) \psi_l^m, \quad L^3 \psi_l^m = m \hbar \psi_l^m \quad (2.62)$$

recognize l -irreps of $\mathfrak{so}(3)$. Use this often:

$$\mathcal{L}^2(\mathbb{R}, d^3x) \simeq \mathcal{L}^2(\mathbb{R}_+, r^2 dr) \otimes \mathcal{H} \quad (2.63)$$

then, natural to use basis functions

$$f(r) \psi_l^m(\theta, \varphi) \quad (2.64)$$

in problems involving rotational symmetry.

Note: $l = \frac{1}{2}, \frac{3}{2}, \dots$ are not allowed *Spin*: Intrinsic angular momentum of particles. Electron has spin described by

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma} \quad (2.65)$$

on \mathbb{C}^2 . (Pauli matrices $\vec{\sigma}$.)

This is just the $j = \frac{1}{2}$ irrep of eq (2.40). Consequently, state space of H-atom is

$$\mathcal{H} = \text{span} \left\{ |nlm\rangle \otimes \left| \frac{1}{2}, s \right\rangle \mid s = \pm \frac{1}{2}, nlm = \dots \right\} \quad (2.66)$$

Similar for other elementary particles

- Bosons \rightarrow integer j
- Fermions \rightarrow half-integer j

No Fermions with $j > \frac{1}{2}$ observed

Example 2.10. For addition of angular momentum:

- H-atom: $|nlm\rangle \otimes \left| \frac{1}{2} \right\rangle \hat{=} |m, s\rangle$, different Basis: $|j_{\text{tot}}, m_{\text{tot}}\rangle : l \otimes \frac{1}{2} = (l + \frac{1}{2}) \oplus (l - \frac{1}{2})$
- Isospin: Δ -Quadruplett ($\Delta^{++}, \Delta^+, \Delta^0, \Delta^-$), nucleon duplett consisting of (p, n). Hypothesis: Made of three $I = \frac{1}{2}$ particles („Quarks“).

Check:

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = (1 \oplus 0) \otimes \frac{1}{2} \quad (2.67)$$

$$\frac{3}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \quad (2.68)$$

Because of the Pauli-principle the second $\frac{1}{2}$ disappears.

$\rightarrow \Delta, N$ from (u, d) quarks.

2.4 Spin $j = n + \frac{1}{2}, n \in \mathbb{N}_0$

Consider rotations around fixed axis. WLOG. z-axis. Generator a_3 in j -irep:

$$J^3 = \begin{pmatrix} j & & & 0 \\ & j-1 & & \\ & & \ddots & \\ 0 & & & -j \end{pmatrix} \quad (2.69)$$

hence

$$\Pi_j = (R_\varphi) e^{i\varphi J^3/\hbar} = \text{diag}(e^{ij\varphi}, e^{i(j-1)\varphi}, \dots, e^{-ih\varphi}) \quad (2.70)$$

This is strange, because for $j = n + \frac{1}{2}, n \in \mathbb{N}_0$

$$\lim_{\varphi \rightarrow 2\pi} \Pi_j(R_\varphi) = \text{diag}(e^{i2\pi j}, e^{i2\pi(j-1)}, \dots, e^{-i2\pi j}) = -\mathbb{1}_{\mathcal{H}_j} \neq \Pi_j(R_0) \quad (2.71)$$

So Π_j defined this way is *not* a representation of $\text{SO}(3)$. Only for $\varphi \rightarrow 4\pi$ would get 1 again. Look at special case $j = \frac{1}{2}$:

$$J^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{\hbar}{2}, J^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\hbar}{2}, J^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (2.72)$$

Notice $j^k = \frac{\hbar}{2} \sigma^k$ with σ^k Pauli notation:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.73)$$

Exponentials $e^{iJ^k \frac{1}{\hbar}}$ are unitary 2x2 matrices, belong to group

Definition 2.7. $\text{SO}(2)$: Group of $U \in M(2 \times 2, \mathbb{C})$

$$U^\dagger = U^{-1}, \det(U) = 1$$

In homework had seen: Group generators are $\tau^k = \frac{i}{2} \sigma^k$

Thus

$$su(2) = \{M \in M(2 \times 2, \mathbb{C}), M^\dagger = -M, \text{tr}(M) = 0\}$$

Had seen:

$$[\tau^k, \tau^l] = \sum_m \epsilon_{klm} \tau^m$$

Set $\tilde{\tau}^k = -\tau^k$. Then: $\tilde{\tau}^k$ are bases of $su(2)$, too. and

$$[\tilde{\tau}^k, \tilde{\tau}^l] = \sum_m -\epsilon_{klm} \tilde{\tau}^m \quad (2.74)$$

Compare with the relations among generators of $\text{SO}(3)$

$$[a^k, a^l] = \sum_m \epsilon_{klm} a^m$$

Exactly the same. Same abstract Lie-algebra, same (irreducible) representation. Thus:

- $SO(3)$ and $SU(2)$ are „same near $\mathbb{1}$ “
- $SO(3)$ and $SU(2)$ differ “globally”

Relations $SO(3)$ - $SU(2)$

Consider $j = 1$ representation of $SU(2)$. Must be 3-dimensional:

$$\Pi_{j=1} \left(e^{\vec{v}\vec{\tau}} \right) := e^{\vec{v}\pi_{j=1}(\vec{\tau})} \quad (2.75)$$

Had already seen that Lie group G acts on its Lie algebra A via

$$\pi(g)b := gb g^{-1} \quad (2.76)$$

called adjoint representation. For $SU(2)$: Note

$$\det(\pi(g)b) = \det \det g^{-1} \det(b) = \det(b)$$

Identically \mathbb{R}^3 with $su(2)$ via

$$\mathbb{R}^3 \ni \vec{v} \mapsto b_{\vec{v}} := \vec{v} \cdot \vec{\tau} = \sum_k v^k \tau^k$$

Then $\det(b_{\vec{v}}) = \frac{1}{4}|\vec{v}|^2$. So (2.76) induces orthogonal transformation on \mathbb{R}^3 . Can show: in $SO(3)$. Moreover:

- is a representation
- $\Pi(SU(2)) = SO(3)$
- is group-homomorphism
- Π is 2 to 1: For $g \in SU(2)$, $-g \in SU(2)$
 $\pi(-g)b = (-1)^2 gb g^{-1} = \pi(g)b$
 so g and $-g$ are mapped at the same element in $SO(3)$.

Finally:

$$\Pi \left(e^{\vec{v}\vec{\tau}} \right) = \Pi_{j=1} \left(e^{\vec{v}\vec{\tau}} \right) = e^{\vec{v}\vec{a}} \quad (2.77)$$

Topological structure of $SO(3), SU(3)$

1. $SO(3) : g = e^{\vec{v}\vec{a}} \hat{=} \text{Rotation around axis given by } \vec{v} \text{ with angle } |\vec{v}|$
 $\Rightarrow SO(3) \hat{=} \text{3d solid ball with opposite points identified on surface.}$
 $\Rightarrow \exists \text{ non-contractible loops, } SO(3) \text{ not simply connected.}$
2. $SU(2) : g = e^{\vec{v}\vec{\tau}}$
 $\Rightarrow SU(2) : \text{Sphere } S^3$
 $\Rightarrow SU(2) \text{ simply connected (no holes)}$
3. 2 - 1 map $SU(2) \rightarrow SO(3)$

Back to representation

For $SU(2)$

$$\Pi_j (e^{\vec{v} \cdot \vec{\tau}}) := e^{\vec{v} \pi_j(\vec{\tau})}$$

gives representation for any j . For $SO(3)$

$$\Pi_j (e^{\vec{a} \cdot \vec{\alpha}}) := e^{\vec{v} \pi_j(\vec{a})}$$

give a rep for $j \in \mathbb{N}_0$. For $j = n + \frac{1}{2}$

$$\Pi_j (e^{\vec{v}_1 \vec{a}}) \Pi_j (e^{\vec{v}_2 \vec{a}}) = C(v_1, v_2) \Pi_j (e^{\vec{v}_1 \vec{a}} e^{\vec{v}_2 \vec{a}}) \quad (2.78)$$

with $C(v_1, v_2) \in \{\pm 1\}$

Definition 2.8. Map Π with (2.78) where C total values on unit circle is called a *projective prep*.

2.5 General form of symmetries

Consider system (\mathcal{H}, O, H) , symmetry group G . Let: $\mathcal{H}_1 = \{v \in \mathcal{H}, \|v\| = 1\}$, $\rho = \{[v], v \in \mathcal{H}\}$, $[v] := \{e^{i\varphi} v, \varphi \in \mathbb{R}\}$.

Definition 2.9.

$$l : \mathcal{H}_1 \rightarrow \rho, v \rightarrow [v] \quad (2.79)$$

Symmetry group comes with rep. Π_ρ , which has (2.80)

$$|\langle [v] | [w] \rangle| = |\langle \Pi_\rho(g)[v] | \pi_\rho(g)[w] \rangle|$$

Given $g \in G$, is there an operator U_g , such that

$$l \circ U_g = \Pi_\rho(g) \circ l \quad (2.80)$$

Theorem 2.11 (Wigner's theorem). For $\Pi_\rho(g)$ with (2.80) there is always U_g fullfilling (2.80), such that U_g is either linear and unitary or anti-linear and anti-unitary.

Definition 2.10. • U with $U(\lambda v + w) = \bar{\lambda} Uv + Uw$ is called anti-linear and with additionally $\langle Uv | Uw \rangle = \langle w | v \rangle$ anti-unitary

- Adjoint U^\dagger of anti-linear operator is given by $\langle v | U^\dagger w \rangle = \overline{\langle Uv | w \rangle} = \langle w | Uv \rangle$

Corollary 2.12. For symmetry group G , U_g given by (2.80) and Wigner's theorem: $\Pi : g \rightarrow U_g$ is a projective representation.

Proof.

$$l \circ U_{gg'} \underbrace{U}_{(2.80)} = \Pi_\rho(gg') \circ l = \Pi_\rho(g)\pi_\rho(g') \circ l \stackrel{(2.80)}{=} \Pi_\rho(g) \circ l \circ U_{g'} \stackrel{(2.80)}{=} l \circ U_g U_{g'}$$

Thus $\Pi(g)\pi(g')\Psi \equiv U_g U_{g'}\Psi = e^{i\phi(g,g',\Psi)} U_{gg'}\Psi \equiv e^{i\phi(\dots)} \Pi(gg')\Psi$ with $\phi(g, g', \Psi) \in \mathbb{R}$.
Actually does not depend on Ψ :

$$\begin{aligned} e^{i\phi(g,g',\Psi_1+\Psi_2)} U_{gg'}(\Psi_1 + \Psi_2) &= U_g U_{g'}\Psi_1 + U_g U_{g'}\Psi_2 \\ &= e^{i\phi(g,g',\Psi_1)} U_{gg'}\Psi_1 + e^{i\phi(g,g',\Psi_2)} U_{gg'}\Psi_2 \\ \Leftrightarrow e^{\pm i\phi(g,g',\Psi_1+\Psi_2)}(\Psi_1 + \Psi_2) &= e^{\pm i\phi(g,g',\Psi_1)}\Psi_1 + e^{\pm i\phi(g,g',\Psi_2)}\Psi_2 \\ \Leftrightarrow \phi(g, g', \Psi_1 + \Psi_2) &= \phi(g, g', \Psi_1) = \phi(g, g', \Psi_2) \end{aligned}$$

□

Remark. • So most general form of a symmetry is a unitary/anti-unitary projective representation on \mathcal{H}

- example for projective rep. as symmetrys: Rotations for $j = n + \frac{1}{2}, n \in \mathbb{N}_0$
- If G is simply connected, can choose phases $\phi = 0$
- For larger class of G , projective rep. is equivalent to normal rep. of covering group

3 Time evolution, propagators, path integrals

Time evolution in QM ruled by Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = H(t)\Psi(t) \quad (3.1)$$

In this section, we will rewrite (3.1) and its solutions in many different and useful ways.

3.1 Review of basic motions

Definition 3.1 (Time evolution operator). For given initial conditions $\Psi(t_0)$ (3.1) has unique solution $\Psi(t)$ and hence we define map

$$U(t, t_0) : \Psi(t_0) \rightarrow \Psi(t) \quad (3.2)$$

This map is linear and satisfies

$$U(t_0, t_0) = \mathbb{1} \text{ and } U^\dagger(t, t_0) = (U(t, t_0))^{-1} \text{ and } U(t, t_1)U(t_1, t_0) = U(t, t_0) \quad (3.3)$$

. $U(t, t_0)$ is called “time evolution operator”.

How to determine $U(t, t_0)$? Plugging $\Psi(t) \equiv U(t, t_0)\Psi(t_0)$ into (3.1), for arbitrary $\Psi(t_0)$.

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t)U(t, t_0) \quad (3.4)$$

which, together with initial condition $U(t_0, t_0) = \mathbb{1}$ defines U uniquely. For $H(t) = H$ time independent can integrate (3.4) easily to get

$$U(t, t_0) = e^{-\frac{i}{\hbar} H(t-t_0)}.$$

For time dependent situation, two cases:

1. $\forall t_1, t_2 : [H(t_1), H(t_2)] = 0$
2. $\exists t_1, t_2 : [H(t_1), H(t_2)] \neq 0$

For 1. solution is

$$U(t, t_0) = \exp\left(-\frac{i}{\hbar} \int_{t_0}^t H(t') dt'\right) \quad (3.5)$$

while for case 2. no simple solution exists, but interesting series expansion: Integrating (3.4) from t_0 to t

$$U(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t dt' H(t') U(t', t_0) \quad (3.6)$$

Iterate (3.6), to get Dyson series

$$\begin{aligned} U(t, t_0) &= \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t dt' H(t') + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 H(t_1) H(t_2) U(t_2, t_0) \underbrace{\equiv \dots}_{\text{recursion}} \\ &= \mathbb{1} + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n H(t_1) \dots H(t_n) \end{aligned} \quad (3.7)$$

Can write this in more compact form, using the time ordered product:

$$T(H(t_1) \dots H(t_n)) := H(t_{\sigma(1)}) H(t_{\sigma(2)}) \dots H(t_{\sigma(n)}) \quad (3.8)$$

with $\sigma \in S_n$ (group of permutations of n objects) s. t. $t_{\sigma(1)} \geq t_{\sigma(2)} \geq \dots \geq t_{\sigma(n)}$

Using this we can write:

$$\begin{aligned} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 T(H(t_1) H(t_2)) &= \underbrace{\int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 H(t_1) H(t_2)}_{(I) \text{ see 5}} + \underbrace{\int_{t_0}^t dt_2 \int_{t_0}^{t_2} dt_1 H(t_2) H(t_1)}_{(II)} \\ &= 2 \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 H(t_1) H(t_2) \end{aligned}$$

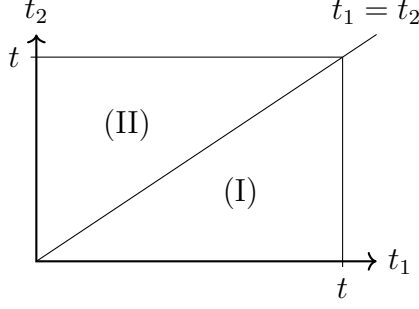


Figure 5: Times in the integrals

Similarly one gets for n integrals:

$$\int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \cdots \int_{t_0}^t dt_n T(H(t_1) \cdots H(t_n)) = n! \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1) \cdots H(t_n)$$

And hence:

$$\begin{aligned} U(t, t_0) &= \mathbb{1} + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \cdots \int_{t_0}^t dt_n T(H(t_1) \cdots H(t_n)) \\ &= \mathbb{1} + \sum_{n=1}^{\infty} \frac{1}{n!} T \left[\left(-\frac{i}{\hbar} \int_{t_0}^t dt' H(t')\right)^n \right] = T \left[e^{-\frac{i}{\hbar} \int_{t_0}^t dt' H(t')} \right] \end{aligned} \quad (3.9)$$

Where we have extended T by linearity. Note that for $[H(t), H(t')] = 0 \forall t, t'$ T is the identity and (3.9) collapses to (3.5). Later we will use this for the case $H = H_0 + V$, where H_0 is simple and V small. Then (3.9) gives good approximation when truncated at finite order.

Heisenberg picture

We can also consider operators to be time dependent, while the states stay constant:

$$\langle A \rangle_{\Psi(t)} = \langle \Psi(t_0) | \underbrace{U^\dagger(t, t_0) A U(t, t_0)}_{=A_H(t)} | \Psi(t_0) \rangle \stackrel{\Psi(t_0)=\Psi}{=} \langle A_H(t) \rangle_{\Psi} \quad (3.10)$$

Using (3.4), we can calculate that $\frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H_H(t), A_H(t)]$. Note that for $[H(t), H(t')] = 0 \forall t, t'$ one has

$$H_H(t) \equiv e^{\frac{i}{\hbar} \int_{t_0}^t dt' H(t')} H(t) e^{-\frac{i}{\hbar} \int_{t_0}^t dt' H(t')} = H(t)$$

For an observable with explicit time dependence $A(t)$:

$$\frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H_H(t), A_H(t)] + \left(\frac{\partial}{\partial t} A \right)_H(t) \quad (3.11)$$

the *Heisenberg equation* in the *Heisenberg picture*.

Had already discussed the constants of motion:

$$0 = \frac{d}{dt}A_H(t) \Leftrightarrow [H_H(t), A_H(t)] + \left(\frac{\partial}{\partial t}A\right)_H(t) = 0 \Leftrightarrow [H(t), A(t)] + \frac{\partial}{\partial t}A = 0$$

Remark. Simplifies to just the commutators if A is not time dependent in the Schrödinger picture.

Interaction picture

Useful if $H(t) = H_0(t) + V(t)$, where H_0 is “trivial” (already known, like spectral decomposition). Then

$$\Psi_I(t) := U_0^\dagger(t, t_0)\Psi(t)$$

where $i\hbar\frac{\partial}{\partial t}U_0(t, t_0) = H_0(t)U_0(t, t_0), U(t_0, t_0) = \mathbb{1}$

i.e. U_0 is the time evolution operator wrt. H_0 . Time evolution:

$$\Psi_I(t) := U_I(t, t'_0)\Psi_I(t'_0)$$

U_I can be calculated to be

$$U_I(t, t'_0) = U_0(t_0, t)U(t, t'_0)U_0(t'_0, t_0) \quad (3.12)$$

Remark. Implicit time dependence on t_0 !

To get a simple form for the expectation value

$$\langle A \rangle_{\Psi(t)} = \langle \Psi_I(t) | \underbrace{U_0^\dagger(t, t_0)A(t)U_0(t, t_0)}_{=: A_I(t)} | \Psi_I(t) \rangle =: \langle A_I(t) \rangle_{\Psi_I(t)} \quad (3.13)$$

Same calculation as the one giving (3.11) from (3.10) here yields

$$\frac{d}{dt}A_I(t) = \frac{i}{\hbar}[H_{0_I}(t), A_I(t)] + \left(\frac{\partial}{\partial t}A\right)_I(t) \quad (3.14)$$

Crucial thing about the interaction picture:

$$\begin{aligned} i\hbar\frac{d}{dt}U_I(t, t'_0) &= i\hbar\frac{d}{dt}(U_0(t, t_0)^{-1}U(t, t'_0)U_0(t'_0, t_0)) = U_0(t_0, t)\underbrace{(H - H_0)}_{V(t)}U(t, t'_0)U_0(t'_0, t_0) \\ &= \underbrace{U_0(t_0, t)V(t)U_0(t, t_0)}_{=: V_I(t)}U_0(t_0, t)U(t, t'_0)U_0(t'_0, t_0) = V_I(t)U_I(t, t'_0) \end{aligned}$$

So

$$i\hbar\frac{d}{dt}U_I(t, t'_0) = V_I(t)U_I(t, t'_0) \text{ and } U_I(t'_0, t'_0) = \mathbb{1} \quad (3.15)$$

$$i\hbar \frac{d}{dt} \Psi_I(t) = V_I(t) \Psi_I(t) \quad (3.16)$$

(3.15) and (3.16) structurally identical to (3.4) and (3.1). But now time evolution is completely given in terms of V . In particular (3.15) is formally solved by (3.9)

$$\begin{aligned} U_I(t, t_0) &= T(e^{-\frac{i}{\hbar} \int_{t_0}^t dt' V_I(t')}) \\ &= \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t V_I(t') dt' + \frac{1}{2} \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^t \int_{t_0}^t dt_1 dt_2 T(V_I(t_1) V_I(t_2)) + \mathcal{O}(V^3) \end{aligned} \quad (3.17)$$

In case V can be considered small, truncating (3.17) gives systematic approximation.

Remark. 1. If $|E_1\rangle, |E_2\rangle$ eigenstates of H_0

$$\begin{aligned} P(E_1, t_1 \rightarrow E_2, t_2) &\equiv |\langle E_2 | U(t_2, t_1) | E_1 \rangle|^2 \\ &= |\langle E_2 | U_0(t_2, t_0) U_I(t_2, t_1) U_0(t_0, t_1) | E_1 \rangle|^2 \\ &= |\langle E_2 | U_I(t_2, t_1) | E_1 \rangle|^2 \end{aligned}$$

with (3.12) which can be expanded using (3.17)

2. This procedure called “time dependent perturbation theory“.

3.2 Propagators

Consider particle in \mathbb{R}^3 . In many situations, $U(t, t_0)$ is given by an integral kernel K :

$$(U(t, t_0)\psi)(x) = \int_{\mathbb{R}^3} d^3x' K(t, x, t_0, x') \Psi(x') \quad (3.18)$$

Can understand K as matrix element of U :

Formally introduce eigenstates $|\vec{x}\rangle$ of \vec{x} and the corresponding decomposition of $\mathbb{1}$

$$\mathbb{1} = \int_{\mathbb{R}^3} d^3x' |\vec{x}'\rangle \langle \vec{x}'|$$

Actually: $|\vec{x}\rangle \langle \vec{x}'| \equiv \delta^{(3)}(\vec{x} - \vec{x}')$. Then:

$$\begin{aligned} \underbrace{(U(t, t_0)\psi)(x)}_{\langle x | U(t, t_0) | \psi \rangle} &= \int_{\mathbb{R}^3} d^3x' \langle x | U(t, t_0) | x' \rangle \langle x' | \psi \rangle \\ &= \int_{\mathbb{R}^3} d^3x' \langle x | U(t, t_0) | x' \rangle \psi(x') \end{aligned}$$

So can identify:

$$K(t, x, t_0, x') = \langle x | U(t, t_0) | x' \rangle \quad (3.19)$$

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

$$\tilde{\psi}(\vec{k}) = \langle p_k \equiv \hbar k | \psi \rangle = \int_{\mathbb{R}^3} e^{-i\vec{k}\vec{x}} \psi(\vec{x})$$

But: K may not be function. \rightarrow Distribution.

Composition property

Combining evolution operators

$$\begin{aligned}
 K(t, x, t_0, x_0) &= \langle x | U(t, t_1) U(t_1, t_0) | x_0 \rangle \\
 &= \int_{\mathbb{R}^3} \langle x | U(t, t_1) | x_1 \rangle \langle x_1 | U(t_1, t_0) | x_0 \rangle d^3 x_1 \\
 &= \int_{\mathbb{R}^3} K(t, x, t_1, x_1) K(t_1, x_1, t_0, x_0) d^3 x_1
 \end{aligned} \tag{3.20}$$

Interpretation of $K(t, x, t_0, x_0)$: probability amplitude for particle to go from x_0 at time t_0 to x at time t . So

$$P(t_0, x_0 \rightarrow t, x) = |K(t, x, t_0, x_0)|^2$$

the probability for this process. Caviat: This might have unexpected properties. (3.18) exposes quantum mechanical superposition principle with the possibility of interference. Therefore K is called a *propagator*. Calculate K for 1d free particle.

$$H = \frac{p^2}{2m}$$

using Fourier Transform:

$$\begin{aligned}
 (\mathcal{F}\psi)(x) &\equiv \tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ikx} \psi(x) dx \\
 (\mathcal{F}^{-1}\tilde{\psi})(x) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ikx} \tilde{\psi}(k) dk
 \end{aligned} \tag{3.21}$$

\mathcal{F} transforms from representation in which x is diagonal to one in which p is indeed:

$$(\mathcal{F}p\psi)(k) = \hbar k \tilde{\psi}(k) \tag{3.22}$$

For

$$|p\rangle(k) = \delta(k - \frac{p}{\hbar}) |k\rangle \tag{3.23}$$

have

$$\langle p | p' \rangle = \delta\left(\frac{p}{\hbar} - \frac{p'}{\hbar}\right) \tag{3.24}$$

and can calculate momentum space propagator:

$$\langle p | U(t, t_0) | p' \rangle = \delta\left(\frac{p-p'}{\hbar}\right) e^{-i \frac{p^2}{2m}(t-t_0)}$$

and hence

$$K(t, x, t_0, x_0) = \frac{1}{2\pi} \int_{\mathbb{R}^3} dk \int_{\mathbb{R}^3} dk' e^{i(k'x' - kx)} \langle p | U(t, t_0) | p' \rangle \tag{3.25}$$

$$= \frac{1}{2\pi\hbar} \int_{\mathbb{R}^3} dp e^{i\frac{p}{\hbar}(x-x')} e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t-t_0)}$$

This integral does not converge in standard sense. Can give meaning as distribution. Replace:

$$i(t-t_0) \equiv iT \text{ with } z = \tau + iT, \tau > 0$$

and consider limit $\tau \rightarrow 0$. This kind of analytic continuation

$$T \rightarrow T - i\tau \quad (3.26)$$

to complex or even imaginary time is called a *Wick-Rotation*. Will study more systematically later. For $\tau > 0$, (3.25) becomes convergent. We have, for $\text{Re}(a) > 0$:

$$\int_{\mathbb{R}^3} dx e^{-\frac{1}{2}ax^2+ibx} = \sqrt{\frac{2\pi}{a}} e^{-\frac{1}{2a}b^2} \quad (3.27)$$

In the current situation:

$$x \rightarrow p, \quad b = \frac{x' - x}{\hbar}, \quad a = \frac{1}{m\hbar}z$$

and hence:

$$K(z, x, x') = \sqrt{\frac{m}{2\pi\hbar z}} e^{-\frac{m}{2\hbar z}(x-x')^2} \quad (3.28)$$

It is possible to take the limit $\tau \rightarrow 0$:

$$K(t, x, t', x') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}} e^{i\frac{m}{2\hbar(t-t')}(x-x')^2} \quad (3.29)$$

But: In case of convergence problems in (3.18):

Treat as distribution, i.e. First $\tau > 0$, then do integral (3.18), then $\lim_{\tau \rightarrow 0}$.

Free particle in \mathbb{R}^3 in tensor product of three 1d particle. Hence:

$$K^{(3d)}(t, \vec{x}, t', \vec{x}') = \left(\frac{m}{2\pi i\hbar(t-t')} \right)^{\frac{2}{3}} e^{i\frac{m}{2\hbar(t-t')}(\vec{x}-\vec{x}')^2}$$

Note the curious property of this propagator: The exponent can be written:

$$i\frac{m}{2\hbar} \frac{(\vec{x} - \vec{x}')^2}{t - t'} = \frac{i}{\hbar} S[\vec{x}_{\text{Cl}}(\cdot)] \quad (3.30)$$

where $S[\vec{x}(\cdot)]$ is the action functional, i.e.:

$$S[\vec{x}(\cdot)] = \int_{t'}^t dt'' L(t'', \vec{x}(t''), \dot{\vec{x}}(t''))$$

with the L Lagrange-function of the free particle. x_{Cl} denotes the classical solution to the equation of motion with boundary values $x_{\text{Cl}}(t) = x, x_{\text{Cl}}(t') = x'$. Turns out: This is true for all systems with quadratic Lagrangians. Reason for this is explained in the following.

3.3 The Feynman path integral

We will show that the propagator can be written as a path integral in a formal sense.

$$K(t, x, t_0, x_0) = \int_{P(t, x, t_0, x_0)} P[x(\cdot)] e^{\frac{i}{\hbar} \int [x(\cdot)]}$$

Will show now: The propagator can be written as an integral over paths, at least in a formal sense.

Consider

$$H = \frac{p^2}{2m} + V(x)$$

Time independent, so

$$U(t, t') = e^{-\frac{i}{\hbar} H(t-t')}$$

only depends on $T := t - t'$. Will with

$$\langle x, U(t, t') | x' \rangle = \langle x | U(T) | x' \rangle \equiv K(T, x, x')$$

Want to rewrite $K(t, x, t_0, x_0)$. Let $N \in \mathbb{N}$, and

$$\epsilon = \frac{t - t_0}{N + 1}$$

Then using (3.20)

$$K(t, x, t_0, x_0) = \int dx_1 \int dx_2 \cdots \int dx_N K(\epsilon, x, x_N) K(\epsilon, x_N, x_{N-1}) \cdots K(\epsilon, x_1, x_0) \quad (3.31)$$

Can make ϵ small by increasing N . So: find approximation for $K(\epsilon, x_N, x_{N-1})$ valid for small ϵ . To do that, from (3.12) with $t'_0 = t_0$

$$U(\epsilon) = U_0(\epsilon) U_I(\epsilon)$$

Moreover

$$U_I(\epsilon) = T \cdot \exp \left(-\frac{i}{\hbar} \int_0^\epsilon V(x_I(t')) dt' \right)$$

with

$$x_I(t') = U_0^\dagger(t') x U_0(t') x = x + \frac{p}{m} t'$$

Now:

$$U_I(\epsilon) = \mathbb{1} - \frac{i}{\hbar} \int_0^\epsilon V(x_I(t')) dt' + \mathcal{O}(\epsilon^2)$$

$$\begin{aligned}
&= \mathbb{1} - \frac{i}{\hbar} V(x)\epsilon + \mathcal{O}(\epsilon^2) \\
&= e^{-\frac{i}{\hbar} V(x)\epsilon} + \mathcal{O}(\epsilon^2)
\end{aligned}$$

Then, for small ϵ :

$$\begin{aligned}
K(\epsilon, x_N, x_{N-1}) &= \langle x_N | U_0(\epsilon) U_I(\epsilon) | x_{N-1} \rangle \\
&\simeq \langle x_N | U_0(\epsilon) e^{-\frac{i}{\hbar} V(x)\epsilon} | x_{N-1} \rangle \\
&= \langle x_N | U_0(\epsilon) | x_{N-1} \rangle e^{-\frac{i}{\hbar} V(x_{N-1})\epsilon} \\
&= \sqrt{\frac{m}{2\pi i \hbar}} \exp \left[i \frac{\epsilon}{\hbar} \left(\frac{m}{2} \left(\frac{x_N - x_{N-1}}{\epsilon} \right)^2 - V(x_{N-1}) \right) \right] \quad (3.32)
\end{aligned}$$

Combining (3.31) and (3.32)

$$K(t, x, t_0, x_0) = \sqrt{\frac{m}{2\pi i \hbar \epsilon}} \int \frac{dx_1}{\sqrt{2\pi i \hbar \frac{\epsilon}{m}}} \cdots \int \frac{dx_N}{\sqrt{2\pi i \hbar \frac{\epsilon}{m}}} e^{i \hbar \Sigma} \quad (3.33)$$

with

$$\Sigma = \epsilon \sum_{n=1}^{N+1} \left(\frac{m}{2} \left(\frac{x_n - x_{n-1}}{\epsilon} \right)^2 - V(x_{n-1}) \right)$$

where we have set $x_{N+1} := x$. σ is the Riemann-sum approximation of the action of the particle:

$$\lim_{N \rightarrow \infty} \Sigma = \int_{t_0}^t dt' \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) = S[x(\cdot)]$$

would hold for $x_N = x(n\epsilon)$ where $x(t)$ is a smooth path. Try to take limit $N \rightarrow \infty$ every where. Have to integrate over positions of the particle at each and all times, i.e. over paths $x(t)$. This is the idea of a path integral (Feynman):

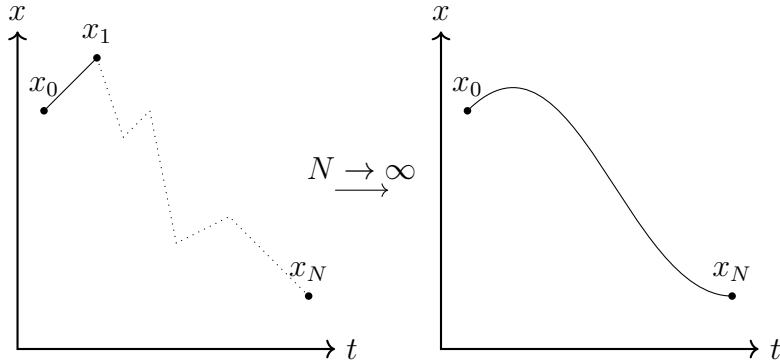


Figure 6: Idea of a path integral

$$\frac{dx_1}{\sqrt{\dots}} \dots \frac{dx_N}{\sqrt{\dots}} \rightarrow D[x(\cdot)]$$

where the measure D is something like

$$D[x(\cdot)] = \lim_{N \rightarrow \infty} \sqrt{\frac{m}{2\pi i \hbar \epsilon}} \prod_{n=1}^N \frac{dx(\epsilon_n)}{\sqrt{2\pi i \hbar \frac{\epsilon}{m}}}$$

Thus we can write:

$$K(x, t, x_0, t_0) = \int_{\mathcal{P}(t, x, t_0, x_0)} D[x(\cdot)] e^{\frac{i}{\hbar} S[x(\cdot)]} \quad (3.34)$$

where the space \mathcal{P} of path to be integrated over consists of paths $x(t)$ with $x(t_0) = x_0, x(t) = x$.

Remark. 1. Up to now, there is no way to make (3.34) literally true for interesting systems, in a well defined math context.

2. (3.34) tremendously important source of correct results
3. Can make “relatives” of (3.34) well defined

Example 3.1. Euclidean path integral \rightarrow later.

Path integral and classical limit

S changes rapidly if $x(\cdot)$ is varied, \rightarrow interference effects that can enhance or decrease amplitude. Consider

$$x(\cdot) = x_0(\cdot) + \epsilon h(\cdot)$$

Taylor expand in ϵ .

$$S[x(\cdot)] = S[x_0(\cdot)] + \underbrace{\epsilon \frac{d}{d\epsilon} \Big|_{\epsilon=0} S[x(\cdot)]}_{(*)} + \mathcal{O}(\epsilon^2) \quad (3.35)$$

For suitable S , $(*)$ will have form:

$$\frac{d}{d\epsilon} \Big|_{\epsilon=0} S[x(\cdot)] = \int F(x_0(t''), \dot{x}(t''), t'' \dots) h(t'') dt'' \quad (3.36)$$

Then one calls S differentiable, and

$$F := \frac{\delta S}{\delta x(\cdot)} \Big|_{x_0(\cdot)}$$

In the path integral, contribution from

$$h(t'') , h(t'') + \frac{\pi \hbar}{F(t'', \dots)(t - t_0)}$$

cancel each other, making contributions from the neighbourhood of x_0 not contribute to the path integral. More precise argument can be given (“Riemann-Lebesgue-Lemma”). Shows: decaying stronger than polynomial in \hbar . These arguments break down if

$$F(t'', \dots) = \left. \frac{\delta S}{\delta x} \right|_{x_0} = 0. \quad (3.37)$$

Then $S[x_0]$ and the quadratic order $\epsilon^2 \int \int h(t')h(t'')$ $\underbrace{G(\dots)}_{= \left. \frac{\delta S}{\delta x(t')\delta x(t'')} \right|_{x(\cdot)=x_0(\cdot)}}$ $dt' dt''$ give non-

vanishing contributions. In fact (3.37) are the Euler-Lagrange-equations of classical mechanics!

So the main contribution come from classical parts.

$$K(t, x, t_0, x_0) \equiv \int_{P(t, x, t_0, x_0)} D(x(\cdot)) e^{iS[x]/\hbar} \underbrace{=} \sum_{x_{Cl}(\cdot)} e^{iS[x_{Cl}(\cdot)]/\hbar} B_{x_{Cl}}(t, x, t', x') \quad (3.38)$$

where

- $S[x_{Cl}(\cdot)] = \int_{t_0}^t L[x_{Cl}(t'), \dot{x}_{Cl}(t'), t'] dt'$ where $x_{Cl}(\cdot)$ solves the EOM, $x_{Cl}(t_0) = x_0$ and $x_{Cl}(t) = x$
- B is the “Gaussian integral” from the second order term in the action, for quadratic Lagrangians: B only depends on $t, t' \rightarrow$ see (3.29)

$$\int D[h] e^{i\epsilon^2 \int \int h h \delta S / \delta x \delta x / \hbar}$$

Quantum mechanical interference

Can be discussed using the path integral: Consider double slit experiment:

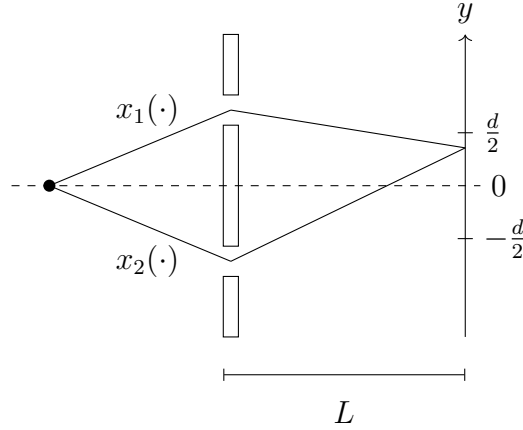


Figure 7: Double slit experiment

for small y (3.38) gives

$$K \approx \left(\underbrace{e^{\frac{imy d}{\hbar 2 \Delta t}}}_{\text{from } x_1(\cdot)} + \underbrace{e^{-\frac{imy d}{\hbar 2 \Delta t}}}_{\text{from } x_2(\cdot)} \right) \propto \cos\left(\frac{1}{2} \frac{my d}{\hbar \Delta t}\right) = \cos\left(\frac{\pi d}{\lambda L} y\right) \quad (3.39)$$

where we have introduced the de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h \Delta t}{m L}$. This will result in an interference pattern with fringes at $y_n = \pm \frac{\lambda L}{d} \left(n + \frac{1}{2}\right)$ (more details in the HW).

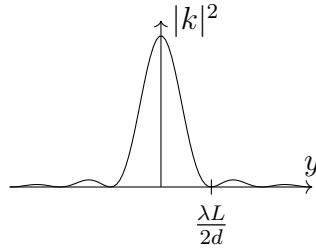


Figure 8: Sinc-function

3.4 Perturbation theory with Feynman diagrams

Perturbation treatment of $H = H_0 + V$,

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 \text{ and } V = \lambda \frac{x^k}{k!} \quad (3.40)$$

x^2 term is included in H_0 so that it has a unique state. Goal: Perturbatively calculate *time ordered n-point functions*

$$\tau(t_1, t_2, \dots, t_n) := \langle \Omega | T(X_H(t_1) X_H(t_2) \dots X_H(t_n)) | \Omega \rangle \quad (3.41)$$

with $|\Omega\rangle$ the ground state of H . This means expressions $|\Omega\rangle$ by $|0\rangle$ (ground state of H_0) and $X_H(t)$ by $X_I(t)$ order by order in λ : Remember for HO:

$$X_H(t) \equiv X_I(t) = \frac{1}{\sqrt{2\omega}} \frac{\hbar}{m} (ae^{-i\omega t} + a^\dagger e^{i\omega t}) \quad (3.42)$$

with $[a, a^\dagger] = 1$ annihilation and creation operator of HO, i.e.

$$a|0\rangle = 0 \quad (3.43)$$

Theorem 3.2 (Magic formula of Gell-Mann and Low). Consider

$$e^{-i/hHT} |0\rangle = e^{-i/hE_0T} |\Omega\rangle\langle\Omega| |0\rangle + \sum_{n>0} e^{-i/hE_nT} |n\rangle\langle n| |0\rangle \quad (3.44)$$

with $|n\rangle$ the higher energy eigenstates of H , so that $E_0 < E_n \forall n$. Thus

$$|\Omega\rangle = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{e^{-i/hHT} |0\rangle}{e^{-i/hE_0T} \langle\Omega|0\rangle} = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{U_I(t_0, -T) |0\rangle}{e^{-i/hE_0(T+t_0)} \langle\Omega|0\rangle}$$

where we have set the zero point of energy such that $H_0 |0\rangle = 0$, and used:

$$e^{-i/hH(T+t_0)} = e^{-i/hH(t_0-(-T))} e^{-i/hH_0(-T-t_0)} e^{i/hH_0(-T-t_0)} = U_I(t_0, -T) e^{i/h(-T-t_0)H_0}.$$

Similarly:

$$\langle\Omega| = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0| U_I(T, t_0)}{e^{-i/hE_0(T-t_0)} \langle 0|\Omega\rangle}$$

Note that this implies:

$$1 = \langle\Omega|\Omega\rangle = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0| U_I(T, -T) |0\rangle}{e^{-2i/hE_0T} |\langle 0|\Omega\rangle|^2}$$

Expressing $X_H(t)$ by $X_I(t)$:

$$X_H(t) = U^\dagger(t, t_0) X U(t, t_0) = U^\dagger(t, t_0) U_0(t, t_0) X_I(t) U_0^\dagger(t, t_0) U(t, t_0) \underbrace{=}_{(3.12)} U_I^\dagger(t, t_0) X_I(t) U_I(t, t_0)$$

Hence for $t_1 > t_2 > \dots > t_n > t_0$

$$T(X_H(t_1) \dots X_H(t_n)) = U_I^\dagger(t_1, t_0) X_I(t_1) U_I(t_1, t_2) X_I(t_2) \dots U_I(t_{n-1}, t_n) X_I(t_n) U_I(t_n, t_0)$$

Putting everything together we get

$$\tau(t_1, \dots, t_n) = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0| U_I(T, t_0) X_I(t_1) U_I(t_1, t_2) X_I(t_2) \dots X_I(t_n) U_I(t_n, -T) |0\rangle}{\langle 0| U_I(T, -T) |0\rangle}.$$

Since T becomes larger and $-T$ smaller than any t_i , we can write

$$\tau(t_1, \dots, t_n)1 = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0|T(\dots)|0\rangle}{\langle 0|T(\dots)|0\rangle}$$

can drop requirement $t_1 > t_2 \dots$! Now we can collect all U_I in the numerator, because time-ordering takes care:

$$\tau(t_1, \dots, t_n) = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0|T(X_I(t_1) \dots X_I(t_n) \exp\left[-\frac{i}{\hbar} \int_{-T}^T V_I(t') dt'\right])|0\rangle}{\langle 0|T(\exp\left[-\frac{i}{\hbar} \int_{-T}^T V_I(t') dt'\right])|0\rangle} \quad (3.45)$$

The “magic” formula of Gell-Mann and Low. Remains to expand RHS of (3.45) in orders of λ . Important information about HO expectation values:

Theorem 3.3 (Wick’s theorem (for the HO)). For $m = n + k$ vertices, where k are internal (λ^k order) and n external (n -point function) vertices.

$$\langle 0|T(X_I(t_1) \dots X_I(t_m))|0\rangle = \begin{cases} 0 & \text{if } m \text{ is odd} \\ \sum_{\substack{\text{partitions of } n \text{ into} \\ \text{unordered pairs}}} \prod_{\substack{\text{pairs} \\ \{p_1, p_2\}}} \langle 0|T(X_I(t_{p_1})X_I(t_{p_2}))|0\rangle \end{cases} \quad (3.46)$$

Example 3.4.

$$\begin{aligned} & \langle 0|T(X_I(1)X_I(2)X_I(3)X_I(4))|0\rangle \\ &= \langle 0|T(X_I(1)X_I(2))|0\rangle \langle 0|T(X_I(3)X_I(4))|0\rangle \\ &+ \langle 0|T(X_I(1)X_I(3))|0\rangle \langle 0|T(X_I(2)X_I(4))|0\rangle \\ &+ \langle 0|T(X_I(1)X_I(4))|0\rangle \langle 0|T(X_I(2)X_I(3))|0\rangle \end{aligned} \quad (3.47)$$

Which will be proofed later.

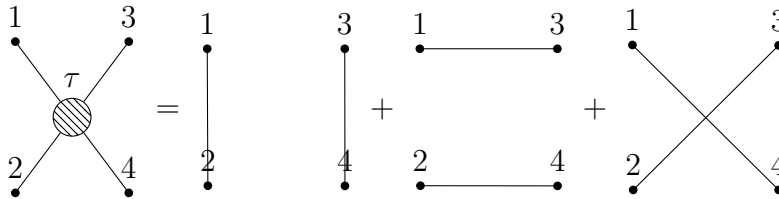
The sole building block of this is the Feynman propagator

$$\tau_0(t_1, t_2) = \langle 0|T(X_I(t_1)X_I(t_2))|0\rangle.$$

Using previous equations (WLOG $t_1 > t_2$)

$$\begin{aligned} \tau_0(t_1, t_2) &= \frac{1}{2\omega} \frac{\hbar}{m} \langle 0|\alpha e^{-i\omega t_1} \alpha^\dagger e^{i\omega t_2}|0\rangle = e^{-i\omega(t_1-t_2)} \frac{1}{2\omega} \frac{\hbar}{m} \\ &= e^{-i\omega|t_1-t_2|} \frac{1}{2\omega} \frac{\hbar}{m} \text{ not necessary to have } t_1 > t_2 \end{aligned}$$

Application of Wick’s theorem can be visualized by diagrams: *Feynman diagrams*. Each line is a Feynman propagator τ_0


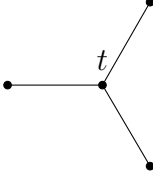


Numerator of (3.45). For definitenes: $K = 4$ in (3.40), $n = 2$ in (3.45)

$$\begin{aligned}
X &:= \langle 0 | T(X_I(t_1)X_I(t_2) \exp \left[-\frac{i}{\hbar} \int_{-T}^T \frac{\lambda(X_I(t))^4}{4!} dt \right]) | 0 \rangle \\
&= \langle 0 | T(X_I(t_1)X_I(t_2) \\
&\quad \left(\mathbb{1} + \left(-\frac{i\lambda}{\hbar 4!} \right) \int (X_I(t))^4 dt + \frac{1}{2} \left(-\frac{i\lambda}{\hbar 4!} \right)^2 \int (X_I(t))^4 (X_I(t'))^4 dt dt' + \dots \right) | 0 \rangle \\
&= \tau_0(t_1, t_2) - \frac{i\lambda}{\hbar 4!} \int \langle 0 | X_I(t_1) X_I(t_2) (X_I(t))^4 | 0 \rangle dt + \dots \\
&= \tau_0(t_1, t_2) - 3 \frac{i\lambda}{\hbar 4!} \tau_0(t_1, t_2) \int_{-T}^T dt \tau_0(t, t) \tau(t, t) \\
&\quad - 12 \frac{i\lambda}{\hbar 4!} \int_{-T}^T dt \tau_0(t_1, t) \tau(t, t_2) \tau(t, t) + \dots \\
&= \begin{array}{c} 1 \quad 2 \\ \bullet \text{---} \bullet \end{array} + \frac{1}{8} \begin{array}{c} 1 \quad 2 \\ \bullet \text{---} \bullet \\ \text{\scriptsize } \circlearrowleft t \\ \bullet \text{---} \bullet \end{array} + \frac{1}{2} \begin{array}{c} 1 \quad 2 \\ \bullet \text{---} \bullet \\ \text{\scriptsize } \circlearrowleft t \end{array} + \dots
\end{aligned}$$

Prefactors $\frac{1}{8}(2*2[\text{one } 2 \text{ per loop}] * 2[\text{switch loops}])$, $\frac{1}{2}$ (one loop) result from absorbing some of the numerical prefactors into the diagram.

Feynman rules

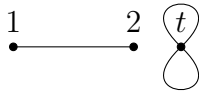
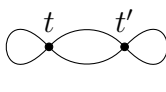
Diagram	name	analytic expression
	propagator	$\tau_0(t, t')$
	internal vertex	$-\frac{i\lambda}{\hbar} \int_{-T}^T dt$
Symmnetries in diagram		divide by symmetry factor (example see above)

To calculate the X:

$$X = \left(\text{Sum over all possible (internal vertices must be 4-valent) diagrams with 2 external vertices} \right) \quad (3.48)$$

Remark. Two different types of diagrams:

- without “vacuum bubbles”: $\begin{array}{c} 1 \quad 2 \\ \bullet \text{---} \bullet \end{array}$ or $\begin{array}{c} 1 \quad 2 \\ \bullet \text{---} \bullet \\ \text{\scriptsize } \circlearrowleft t \end{array}$



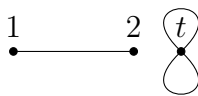
- with “vacuum bubbles”:  or 

Where a “vacuum bubble” is a component (sub-)diagram without external legs.

Combinatorics gives:

$$\left(\sum \text{all possible Feynman diagrams with } n \text{ external legs} \right) = \left(\sum \text{all diagrams without vacuum bubbles} \right) \cdot \underbrace{\exp \left(\sum \text{all vacuum bubble diags.} \right)}_{= (*)} \quad (3.49)$$

where multiplication is the union of diagrams.

Example 3.5.  \cdot  = 

$$\begin{aligned} \text{So } (*) &= 1 + \underbrace{\left(\text{vacuum bubble} + \text{vacuum bubble} + \text{vacuum bubble} + \dots \right)}_{(a)} + \frac{1}{2}(a)^2 + \dots \\ &= 1 + (a) + \left(\text{vacuum bubble} \text{ } \text{vacuum bubble} + \text{vacuum bubble} \text{ } \text{vacuum bubble} + \dots \right) + \dots \end{aligned}$$

Furthermore: Denominator in (3.45)

$$\langle 0 | T \left(\exp \left[-\frac{i}{\hbar} \int_{-T}^T \frac{\lambda (X_I(t))^4}{4!} dt \right] \right) | 0 \rangle = \exp \left(\sum \text{all vacuum bubbles} \right) \quad (3.50)$$

(One can proof this, see reference) Thus we finally find

$$\tau(t_1, \dots, t_n) = \lim_{T \rightarrow \infty(1-i\epsilon)} \left(\sum \text{all possible ("connected") Feynman diagrams with } n \text{ ext. legs without vacuum bubbles} \right) \quad (3.51)$$

Remark. • many terms subsumed under a single diagram

- No guaranty that power series in λ converges
- No guaranty that the integral for a single Feynman diagram converges (\rightarrow Problem of renormalisation in QFT)
- Standard pertubation approach in QFT \rightarrow Scattering amplitudes

Feynman rules in general cases

For general k , rule for internal vertices

$$\text{k legs} \left[\text{diagram} \right] \leftrightarrow \frac{-i\lambda}{\hbar} \int_{-\tau}^{\tau} dt$$

More generally, $V = \sum_k \lambda_k \frac{x^k}{k!}$ gives different types of internal vertices:

$$\text{k legs} \left[\text{diagram} \right] \leftrightarrow \frac{-i\lambda_k}{\hbar} \int_{-\tau}^{\tau} dt$$

Finally, we would have $H = H_0^{(1)} \otimes H_0^{(2)} \otimes \dots \otimes H_0^{(l)} + V$ with harmonic oscillators $H_0^{(i)}, i \in \{1, \dots, l\}$ and $V = \lambda \prod_{i=1}^l \frac{(x^{(i)})^{k_i}}{k_i!}$. Then Feynman rules become:

Diagram	analytic expression
t_1 (i) t_2 	$\tau_0^{(i)}(t, t')$
	$-\frac{i\lambda_k}{\hbar} \int_{-T}^T dt$

Often different lines for different Feynman propagators

$$\begin{array}{l}
 t_1 \text{ (1) } t_2 \leftrightarrow t_1 \text{ --- } t_2 \\
 t_1 \text{ (2) } t_2 \leftrightarrow t_1 \text{ --- } t_2
 \end{array}$$

In QFT this would correspond to different particle species.

4 Scattering Theory

Theoretical description of scattering experiment:

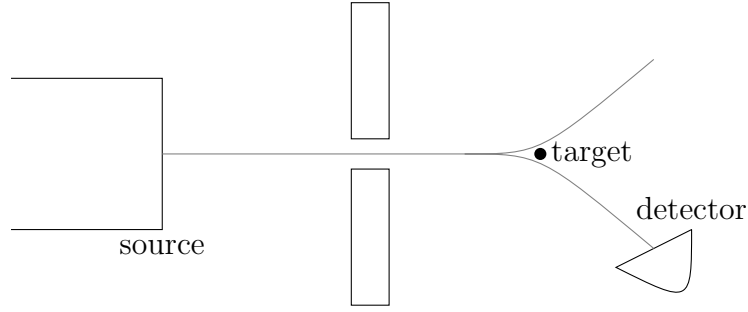


Figure 9: Scattering apparatus

Main assumption

Interaction between particles and target falls off fast, such that particles are approximately free away from vicinity of the target.

Main goal

Calculation of *scattering cross section*: Consider a particle bunch B scattering off of target bunch A with velocity v :

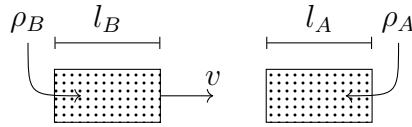


Figure 10: Scattering apparatus

There is a cross section area A_C common to both bunches, then:

$$\sigma := \frac{N}{\rho_A l_A \rho_B l_B A_C} \tag{4.1}$$

the scattering cross section, where N is the number of observed scattering events. Scattering events are usually selected according to parameters, i.e. energy, particle-content, scattering angle, $\dots \rightarrow \sigma$ becomes dependent on the selection of parameters. Most important for QM: angular selection: $\sigma = \sigma(\Omega)$, where Ω is the solid angle (area on the unit sphere).

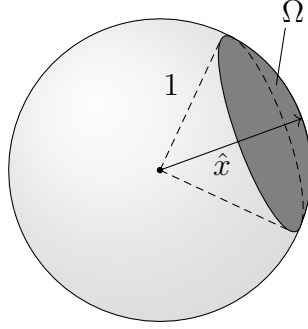


Figure 11: Solid angle on the unit sphere

Then $\frac{d\sigma}{d\Omega}(\hat{x})$ the *differential cross section* in direction of \hat{x} (unit vector) is also relevant.

Remark. σ has units of an area. We can indeed imagine every particle of A as a scattering area σ of bunch B:

$$N = N_A \sigma \rho_B l_B, N_A = \rho_A l_A A_C \quad (4.2)$$

In principle: scattering of wave packets:

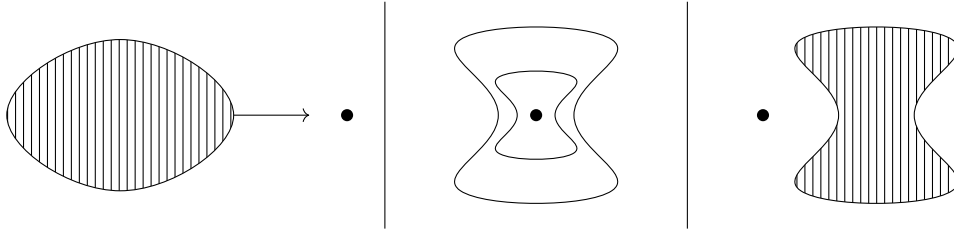


Figure 12: Scattering of a wave packet (before — during — after)

It turns out, that we can analyse the situation for wave packets by considering the stationary case (wave packet \rightarrow plane wave). We will find a solution to the Schrödinger

$$\Psi_k^+(\vec{x}) \approx e^{ik\vec{x}} + f_k(\hat{x}) \frac{e^{ikr}}{r} \quad (4.3)$$

with $\hat{x} = \vec{x}/|\vec{x}|$, $r = |\vec{r}|$. We will calculate the scattering amplitude $f_k(\hat{x})$ in various approximations. The differential cross section will be given by

$$\frac{d\sigma}{d\Omega}(\hat{x}) = |f_k(\hat{x})|^2 \quad (4.4)$$

4.1 S -matrix, scattering amplitudes

Consider $H = H_0 + V$, $H_0 = \frac{p^2}{2m}$ with *short range potential* V , such that

$$\lim_{|\vec{x}| \rightarrow \infty} |\vec{x}| |V(\vec{x})| = 0 \quad (4.5)$$

Remark. This excludes the Coulomb potential, but it is possible to treat the Coulomb potential with a similar formalism (see tutorial).

We can expand the wave function in terms of eigenbasis of H_0 ,

$$|\vec{k}\rangle(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{x}\vec{k}} \quad (4.6)$$

with

$$\langle \vec{k} | \vec{k}' \rangle = \delta(\vec{k} - \vec{k}'), H_0 |\vec{k}\rangle = \frac{\hbar^2 \vec{k}^2}{2m} |\vec{k}\rangle =: E_0(\vec{k}) |\vec{k}\rangle.$$

We now consider a wave packet in the interaction picture:

$$\Psi_I(t, \vec{x}) = \int C(t, \vec{k}) |\vec{k}\rangle(\vec{x}) d^3k$$

Remark. $C_{\pm}(\vec{k}) := \lim_{t \rightarrow \pm\infty} C(t, \vec{k})$ is well defined because Ψ_I becomes constant in t for large/small t (Ψ_I evolves with V_I , which becomes negligible far away from the target). All information about scattering is in the map $C_- \rightarrow C_+$. In fact:

$$C_+(\vec{k}') = \int C_-(\vec{k}) S(\vec{k}, \vec{k}') d^3k \text{ with}$$

$$S(\vec{k}, \vec{k}') = \langle \vec{k} | S | \vec{k}' \rangle, S = \text{T exp} \left(\int_{-\infty}^{\infty} dt V_I(t) \right), \quad (4.7)$$

where S as well as the matrix elements $S(\vec{k}, \vec{k}')$ are called *S-matrix* (scattering matrix).

We now set the reference time $t_0 = 0$, and interpret the $|k\rangle$ as Schrödinger states at $t = 0$,

$$S(\vec{k}, \vec{k}') = \lim_{t \rightarrow \infty, t' \rightarrow -\infty} \langle \vec{k} | e^{i\hbar H_0 t} e^{-i\hbar H(t-t')} e^{-i\hbar H_0 t'} | \vec{k}' \rangle =^{(-)} \langle \vec{k} | \vec{k}' \rangle^{(+)} \quad (4.8)$$

$$\text{with } |\vec{k}\rangle^{(\pm)} = \lim_{t' \rightarrow \pm\infty} U(0, t') U_0(t', 0) |\vec{k}\rangle \quad (4.9)$$

Interpretation: $|\vec{k}\rangle^{(+)}$ was a plane wave in the distant past, while $|\vec{k}\rangle^{(-)}$ will be a plane wave in the distant future. The operators involved in (4.9)

$$\Omega^{(\pm)} := \lim_{t' \rightarrow \pm\infty} U(0, t') U_0(t', 0) \quad (4.10)$$

are called *Moeller operators* (Wave operators) and have a remarkable property

$$\Omega^{(\pm)} H_0 = H \Omega^{(\pm)} \quad (4.11)$$

$$\text{since } S = (\Omega^{(-)})^\dagger \Omega^{(+)} \quad (4.12)$$

it follows that $[S, H_0] = 0$. That means $S(\vec{k}, \vec{k}') \propto \delta(\vec{k}, \vec{k}')$, and we parametrize

$$S(\vec{k}, \vec{k}') =: \langle \vec{k} | \vec{k}' \rangle - 2\pi i \delta(\underbrace{E_{\vec{k}'} - E_{\vec{k}}}_{\equiv E_0(\vec{k}')}) \Gamma(\vec{k}', \vec{k}) \quad (4.13)$$

First term \propto wave going through without scattering, while we still have to calculate the second one.

4.2 Lippman-Schwinger equation

At first we need some technology

Advanced and retarded propagators

$$\begin{aligned} G^{(\pm)}(t) &:= \mp \frac{i}{\hbar} \Theta(\pm t) U(t) \equiv U(t, 0) \\ G_0^{(\pm)}(t) &:= \mp \frac{i}{\hbar} \Theta(\pm t) U_0(t) \end{aligned} \quad (4.14)$$

the retarded (+) and advanced (-) full and free (0) propagators Greens functions of the Schrödinger equation:

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t} - H \right) G^\pm(t) &= \delta(t) \\ \left(i\hbar \frac{\partial}{\partial t} - H_0 \right) G_0^\pm(t) &= \delta(t) \end{aligned}$$

Need \mathcal{F} -transforms of these

$$G_{(0)}^\pm(E) \stackrel{?}{:=} \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} Et} G_{(0)}^{(\pm)}(t)$$

Integral will not be convergent in general. Define this (distribution!) by adding a small imaginary part to the energy

$$G_{(0)}^\pm(E) \stackrel{!}{:=} \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar} (E \pm i\epsilon)t} G_{(0)}^{(\pm)}(t)$$

Example 4.1. Carry out the integration

$$G_{(0)}^+(E) = \lim_{\epsilon \rightarrow 0^+} -\frac{i}{\hbar} \int_0^{\infty} dt e^{\frac{i}{\hbar} (E + i\epsilon - H_{(0)})t} = \lim_{\epsilon \rightarrow 0^+} \frac{1}{E - H_{(0)} + i\epsilon} \quad (4.15)$$

$$G_{(0)}^-(E) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{E - H_{(0)} - i\epsilon} \quad (4.16)$$

Will also need $G_0^{(+)}$ in position representation. In k -rep. we have

$$\langle \vec{k} | G_0^{(+)}(E) | \vec{k}' \rangle = \lim_{\epsilon \rightarrow 0^+} \frac{1}{E - E_{\vec{k}} + i\epsilon} \delta(\vec{k} - \vec{k}')$$

from this we get for $\epsilon > 0$

$$G_0^{(+)}(E, \vec{x} - \vec{x}') := \langle \vec{x} | G_0^{(+)}(E) | \vec{x}' \rangle = \int d^3k \frac{1}{(2\pi)^3} \frac{1}{E - E_{\vec{k}} + i\epsilon} e^{i\vec{k}(\vec{x} - \vec{x}')}$$

Use spherical coordinates to carry out θ, φ integrals for $\epsilon > 0$

$$G_0^{(+)}(E, \vec{x}) = \frac{1}{(2\pi)^2} \frac{1}{i|\vec{x}|} \int_{-\infty}^{\infty} dk \frac{k e^{ik|\vec{x}|}}{E - E_k + i\epsilon}$$

Interpret as contour integral in the complex k -plane. Closing the contour in the upper half plane, use of the theorem of residues yield

$$G_0^{(+)}(E_{\vec{k}}, \vec{x}) = -\frac{m}{2\pi\hbar} \frac{e^{ik|\vec{x}|}}{|\vec{x}|} \quad (4.17)$$

First thing to note

$$\begin{aligned} \Omega^{(+)} &\equiv \frac{\hbar}{i} \int_{-\infty}^{\infty} \frac{d}{dt} [G^{(+)}(-t)U_0(t)] dt = \int_{-\infty}^{\infty} G^+(-t)(H - H_0)U_0(t)dt + 1 \\ &= 1 + \int_{-\infty}^{\infty} G^+(t)VU_0(-t)dt \end{aligned} \quad (4.18)$$

Now we apply this to $|\vec{k}\rangle$

$$\begin{aligned} \Omega^+ |\vec{k}\rangle &= \lim_{\epsilon \rightarrow 0} \left(1 + \frac{1}{E_{\vec{k}} - H + i\epsilon} V \right) |\vec{k}\rangle = \lim_{\epsilon \rightarrow 0} \frac{1}{E_{\vec{k}} - H + i\epsilon} (E_{\vec{k}} - H + V + i\epsilon) |\vec{k}\rangle \\ &= \lim_{\epsilon \rightarrow 0} \frac{i\epsilon}{E_{\vec{k}} - H + i\epsilon} |\vec{k}\rangle \end{aligned} \quad (4.19)$$

Finally we get

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \frac{E_{\vec{k}} - H + i\epsilon}{E_{\vec{k}} - H + i\epsilon} \Omega^+ |\vec{k}\rangle &= |\vec{k}\rangle \text{ and hence} \\ \Leftrightarrow \Omega^+ |\vec{k}\rangle &= |\vec{k}\rangle + \lim_{\epsilon \rightarrow 0} \frac{1}{E_{\vec{k}} - H + i\epsilon} V \Omega^+ |\vec{k}\rangle = |\vec{k}\rangle + G_0^+(E_{\vec{k}}) V \Omega^+ |\vec{k}\rangle \end{aligned} \quad (4.20)$$

the Lippmann-Schwinger equation. We can iterate

$$|\vec{k}\rangle^+ = \lim_{\epsilon \rightarrow 0^+} \left(|\vec{k}\rangle + \frac{1}{E_{\vec{k}} - H_0 + i\epsilon} V |\vec{k}\rangle + \left[\frac{1}{E_{\vec{k}} - H_0 + i\epsilon} V \right]^2 |\vec{k}\rangle + \dots \right) \quad (4.21)$$

Remark. • Heuristic interpretation: $0 \times$ scattering $+1 \times$ scattering $+\dots$

- Perturbation treatment: cut off after finitely many terms

Also

$$|\vec{k}\rangle^+ = |\vec{k}\rangle + |\vec{k}\rangle_{sc}$$

where $|\vec{k}\rangle_{sc}$ is the scattered contribution. Plugging (4.17) in (4.20)

$$|\vec{k}\rangle^+(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}} - \frac{m}{2\pi\hbar^2} \int d^3x' \frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} V(\vec{x}') |\vec{k}\rangle^+(\vec{x}') \quad (4.22)$$

4.3 Scattering amplitude and scattering cross section

Since $V(\vec{x})$ is short range, we can approximate:

$$|\vec{x}-\vec{x}'| \approx r - \hat{x}\hat{x}', \hat{x} = \frac{\vec{x}}{|\vec{x}|}, |\vec{x}| = r$$

in (4.22) for points \vec{x} far from target.

$$|\vec{k}\rangle^+(\vec{x}) \approx \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}} + \frac{1}{(2\pi)^{3/2}} f_{\vec{k}}(\hat{x}) \frac{e^{ikr}}{r}(\vec{x})$$

where

$$f_{\vec{k}}(\hat{x}) = -\frac{\sqrt{2\pi}m}{\hbar^2} \int d^3x' e^{-ik\hat{x}\hat{x}'} V(\vec{x}') |\vec{k}'\rangle^+(\vec{x}') = -\frac{\sqrt{2\pi}m}{\hbar^2} \langle \vec{k}' | V | \vec{k} \rangle^+ \quad (4.23)$$

with $\vec{k}' = |\vec{k}|\hat{x}$. $f_{\vec{k}}(\hat{x})$ is called the *scattering amplitude*.

Connection to the scattering cross-section

QM-probability current:

$$\vec{j} = \frac{\hbar}{2mi} [\bar{\Psi} \nabla \Psi - (\nabla \bar{\Psi}) \Psi] \quad (4.24)$$

Fullfills the continuity equation

$$\dot{\rho} + \nabla \cdot \vec{j} = 0 \text{ with } \rho = \bar{\Psi} \Psi$$

A plane wave has

$$\vec{j}_{\vec{k}} = \frac{1}{(2\pi)^3} \frac{\hbar \vec{k}}{m} = \frac{1}{(2\pi)^3} \vec{V}$$

For the scattered wave $|\vec{k}\rangle_{\text{sc}}$, we find

$$\vec{j}_{\text{sc}}(\vec{x}) = \frac{\hbar|\vec{k}|}{m} \frac{1}{r^2} |f_{\vec{k}}(\hat{x})|^2 \hat{x} + \mathcal{O}\left(\frac{1}{r^3}\right)$$

For the (differential) cross section:

$$\sigma(\hat{x}, r, \Omega) = \frac{\vec{j}_{\text{sc}} \hat{x} r^2 \Omega}{|\vec{j}_{\vec{k}}|} \text{ and } \frac{d\sigma}{d\Omega} = \frac{\vec{j}_{\text{sc}} \hat{x} r^2 \hat{x}}{|\vec{j}_{\vec{k}}|^2} \approx |f_{\vec{k}}(\hat{x})|^2 \quad (4.25)$$

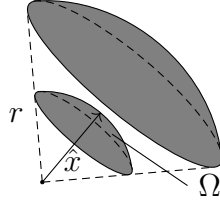


Figure 13: Angle

Born approximation

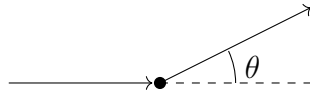
We iterate only once

$$f_{\vec{k}}(\hat{x}) \approx -\frac{(2\pi)^2 m}{\hbar^2} \langle \vec{k}' | V | \vec{k} \rangle = -\frac{(2\pi)^2 m}{\hbar^2} \frac{1}{(2\pi)^{3/2}} \tilde{V}(\vec{k}' - \vec{k}) \quad (4.26)$$

For $V(\vec{x}) \equiv V(|\vec{x}|)$

$$f_k(\theta) = -\frac{2m}{\hbar^2 q} \int_0^\infty dr' r' V(r') \sin(qr')$$

with $q = 2k \sin\left(\frac{\theta}{2}\right)$



For $V(\vec{x}) \equiv V(|\vec{x}|)$ we can partially calculate:

$$\begin{aligned} \frac{1}{(2\pi)^{3/2}} \tilde{V}(\vec{k}' - \vec{k}) &= \frac{1}{(2\pi)^{3/2}} \int d^3x e^{-i\vec{q}\vec{x}} V(\vec{x}) \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty dr' \int_0^\pi d\theta \int_0^{2\pi} d\varphi r' \sin(\theta) e^{-iqr' \cos(\theta)} V(r') \\ &= \frac{2}{(2\pi)^2 q} \int_0^\infty dr' r' \sin(qr') V(r') \end{aligned}$$

with $q = |\vec{q}|$, $\vec{q} = \vec{k}' - \vec{k}$ can be interpreted as the momentum exchanged in the scattering process.

$$q^2 = \vec{k}^2 + \vec{k}'^2 - 2|\vec{k}||\vec{k}'|\cos(\theta) = \dots = 4k^2 \sin^2\left(\frac{\theta}{2}\right)$$

Then we have

$$f_k(\theta) = -\frac{2m}{\hbar^2 q} \int_0^\infty dr' r' \sin(qr') V(r') \quad (4.27)$$

Partial wave decomposition

Useful for $V(\vec{x}) \equiv V(|\vec{x}|)$. Then $[\vec{L}, H] = 0$ and we can decompose into \vec{L} -eigenfunctions.

$$|\vec{k}\rangle^+(\vec{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_{\vec{k}lm}(r) \Psi_{lm}(\theta, \varphi)$$

For $\vec{k}^+ \equiv k\vec{e}_z$, only $m = 0$ contributes, so we get

$$|\vec{k}\rangle^+ = \sum_{l=0}^{\infty} \frac{U_{kl}(r)}{r} P_l(\cos(\theta)) \quad (4.28)$$

From (4.11): $|\vec{k}\rangle^+$ eigenstate of H with eigenvalue $E_{\vec{k}}$. Plugging in (4.28) into the Schrödinger eq.

$$\begin{aligned} u''_{kl}(r) + (k^2 - V_l(r))u_{kl}(r) &= 0 \\ V_l(r) &= \frac{2m}{\hbar^2} V(r) + \frac{\hbar l(l+1)}{2mr^2} \end{aligned} \quad (4.29)$$

Equations decouple, typically solve only for low l . In particular, $l = 0$: “S-wave scattering”.

Scattering phases

Connection between $f_k(\theta)$ and $U_{kl}(r)$. We expand

$$|\vec{k}\rangle^+(\vec{x}) \approx \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}} + \frac{1}{(2\pi)^{3/2}} \frac{e^{ikr}}{r} f_{\vec{k}}(\hat{x})$$

in Legendre polynomials.

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1) f_k(l) P_l(\cos(\theta))$$

Moreover

$$e^{i\vec{k}\vec{x}} = e^{ikr \cos(\theta)} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos(\theta)) \quad (4.30)$$

with $j_l(\cdot)$ a spherical Bessel function. For large r :

$$j_l(kr) \approx (e^{i(kr-l\frac{\pi}{2})} - e^{-i(kr-l\frac{\pi}{2})}) / (2ikr)$$

and hence

$$\left| \vec{k} \right\rangle^+ (\vec{x}) \approx \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos(\theta))}{2ik} \left[\underbrace{(1 + 2ik f_k(l))}_{=: S_k(l)} \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right] \quad (4.31)$$

Effects of scattering all in outgoing wave. We can show by considering the probability current $j(\vec{x})$ corresponding to $\left| \vec{k} \right\rangle^+ (\vec{x})$, that $|S_k(l)| = 1$. Define *scattering phase shift* $\delta_l(k)$

$$S_k(l) = e^{i2\delta_l(k)} \quad (4.32)$$

It follows that

$$f_k(l) = \frac{e^{i\delta_l(k)} \sin(\delta_l(k))}{k}$$

and

$$f_k(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l(k)} \sin(\delta_l(k)) P_l(\cos(\theta)) \quad (4.33)$$

For small δ_l : $f_k(l) \approx \frac{f_l}{k}$ is small. For $\delta_l \approx \frac{\pi}{2}$: $f_k \approx \frac{i}{k} \rightarrow$ Resonances. Formula for $\frac{d\sigma}{d\Omega}$ in terms of δ_l 's not particularly enlightening. But

$$\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega} d\Omega = \sum_{l=0}^{\infty} \sigma_l \text{ with } \sigma_l = \frac{2\pi}{k^2} (2l+1) \sin^2(\delta_l) \quad (4.34)$$

shows independence of partial waves. Also

$$\sigma_l \leq \frac{4\pi}{k^2} (2l+1) \propto \frac{1}{E_k}$$

To calculate the phase shifts, we solve (4.29). Far away from 0:

$$\left| k \right\rangle^+ \approx \frac{1}{(2\pi)^{3/2}} \sum_l \underbrace{A_{kl}(r)}_{=\frac{u_{kl}}{r}} P_l(\cos(\theta))$$

$$A_{kl}(r) \approx i^l (2l+1) e^{i\delta_l} (\cos(\delta_l) j_l(kr) - \sin(\delta_l) n_l(kr)) \quad (4.35)$$

with $n_l(\cdot)$ a Hankel function. Match continuously (1), differentiable (2) to solution of (4.29) with $u_{kl}|_{r=0} = 0$. This yields 3 equations for 3 unknowns. 2 initial conditions for $u_{kl}(\cdot)$ and the $\delta_l \Rightarrow \delta_l$ is determined.

***S*-matrix and optical theorem**

We can obtain $f_k(\theta)$ directly from the S -matrix: First:

$$\Omega^\pm |k\rangle = (1 + G^{(\pm)}(E_k)V) |k\rangle \quad (4.36)$$

Then

$$(G^+(E) - G^-(E)) \Omega^{(+)} |k\rangle = -2\pi i \delta(E - E_k) \quad (4.37)$$

Finally

$$\langle k|^{(-)} = \langle k| V (G^+(E) - G^-(E)) +^+ \langle k|$$

And using this and the definitions of $S(\vec{k}, \vec{k}')$

$$S(\vec{k}, \vec{k}') = \delta^{(3)}(\vec{k} - \vec{k}') + 2\pi i \delta(E_{\vec{k}} - E_{\vec{k}'}) \frac{\hbar^2}{(2\pi)^2 m} f_{\vec{k}}(\theta) \quad (4.38)$$

From unitarity of S

$$\delta^3(\vec{k} - \vec{k}') = \int d^3 k'' \langle \vec{k}' | S | \vec{k}'' \rangle \langle \vec{k}'' | S^\dagger | \vec{k} \rangle$$

and (4.23) and (4.38) we obtain the *optical theorem*

$$\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im}(f_k(\theta = 0)) \quad (4.39)$$

5 Identical Particles

5.1 Introduction

Elementary particles of same species: experimentally indistinguishable: same mass, same charge, ... Classically they are distinguishable by their position. In quantum mechanics this is not well defined.

Example 5.1. Scattering

1. Classical

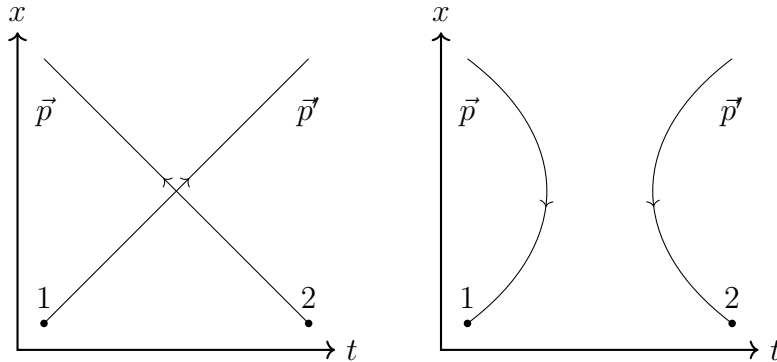


Figure 14: Classical scattering

2. QM

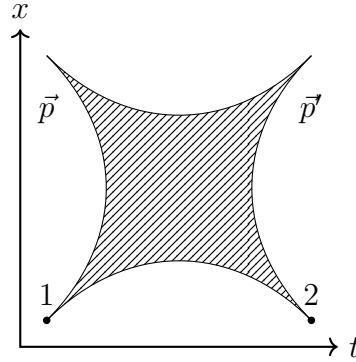


Figure 15: QM scattering

The two end states can be distinguished, in QM, particles are initially distinguished, but not after scattering.

More formally:

Exchange degeneracy

Two identical particles $\mathcal{H} = h_1 \otimes h_2, h_1 = h_2 = h$ ONB (orthonormal basis) of h : $|\underline{k}\rangle$ with $\underline{k} = (k_1, k_2, \dots)$ eigenvalues of complete set of observables \underline{Q} . Exchange operator:

$$T_{12} : |\underline{k}_1\rangle \otimes |\underline{k}_2\rangle = |\underline{k}_2\rangle \otimes |\underline{k}_1\rangle$$

Where only the observables \underline{Q} with

$$[\underline{Q}, T] = 0 (T = T_{12}) \quad (5.1)$$

are experimentally accessible. Let $\phi \in \mathcal{H}$ with $\langle \phi | T | \phi \rangle = 0, \|\phi\| = 1$. (for example $\phi = |\underline{k}\rangle \otimes |\underline{k}\rangle$ with $\underline{k}' \neq \underline{k}$) Then we have

$$\Psi = \alpha\phi + \beta T\phi, |\alpha|^2 + |\beta|^2 = 1 \quad (5.2)$$

These states are indistinguishable for observables with (5.1) (same expectation values etc.). This is called exchange degeneracy.

Boson-Fermion alternative

Note that since

$$T^\dagger = T, T^2 = \mathbb{1}$$

we can compose into eigenspaces

$$\mathcal{H} = \mathcal{H}_+ \otimes \mathcal{H}_-, T \Big|_{\mathcal{H}_\pm} = \pm \mathbb{1}_{\mathcal{H}_\pm} \quad (5.3)$$

Law of nature: Not all states in \mathcal{H} are allowed. Only:

- Bosons: states in \mathcal{H}_+
- Fermions: states in \mathcal{H}_-

This means that identical particles have smaller state spaces. We will see many consequences of this.

Spin-statistics correspondence

In relativistic QFT, in dimension $d \geq 3 + 1$ one can approximately prove, that

- integer spin/helicity \leftrightarrow bosons
- half-integer spin \leftrightarrow fermions

using the understanding of T as physical (spatial) exchange of particles. In lower dimensions, how many ways to exchange particles on spatial paths

- $3 + 1$: one way up to deformations of path
- $2 + 1$: many, SKETCH, would be different path exchanges different, could have states between fermions and bosons
- $1 + 1$: none

Boson-Fermion alternative does not hold in $2 + 1$ and $1 + 1$ dimensions.

5.2 n identical particles

$$S_n = \{\text{Permutations of } n \text{ things}\} = \{\text{Bijective maps on } n\text{-element sets}\}$$

- S_n is a group wrt. concatenation of permutations:

$$(P_1 \cdot P_2)(x) = P_1(P_2(x)), \text{ with } P_1, P_2 \in S_n$$

- every finite group is a subgroup of some S_n

Notation. 1. $S_n \ni P = \begin{pmatrix} 1 & 2 & \cdots & n \\ P(1)P(2) & \cdots & P(n) & \end{pmatrix}$ (where $P(i) \in 1, 2, \dots, n$)

2. $P = (12)(3)\cdots$: Cycle notation, by considering P, P^2, P^3, \dots

Special case: Transposition $\underbrace{T_{ij}}_{=P_{ij}} \equiv (ij) \equiv \begin{pmatrix} 1 \cdots i \cdots j \cdots n \\ 1 \cdots j \cdots i \cdots n \end{pmatrix}$

Definition 5.1 (Signature). The *signature* is an important property of permutations

$$\text{sign}(P) = (-1)^{I(P)} \tag{5.4}$$

with $I = |\{(x, y) \in 1, 2, \dots, n^2 : x < y, P(x) > P(y)\}|$

Lemma 5.2. 1.

$$\text{sign}(P) = (-1)^{\text{T}(P)} \quad (5.5)$$

where $P = \underbrace{P_{i_1 j_1} \cdot P_{i_2 j_2} \cdots}_{\text{T}(P)\text{transpositions}}$

2. sign is a group homomorphism:

$$\text{sign}(P_1 P_2) = \text{sign}(P_1) \text{sign}(P_2) \quad (5.6)$$

State space for n identical particles

State with

$$\mathcal{H} = \otimes_{k=1}^n h$$

with $\{|\underline{k}\rangle\}$ a basis of h as before.

Notation. $|\underline{k}_1\rangle \otimes \cdots \otimes |\underline{k}_n\rangle \equiv |\underline{k}_1, \cdots, \underline{k}_n\rangle$

Important subspace of \mathcal{H}

Let $n = \sum_{i=1}^m n_i, n_i \in \mathbb{N}, n_i \neq 0, \underline{l}_1, \cdots, \underline{l}_m$ with $\underline{l}_i \neq \underline{l}_k$ for $i \neq k$ (\underline{l}_i are the numbers that describe a physical state). Then we define

$$\mathcal{H}(n_1, \underline{l}_1, \cdots, n_m, \underline{l}_m) := \{|\underline{k}_1, \cdots, \underline{k}_n\rangle \mid n_i \text{ many of the } \underline{k}_j \text{'s are equal to } \underline{l}_i\} \quad (5.7)$$

Then $\dim \mathcal{H}(n_1, \underline{l}_1, \cdots) =$ exchange degeneracy for the ‘‘physical’’ state $n_1 \underline{l}_1, \cdots, n_m \underline{l}_m$
 S_n acts on \mathcal{H} :

$$\Pi(P) |\underline{k}_1\rangle \otimes \cdots \otimes |\underline{k}_n\rangle = |\underline{k}_{P(1)}\rangle \otimes \cdots \otimes |\underline{k}_{P(n)}\rangle$$

Lemma 5.3. $\Pi(\cdot)$ is a unitary representation of S_n . For identical particles, we must have

$$[\Pi(P), O] = 0 \forall P \in S_n \quad (5.8)$$

, in particular for $O = H$, the Hamiltonian.

Lemma 5.4. Π leaves the $\mathcal{H}(n_1, \underline{l}_1, \cdots)$ invariant.

(Anti-)symmetrizer

$$S = \frac{1}{n!} \sum_{P \in S_n} \Pi(P) \text{ and } A = \frac{1}{n!} \sum_{P \in S_n} \text{sign}(P) \Pi(P) \quad (5.9)$$

Lemma 5.5. 1. S and A are projections

$$S^\dagger = S, S^2 = S \text{ and } A^\dagger = A, A^2 = A \quad (5.10)$$

2.

$$\Pi(P)S = S\Pi(P) = S \quad (5.11)$$

$$\Pi(P)A = A\Pi(P) = \text{sign}(P)A \quad (5.12)$$

Bose-Fermi-alternative: Not all states of \mathcal{H} are allowed, only

$$\begin{aligned} \mathcal{H}_+ &:= S\mathcal{H} \text{ for Bosons} \\ \mathcal{H}_- &:= A\mathcal{H} \text{ for Fermions} \end{aligned}$$

5.3 Fermi- and Bose-Einstein statistics

Fermi-statistics: Obtain ONB of \mathcal{H}_- by anti-symmetrizing states of $\mathcal{H}(n_1, l_1, n_2, l_2, \dots)$ [Remember: Take $n_i \neq 0$ in our notation].

Lemma 5.6. 1. if $n_i > 1$ for some i , then $A\mathcal{H}(n_1, l_1, \dots) = 0$.

2. if all $n_i = 1$, then there is a unique (up to normalisation) anti-symmetric state in $\mathcal{H}(n_1, l_1, \dots)$

$$\sqrt{n!}A |l_1, l_2, \dots, l_n\rangle \quad (5.13)$$

is a normalized representative.

Proof. 1. Let $\psi \in \mathcal{H}(n_1, l_1, \dots)$ be of the form $\psi = \left| \dots, \underbrace{e_i}_k, \dots, \underbrace{e_i}_l, \dots \right\rangle$

Then $\Pi(P_{(kl)})\psi = \psi$, thus $A\Pi(P_{(kl)})\psi = A\psi$, but because (5.12): $A\Pi(P_{(kl)})\psi = -A\psi$

$\Rightarrow A\psi = 0$. If $n_i > 1$ for some i , then all states in $\mathcal{H}(l_1, n_1, \dots)$ are linear combination of states of the above form (for various k, l).

2. Uniqueness is obvious. Check normalisation

$$\begin{aligned} \|A |l_1, l_2, \dots\rangle\|^2 &= \frac{1}{(n!)^2} \sum_{P, P'} \text{sign}(P)\text{sign}(P') \underbrace{\langle l_{P(1)}, l_{P(2)} | l_{P'(1)}, l_{P'(2)} \rangle}_{\delta_{P, P'}} = \\ &= \frac{1}{(n!)^2} \sum_P (\text{sign}P)^2 \frac{1}{n!} \end{aligned}$$

gives normalisation of (5.13)

□

Remark. 1. First statement gives Pauli-exclusion-principle!

This helps to explain the structure of atoms: For atom with n electrons:

- $\mathcal{H} = (\mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^2)^{\otimes n}$
- $\underline{K} = (n, l, m, s)$
- Neglect interactions between electrons: $\mathcal{H}(n_1, \underline{l}_1, \dots)$ eigenspaces of energy.
- Lemma says: all n have to be 1.

Bose-Einstein-statistics: Consider symmetrization of $\mathcal{H}(n_1, \underline{l}_1, \dots)$

Lemma 5.7. There is, up to phase, one normalized totally symmetric state in $\mathcal{H}(n_1, \underline{l}_1, \dots)$:

$$\sqrt{\frac{n!}{n_1!n_2!\dots n_m!}} S \left| \underbrace{\underline{l}_1, \underline{l}_1, \dots, \underline{l}_1}_{n_1 \text{ times}}, \underbrace{\underline{l}_2, \underline{l}_2, \dots, \underline{l}_2}_{n_2 \text{ times}}, \dots \right\rangle \quad (5.14)$$

Proof. Uniqueness up to phase:

$$\psi = \sum_P c_P \Pi(P) \left| \underbrace{\underline{l}_1, \underline{l}_1, \dots, \underline{l}_1}_{n_1}, \underbrace{\underline{l}_2, \dots, \underline{l}_2}_{n_2} \right\rangle$$

But because (5.11):

$$S\psi = \sum_P c_P \underbrace{S\Pi(P)}_S |\rangle = c_S \left| \underbrace{\underline{l}_1, \underline{l}_1, \dots, \underline{l}_1}_{n_1}, \underbrace{\underline{l}_2, \underline{l}_2, \dots, \dots}_{n_2} \right\rangle$$

So that shows uniqueness up to phase. Normalisation:

$$\begin{aligned} \|S|\underline{l}_1, \dots, \underline{l}_2, \dots\rangle\|^2 &= \frac{1}{(n!)^2} \sum_{P, P'} \langle \underline{l}_{P(1)}, \underline{l}_{P(2)}, \dots | \underline{l}_{P'(1)}, \underline{l}_{P'(2)}, \dots \rangle \\ &= \frac{1}{(n!)^2} \sum_P (n_1!)(n_2!) \dots (n_m!) = \frac{(n_1!)(n_2!) \dots (n_m!)}{n!} \end{aligned}$$

which constitute normalisation of (5.14) □

Remark. Note that in both, Fermi and Boson case, exchange symmetry is removed.

5.4 Fermi and Boson gas

n identical particles, weakly interacting:

$$H \simeq \sum_{k=1}^n h_k, \quad h_k = \mathbb{1} \otimes \mathbb{1} \otimes \dots \otimes h \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} \quad (5.15)$$

with h the Hamiltonian for one particle. Denote E_m , $m \in \mathbb{N}_0$ spectrum of h . For simplicity, assume non-degeneracy. Then spectrum of H is

$$E = \sum_k n_k E_k, \quad n_k \geq 0, \quad \sum_k n_k = n$$

Now allow energy exchange with heat bath. Expectation values are governed by density matrix

$$\rho = \frac{e^{-\beta H}}{Z(\beta)}, \quad Z(\beta) = \text{tr}(e^{-\beta H}) \quad (5.16)$$

Consider Fermions first:

$$\langle n_k \rangle = \frac{\sum_{\underline{n}} n_k \exp(-\beta \sum_l n_l E_l)}{\sum_{\underline{n}} \exp(-\beta \sum_l n_l E_l)} = -\frac{1}{\beta} \frac{\partial \ln(Z(\beta))}{\partial E_k} \quad (5.17)$$

where $\sum_{\underline{n}}$ is over (n_1, n_2, \dots) with $n_i \in \{0, 1\}$, $\sum_i n_i = n$.

Definition 5.2.

$$Z_k(N) := \sum_{\underline{n}: n_k=0, \sum_l n_l=N} e^{-\beta \sum_l n_l E_l}$$

Then:

$$\langle n_k \rangle = \frac{e^{-\beta E_k} Z_k(n-1)}{Z_k(n) + e^{-\beta E_k} Z_k(N-1)}$$

Now treat N as continuous variable, and Taylor ($n \gg 1$) expand:

$$\begin{aligned} \ln(Z_k(n-1)) &\approx \ln(Z_k(n)) - \alpha_k \quad \text{with } \alpha_k = \frac{\partial \ln(Z_k(n))}{\partial n} \\ \text{or } Z_k(n-1) &\approx Z_k(n) e^{-\alpha_k} \end{aligned}$$

Furthermore, assume that $\alpha_k \simeq \alpha$. Then

$$\langle n_k \rangle = \frac{1}{e^{\alpha + \beta E_k} + 1} \quad (5.18)$$

with α given by

$$\sum_k \langle n_k \rangle = n$$

Similar calculation for the Boson gives

$$\langle n_k \rangle = \frac{1}{e^{\alpha + \beta E_k} - 1} \quad (5.19)$$

For high temperature (small β) behaviour is similar. For low temperature very different behaviour.

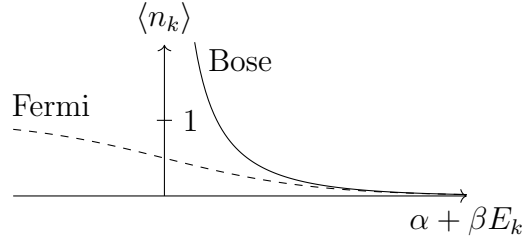


Figure 16: Fermi-Dirac and Bose-Einstein distributions

5.5 Fock space

Often it is useful not to fix the particle number. As before, we have h the one particle Hilbert space and $\mathcal{H}_n := h^{\otimes n}$, $\mathcal{H}_n^A := A \mathcal{H}_n$, $\mathcal{H}_n^S := S \mathcal{H}_n$ the Hilbert spaces for n (identical) particles. Let's agree that

$$\mathcal{H}_0 = \mathcal{H}_0^A + \mathcal{H}_0^S = \mathbb{C} \quad (5.20)$$

, then we get

$$\begin{aligned} \mathcal{F}(h) &:= \bigoplus_{n=0}^{\infty} \mathcal{H}_n \text{ Fock space} \\ \mathcal{F}_S(h) &:= \bigoplus_{n=0}^{\infty} \mathcal{H}_n^S \text{ Bosonic Fock space} \\ \mathcal{F}_A(h) &:= \bigoplus_{n=0}^{\infty} \mathcal{H}_n^A \text{ Fermionic Fock space} \end{aligned} \quad (5.21)$$

the Hilbert spaces for arbitrary numbers of particles.

- states in different n -sectors are orthogonal
- linear combinations of states with different particle number possible

There are two ways a operator in h can operate in $\mathcal{F}(h)$:

1. B operator on h , then $\Gamma(B)$ is an operator on $\mathcal{F}(h)$ by

$$\Gamma(B) \Big|_{\mathcal{H}_n} = \underbrace{B \otimes \cdots \otimes B}_{n\text{-times}} \quad (5.22)$$

and linear extension. This is well defined as $[A, B^{\otimes n}] = 0 = [S, B^{\otimes n}]$.

Remark. $\Gamma(BC) = \Gamma(B)\Gamma(C)$, $\Gamma(B)^\dagger = \Gamma(B^\dagger)$, etc.

2. $d\Gamma(B)$ operator on $\mathcal{F}(h)$ via

$$d\Gamma(B)\Big|_{\mathcal{H}_n} = \sum_{i=1}^n \mathbb{1} \otimes \cdots \otimes \underbrace{B}_i \otimes \mathbb{1} \cdots \otimes \mathbb{1} =: \sum_{i=1}^n B_i \quad (5.23)$$

Remark. if we set $\Gamma(B)\Big|_{\mathcal{H}_0} := \mathbb{1}$, $d\Gamma(B)\Big|_{\mathcal{H}_0} := 0$

$$\Gamma(e^{iB}) = e^{id\Gamma(B)} \quad (5.24)$$

Example 5.8. • Non-interacting particles, one-particle Hamiltonian h :

- $d\Gamma(h)$ = Hamiltonian on $\mathcal{F}(h)$
- $\Gamma(e^{ith})$ = time evolution op. on $\mathcal{F}(h)$

• Number operator:

$$N := d\Gamma(\mathbb{1}_h) \quad (5.25)$$

The observable corresponding to particle number. n -particle space \mathcal{H}_n are eigenspaces of N :

$$N\Big|_{\mathcal{H}_n} = n \mathbb{1}\Big|_{\mathcal{H}_n}$$

kernel of N is \mathcal{H}_0 “*Vacuum*”

Remark. Γ in particular and also the whole formalism in general is sometimes called “*second quantization*” Many interesting operators on $\mathcal{F}(h)$ don’t come from operators on h !

Creation and annihilation operators

From now on $\mathcal{F}(h) = \left\{ F_S(h) \mathcal{F}_A(h) \right\}$ with

$$\mathcal{F}(h) \ni \Psi = (\Psi_0, \Psi_1, \Psi_2, \dots) \text{ with } \Psi_k \in \mathcal{H}_k^i$$

Thus for $\varphi \in h$

$$a^\dagger(\varphi)(\Psi_0, \Psi_1, \dots) = (0, \Psi'_1, \Psi'_2, \dots), \text{ with } \Psi'_k = \sqrt{k}S(\Psi_{k-1} \otimes \varphi) \text{ (bosonic)} \quad (5.26)$$

$$c^\dagger(\varphi)(\Psi_0, \Psi_1, \dots) = (0, \Psi'_1, \Psi'_2, \dots), \text{ with } \Psi'_k = \sqrt{k}A(\Psi_{k-1} \otimes \varphi) \text{ (bosonic)} \quad (5.27)$$

These create a new particle in state φ , in each sector and are thus called *creation operator*. Indeed we see, choosing some ONB $\{\varphi_i\}$ of h ($i \leftrightarrow \underline{k}, \underline{l}$ from before), denote for $\sum_i n_i = n$, allowing $n_i = 0$,

$$|n_1, n_2, \dots\rangle. \in \mathcal{H}_n^i$$

the normalized state from lemmas, (5.13) and (5.14), then

$$\begin{aligned} a^\dagger(\varphi_i) |n_1, n_2, \dots\rangle_S &= \sqrt{n_i + 1} |n_1, \dots, n_{i-1}, n_i + 1, n_{i+1}, \dots\rangle_S \\ c^\dagger(\varphi_i) |n_1, n_2, \dots\rangle_A &= (1 - n_i) (-1)^{\sum_{k < i} n_k} |n_1, \dots, n_{i-1}, n_i + 1, n_{i+1}, \dots\rangle_A \end{aligned}$$

And the *annihilation operator* is the adjoint of the creation operator:

$$\begin{aligned} a(\varphi) &:= (a^\dagger(\varphi))^\dagger \\ c(\varphi) &:= (c^\dagger(\varphi))^\dagger \end{aligned}$$

Remark. Annihilation op. is anti-linear in φ . Also one can workout that

$$\begin{aligned} a(\varphi)S(v_1 \otimes \dots \otimes v_n) &= \frac{1}{\sqrt{n}} \sum_{k=1}^n \langle \varphi | v_k \rangle_h S(v_1 \otimes v_2 \otimes \dots \otimes \cancel{v_k} \otimes \dots \otimes v_n) \text{ for } n \geq 1 \\ a(\varphi) \Big|_{\mathcal{H}_0} &= 0 \end{aligned} \tag{5.28}$$

and for $c(\varphi)$

$$\begin{aligned} c(\varphi)A(v_1 \otimes \dots \otimes v_n) &= \frac{1}{\sqrt{n}} \sum_{k=1}^n (-1)^{n-k} \langle \varphi | v_k \rangle_h A(v_1 \otimes v_2 \otimes \dots \otimes \cancel{v_k} \otimes \dots \otimes v_n) \text{ for } n \geq 1 \\ a(\varphi) \Big|_{\mathcal{H}_0} &= 0 \end{aligned} \tag{5.29}$$

As always $\varphi \in \mathfrak{h}$. in the occupation number basis (wrt. ONB $\{\varphi_i\}$)

$$\begin{aligned} a(\varphi_i) |n_1, n_2, \dots\rangle_S &= \sqrt{n_i} |n_1, \dots, n_{i-1}, n_i - 1, n_{i+1}, \dots\rangle_S \\ c(\varphi_i) |n_1, n_2, \dots\rangle_A &= n_i (-1)^{\sum_{k < i} n_k} |n_1, \dots, n_{i-1}, n_i - 1, n_{i+1}, \dots\rangle_A \end{aligned} \tag{5.30}$$

One can work out commutation relations

$$\begin{aligned} [a(\varphi), a(\varphi)] &= 0 = [a^\dagger(\varphi), a^\dagger(\varphi)] \\ [a(\varphi), a^\dagger(\Psi)] &= \langle \varphi | \Psi \rangle_h \mathbb{1}_{\mathcal{F}_s(\mathfrak{h})} \end{aligned} \tag{5.31}$$

and for Fermionic fock space one has

$$(c^\dagger(\varphi))^2 = 0 = (c(\varphi))^2 \tag{5.32}$$

$$\begin{aligned} [c(\varphi), c(\Psi)] &= 0 = [c^\dagger(\varphi), c^\dagger(\Psi)] \\ \{c(\varphi), c^\dagger(\Psi)\} &= \langle \varphi | \Psi \rangle_h \mathbb{1}_{\mathcal{F}_A(\mathfrak{h})} \end{aligned} \tag{5.33}$$

with $\{\cdot, \cdot\}$ the anti-commutator ($\{A, B\} = AB + BA$)

Example 5.9. (mathematical) harmonic oscillator $\mathcal{H} = l^2(\mathbb{C}) = \mathcal{F}_S(\mathbb{C})$, a, a^\dagger the usual annihilation and creation operators.

Remark. We can write $d\Gamma$ in terms of a, a^\dagger

$$d\Gamma(B) = \sum_{i,j} \langle \varphi_i | B | \varphi_j \rangle a^\dagger(\varphi_i) a(\varphi_j) \quad (5.34)$$

This leads to the term “second quantization”.

Example 5.10.

$$h = \frac{\vec{p}^2}{2m} + V(\vec{x}), \varphi_i \rightarrow \delta_{\vec{x}}^3(\cdot) \text{ and } a^\dagger(\delta_{\vec{x}}^3) =: a^\dagger(\vec{x})$$

Then

$$H := d\Gamma(h) = \int d^3x a^\dagger(\vec{x}) \left(\frac{\vec{p}^2}{2m} + V(\vec{x}) \right) a(\vec{x})$$

looks like “ $\langle h \rangle_a$ ”. But $a(\vec{x})$ is nor operator, nor a wave function \rightarrow “second quantization”!

6 Relativistic Quantum Mechanics

In this chapter, we set

- $c = 1$
- Space-time indices $\mu, \nu, \dots = 0, 1, 2, 3$
- spatial indices $a, b, c, \dots = 1, 2, 3$

and use the einstein summation convention

$$\sum_{\mu=0}^3 T^{\dots \mu \dots} W^{\dots \mu \dots} \equiv T^{\dots \mu \dots} W^{\dots \mu \dots}$$

where the position of the spacetime indices matters!

6.1 Short review of special relativity

- *Newton*: Theory of mechanics: Form-invariant under Galilei-trafos
- *Maxwell*: Theory of electro-dynamics: Form-invariant under Poincaré-transformations
- *Einstein*: Relativistic mechanics: same as e-dyn.

The essence of special relativity (SR) is the Form-invariance of physics under Poincaré-trafos. This means that there are no preferred inertial observers.

Definition 6.1 (Coordinate changes). $x^\mu \rightarrow x'^\mu(x)$ induce changes in components of physical quantities. One simple class are tensors

$$T'^{\mu_1, \dots, \mu_m}_{\nu_1, \dots, \nu_n}(x') = \frac{\partial x'^{\mu_1}}{\partial x^{\alpha_1}} \cdots \frac{\partial x'^{\mu_m}}{\partial x^{\alpha_m}} \frac{\partial x^{\beta_1}}{\partial x'^{\nu_1}} \cdots \frac{\partial x^{\beta_n}}{\partial x'^{\nu_n}} T^{\alpha_1 \dots \alpha_m}_{\beta_1 \dots \beta_n}(x) \quad (6.1)$$

Partial derivatives $\frac{\partial x'}{\partial x}, \frac{\partial x}{\partial x'}$ are inverses, as matrices:

$$\frac{\partial x'^\mu}{\partial x^\alpha} \frac{\partial x^\alpha}{\partial x'^\nu} = \delta^\mu_\nu \quad \text{and} \quad \frac{\partial x'^\mu}{\partial x^\nu} \frac{\partial x^\nu}{\partial x'^\mu} = \delta^\beta_\nu \quad (6.2)$$

Also note

$$\frac{\partial}{\partial x'^\mu} = \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial}{\partial x^\alpha} \quad (6.3)$$

Definition 6.2 (Poincaré trafos).

$$x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu \quad (6.4)$$

with arbitrary shift $a^\mu \in \mathbb{R}^4$, and Λ st.

$$\Lambda^\mu_\nu \Lambda^\alpha_\beta \eta_{\mu\alpha} = \eta_{\nu\beta} \quad (6.5)$$

where

$$\eta = \text{diag}(-1, 1, 1, 1) \quad (6.6)$$

The physical interpretation of the form invariance is the change of the inertial observer. The technical reason for the form-invariance: The geometry for the laws of nature is provided by metric (6.6). Poincaré-trafos are precisely the coordinate transformations that have (6.6) form-invariant (“isometries”). Trafos (6.4) form a group called Poincaré-group $\mathcal{P}(3, 1)$ (actually: (matrix) Lie group). Lie algebra of $\mathcal{P}(3, 1)$

$$p(3, 1) = \{(\omega^\mu_\nu, t^\alpha) \in M(4 \times 4, \mathbb{R}) \times \mathbb{R}^4 \mid \omega^{\mu\nu} = -\omega^{\nu\mu}\} \quad (6.7)$$

where

$$\omega^\mu_\nu \eta^{\nu\alpha} =: \omega^{\mu\alpha} \quad \text{and} \quad \omega^\mu_\nu \eta_{\mu\alpha} =: \omega_{\alpha\nu} \quad \text{with} \quad \eta^{\mu\nu} = (\eta^{-1})^{\mu\nu} = \text{diag}(-1, 1, 1, 1)$$

with the Lie product between

- ω 's: matrix commutator
- t 's: $[t^\alpha, t'^\beta] = 0$
- $[\omega, t] := \omega \cdot t$ ($[\omega, t] = t'$, with $t'^\alpha = \omega^\alpha_\beta t^\beta$ and $[t, \omega] := -\omega t$)

Trafos with $a^\mu = 0$ form a subgroup, Lorentz-group $O(3, 1)$, with Lie algebra just consisting of the ω 's, i.e. $t = 0$ in (6.7).

Relativistic mechanics

One defines the 4-velocity of a particle

$$u^\mu := \frac{dx^\mu}{d\tau}$$

with τ the *proper time* (ie. η -length along the world line [trajectory in 4-dim space] of the particle)

$$\begin{aligned} \frac{d\tau}{dt} &= \sqrt{1 - \vec{v}^2}, \quad \vec{v} = \frac{d\vec{x}}{dt} \\ \tau &= \int dt \sqrt{-\eta_{\mu\nu} \frac{dx^\mu}{dt} \frac{dx^\nu}{dt}} + \text{const} \end{aligned} \quad (6.8)$$

Additionally the 4-momentum

$$p^\mu = m u^\mu \equiv p_{\text{kin}}^\mu$$

which can be interpreted $p^\mu = (E, \vec{p})$. Thus as $u^\mu u_\mu = -1$, we get

$$m^2 = E^2 - \vec{p}^2 \quad (6.9)$$

Hamiltonian form of particle kinematics

From the action

$$S = -m \int d\tau = -m \int dt \sqrt{-\eta_{\mu\nu} \frac{dx^\mu}{dt} \frac{dx^\nu}{dt}}$$

we can read of the Lagrangian, and then we get the Hamiltonian

$$H = \sqrt{\vec{p}^2 + m^2} \left(\approx m + \frac{\vec{p}^2}{2m} \text{ for } \vec{p}^2 \ll m^2 \right)$$

Coupling to EM fields gives an additional term in the action

$$S = -m \int d\tau + q \int d\tau u^\mu A_\mu(x(\tau))$$

which leads to a modified canonical momentum

$$p^\mu = p_{\text{kin}}^\mu + q A^\mu \quad (6.10)$$

and the Hamiltonian

$$H = \sqrt{(\vec{p} - q\vec{A})^2 + m^2} + qA^0. \quad (6.11)$$

This yields the EOM

$$\frac{dp_{\text{kin}}^\mu}{d\tau} = q F^{\mu\nu} u_\nu$$

with the field strength tensor F of the EM field

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.$$

Equation (6.9) (“mass shell condition”) becomes

$$m^2 = (E - qA^0)^2 - (\vec{p} - q\vec{A})^2 \quad (6.12)$$

6.2 Some representations of $\mathcal{P}(3, 1)$ and $O(3, 1)$

Let $\phi(x)$ be some n -component field or wave function. Representations of $\mathcal{P}(3, 1)$ on $\{\phi(x)\}$ given by

$$(\Pi(\Lambda, a)\phi)(x) = \Pi_n(\Lambda)\phi(\Lambda^{-1}(x - a)) \quad (6.13)$$

Here (Λ, a) denotes elements of $\mathcal{P}(3, 1)$ and Π_n is an n -dim representation of $O(3, 1)$.

Example 6.1. (4-)vector fields, such as $A^\mu(x)$, then $n = 4$, $\Pi_4(\Lambda) = \Lambda$

Irreducible representations of $O(3, 1)$

First we choose Irr. reps. of $o(3, 1)$ a Basis

$$M_a = \begin{pmatrix} 0 & \vec{0}^T \\ \vec{0} & \epsilon_a \end{pmatrix}, \text{ with } (\epsilon_a)^b{}_c = \epsilon_a{}^b{}_c \text{ and } N_a = \begin{pmatrix} 0 & \epsilon_a^T \\ \epsilon_a & \mathbf{0} \end{pmatrix}, \text{ with } (\epsilon_a)_b = \delta_{ab} \quad (6.14)$$

and $\epsilon_{abc} = \begin{cases} \text{sign}(P) \text{ for } (abc) = (P(1)P(2)P(3)), P \text{ a perm.} \\ 0 \text{ else} \end{cases}$

and indices of ϵ are raised and lowered with δ ($\epsilon_a{}^b{}_c := \delta^{bd}\epsilon_{adc}$). Then we get

$$\Lambda(\vec{\alpha}, \vec{v}) = \mathbb{1} + \alpha^a M_a + v^b N_b + \mathcal{O}(\alpha^2, v^2) \quad (6.15)$$

where $\vec{\alpha}$ parameterises a rotation and \vec{v} the boost velocity. We have the commutation relation:

$$[M_a, M_b] = -\epsilon_{ab}{}^c M_c \text{ and } [N_a, N_b] = \epsilon_{ab}{}^c M_c \text{ and } [N_a, M_b] = -\epsilon_{ab}{}^c N_c \quad (6.16)$$

this is up to a sign in $[N, N]$ the same structure as found in $o(4)$ (see homework!) and as such can do the same trick

$$L_a^\pm := \frac{1}{2} (M_a \pm iN_a) \quad (6.17)$$

with the commutators

$$[L_a^\pm, L_b^\pm] = -\epsilon_{ab}{}^c L_c^\pm \text{ and } [L_a^\pm, L_b^\mp] = 0. \quad (6.18)$$

Lemma 6.2. A, B Lie-alg., π_1, \mathcal{H}_2 rep. of B , then

1. $A \oplus B$ is a Lie-alg., via $[a \oplus b, c \oplus d] := [a, c] \oplus [b, d]$
2. Rep. π_{12} on $\mathcal{H}_1 \otimes \mathcal{H}_2$ of $A \oplus B$ via $\pi(a \oplus b) := \pi_1(a) \otimes \mathbb{1} + \mathbb{1} \otimes \pi_2(b)$

which can be proved by simple calculation.

Now we see $o(3, 1) = su(2) \oplus su(2)$. Furthermore we can show, that Irreps. of $o(3, 1)$ are of the form π_{12} as above with π_1, π_2 irreps. of $su(2)$. From this we conclude that irreps of $o(3, 1)$ can be described by a pair $(j^+, j^-) \in (\frac{1}{2} \mathbb{N}_0)^2$, and

$$\dim(\pi_{(j^+, j^-)}) = (2j^+ + 1)(2j^- + 1).$$

Rewriting (6.15) in terms of L^\pm we find

$$\Lambda(\vec{\alpha}, \vec{v}) = \mathbb{1} + (\vec{\alpha} - i\vec{v})\vec{L}^+ + (\vec{\alpha} + i\vec{v})\vec{L}^- + \dots$$

and

$$\pi_{(j^+, j^-)}(\Lambda(\vec{\alpha}, \vec{v})) = \mathbb{1}_{j^+ \otimes j^-} + (\vec{\alpha} - i\vec{v})\pi_{j^+}(\vec{L}^+) \otimes \mathbb{1}_{j^-} + (\vec{\alpha} + i\vec{v})\mathbb{1}_{j^+} \otimes \pi_{j^-}(\vec{L}^-) + \dots$$

Coefficient of $\vec{\alpha}$ is just

$$\pi_{j^+}(\vec{L}^+) \otimes \mathbb{1} + \mathbb{1} \otimes \pi_{j^-}(\vec{L}^-).$$

This is just the tensor product rep. $j^+ \otimes j^-$ of the rotation generators. So we have

$$\pi_{(j^+, j^-)} \Big|_M = \pi_{j^+} \otimes \pi_{j^-} = \bigoplus_{k=|j^+ - j^-|}^{j^+ + j^-} \pi_k$$

Example 6.3. 1. $\pi_{\frac{1}{2}, \frac{1}{2}} : 4d$ -rep. for the rotation subalgebra

$$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$$

We recognise defining rep. of $o(3, 1)$, with 0, 1 the time- and space component of a 4-vector

$$A^\mu = (A^0, \vec{A})$$

2. $\pi_{(\frac{1}{2}, 0)}$ and $\pi_{(0, \frac{1}{2})}$ two $2d$ -reps. where rotations act as in

$$\frac{1}{2} \otimes 0 = \frac{1}{2} \text{ "Weyl-spinors"}$$

3. $\pi_{(0, 0)} 1 - dim. scalar$

4. $\pi_{(\frac{1}{2}, 0)} \oplus \pi_{(0, \frac{1}{2})}$ 4-dim. reducible rep. "Dirac spinor"

Remark. Representations of $O(3, 1)$ are complicated due to

1. (6.5) allows also for reflections, in particular parity P and time reversal T . $O(3, 1)$ consists of 4 components

$$O(3, 1) = \mathcal{L}_+^\uparrow \dot{\cup} P\mathcal{L}_+^\uparrow \dot{\cup} T\mathcal{L}_+^\uparrow \dot{\cup} PT\mathcal{L}_+^\uparrow \text{ with } \mathcal{L}_+^\uparrow = \{\Lambda \in O(3, 1) | \det \Lambda = 1, \Lambda^0_0 \geq 1\}$$

2. \mathcal{L}_+^\uparrow is not simply connected It follows that $\Pi_{(j^+, j^-)}$ in general only a rep. for the covering group of \mathcal{L}_+^\uparrow . Suitable rep. for P and T has to be found separately. (Some more remarks on this later)

6.3 Klein-Gordon equation

Try to guess a relativistic version of the Schrödinger equation. Starting with the simplest idea which assumes a 1-component Wave-function: $\Pi_n = \Pi_{(0,0)}$ in (6.13). Now use (6.12) together with heuristics $E \leftrightarrow i\hbar \frac{\partial}{\partial t}$, $\vec{p} \leftrightarrow -i\hbar \vec{\nabla}$ this suggests the Klein-Gordon equation

$$\left(\square - \frac{m^2}{\hbar^2}\right)\Psi = 0 \quad (6.19)$$

with

$$\square = \eta^{\mu\nu} (\partial_\mu + iqA_\mu(x)) (\partial_\nu + iqA_\nu(x)) \quad (6.20)$$

for the wave function Ψ of a particle with mass m . Can this make sense? (in the following $\hbar = 1$)

Non-relativistic limit

The Klein-Gordon (6.19) is second order in time. So we need to specify $\Psi(t_0, \vec{x})$, $\dot{\Psi}(t_0, \vec{x})$ to have a well defined evolution. How can the Schrödinger equation emerge in the non-relativistic limit? Let $A_\mu = 0$ and then consider

$$\phi_1 = \Psi + \frac{i}{m} \dot{\Psi}, \phi_2 = \Psi - \frac{i}{m} \dot{\Psi}. \quad (6.21)$$

Then using $\Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$ the Klein-Gordon eq. takes the form

$$i \frac{\partial}{\partial t} \Phi = \left[\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{\Delta}{2m} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} m \right] \Phi \quad (6.22)$$

For slow particles, first term in Hamiltonian decouples. ϕ_1, ϕ_2 are wave functions for two independent particles. For higher energy, these particles interact. Analysis with $A_\mu \neq 0$: Particles have same mass, but opposite charge $q, -q$. One can interpret these as the particle and the corresponding anti-particle.

Probability interpretation

For Schrödinger equation, had conserved prob. current

$$\partial_t \rho + \nabla \cdot \vec{j} = 0$$

with $\rho = |\Psi|^2$. (6.19) also implies a conserved current

$$j^\mu = i (\bar{\Psi} \partial^\mu \Psi - \Psi \partial^\mu \bar{\Psi} - 2iqA^\mu \bar{\Psi} \Psi) \text{ with current conservation } \partial_\mu j^\mu = 0.$$

The density

$$\rho = j^0 = i (\bar{\Psi} \dot{\Psi} - \Psi \dot{\bar{\Psi}} - 2iqA^0 \bar{\Psi} \Psi)$$

is not positive definite. For $A_\mu = 0$, then

$$\rho = 2m (|\phi_1|^2 - |\phi_2|^2) \quad (6.23)$$

Probability interpretation can perhaps be given for low energy, but not in general. So ρ will be interpreted as the charge density.

Negative energy solutions

(6.19) has plane wave solutions $\Psi_{\vec{p}} = e^{-i(Et - \vec{p}\vec{x})}$ with

$$E = \pm \sqrt{\vec{p}^2 + m^2} \quad (6.24)$$

Remark. We can quantize the relativistic Hamiltonian (6.11) Then we get

$$H\Psi_{\vec{p}} = E\Psi_{\vec{p}}$$

So (6.24) gives energy spectrum of the KG (Klein-Gordon) particles. Support of solutions in Fourier space:

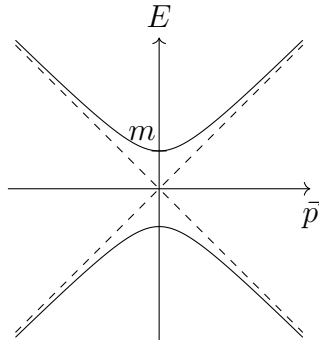


Figure 17: $E(\vec{p}, m)$ (dashed for $m = 0$)

Negative mass shell is physically problematic: Upon coupling to EM field, system can emit arbitrary amounts of energy, by populating the neg. mass shell and as such the system is unstable. But the equation is still useful for some approximate calculation and the occurring problems are fully resolved in QFT.

6.4 Dirac equation

Looking for relativistic covariant (forminvariant under Poincare) wave equation for spin- $\frac{1}{2}$ particles. We expect something of the form

$$\Psi = \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_N \end{pmatrix} \in \mathcal{H}_{\text{orbital}} \otimes \mathcal{H}_{\text{spin}} \quad (6.25)$$

which in the simplest case yields $(\frac{1}{2}, 0)$ or $(0, \frac{1}{2})$ for Π_n of (6.13). The first idea $\square\Psi - m^2\Psi = 0$, but this would just be a couple of KG particles and as such would have the negative energy problems.

The second idea is to try a first order equation

$$\partial_\mu\Psi = 0.$$

Here we would get too many equations such that the equation is not physical. So we get the idea to contract ∂_μ over μ with something. For this we can show:

Lemma 6.4. Let

$$\sigma^\mu := (\mathbb{1}_{2\times 2}, \vec{\sigma}) \quad \bar{\sigma}^\mu := (\mathbb{1}_{2\times 2}, -\vec{\sigma}) \quad (6.26)$$

with $(\vec{\sigma})_a = \Sigma_a =$ the a Pauli matrix. Then we get

- if Ψ transforms under $(\frac{1}{2}, 0) \Rightarrow \bar{\sigma}^\mu\partial_\mu\Psi$ transforms under $(0, \frac{1}{2})$
- if Ψ transforms under $(0, \frac{1}{2}) \Rightarrow \sigma^\mu\partial_\mu\Psi$ transforms under $(\frac{1}{2}, 0)$

Proposition 6.5.

$$\sigma^\mu\partial_\mu\Psi_R = 0 \text{ or } \bar{\sigma}^\mu\partial_\mu\Psi_L = 0 \quad (6.27)$$

where Ψ_R transform under $(0, \frac{1}{2})$ and Ψ_L under $(\frac{1}{2}, 0)$. (6.27) is called *Weyl equation*, Ψ_R, Ψ_L are *right-/left-handed Weyl spinors*.

The mass term $m\Psi = m\mathbb{1}_{2\times 2}\Psi$ transforms under *same* rep. as Ψ . Thus

$$-i\bar{\sigma}^\mu\partial_\mu\Psi + m\Psi = 0$$

is *not* forminvariant under P-trafos.

Remark. (6.27) seems useless to describe electrons (because they are massive!). However in the standard model fermions are “born” as Weyl spinors, acquire mass via Higgs mechanism.

Now we look for other options

1. $(\frac{1}{2}, \frac{1}{2})$: has the wrong rotation rep. $\frac{1}{2} \otimes \frac{1}{2} = 1 \otimes 0$
2. $(\frac{1}{2}, 1)$: has too many components ($\frac{3}{2}$ part): Rot. $\frac{1}{2} \otimes 1 = \frac{3}{2} \otimes \frac{1}{2}$

Could one have one equation with both, Ψ_R, Ψ_L ? That corresponds to $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$ where we indeed find

$$-i\sigma^\mu\partial_\mu\Psi_R + m\Psi_L = 0 \quad -i\bar{\sigma}^\mu\partial_\mu\Psi_L + m\Psi_R = 0 \quad (6.28)$$

forminvariant set of 4 equations for 4 wave-functions Ψ_L, Ψ_R .

Introduce the γ -matrices:

$$\gamma^\mu := -i \begin{pmatrix} 0_{2 \times 2} & \sigma^\mu \\ \bar{\sigma}^\mu & 0_{2 \times 2} \end{pmatrix} \quad (6.29)$$

Then (6.28) becomes

$$(\gamma^\mu \partial_\mu + m) \Psi = 0 \quad (6.30)$$

$$\text{with } \Psi(x) = \begin{pmatrix} \Psi_L(x) \\ \Psi_R(x) \end{pmatrix} \in \mathbb{C}^4 \quad (6.31)$$

Where (6.30) is the covariant form of the *Dirac equation*, Ψ is called *bi-spinor* or *Dirac spinor*. It transforms under $\Pi_4 = (\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$ in (6.13). Sometimes one writes $\gamma^\mu \partial_\mu = \not{\partial}$. Coupling to an EM-field is achieved by “minimal substitution” $\not{\partial} \rightarrow \not{\nabla} = \gamma^\mu (\partial_\mu + iqA_\mu)$ in (6.30). Basis change in spinor space changes form of γ -matrices. (6.29) is the *chiral form*. Another useful form is the *Dirac form*, with $\gamma^a, a = 1, 2, 3$ unchanged and

$$\gamma^0 = -i \begin{pmatrix} \mathbb{1}_{2 \times 2} & 0 \\ 0 & -\mathbb{1}_{2 \times 2} \end{pmatrix} \quad (6.32)$$

Clifford relations

Basis independent property that leads to correct transformation behavior is

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu} \mathbb{1}_{4 \times 4} \quad (6.33)$$

Objects that satisfy (6.33) span the *Clifford-algebra* $Cl(3, 1)$. The γ 's we found are a 4d representation of this algebra. This generalizes to other dimensions and signatures.

Proposition 6.6. Only one irreducible rep. of (6.33) exists, up to basis changes. I.e. for irreducible solutions γ^μ, γ'^μ of (6.33) there is $A \in GL(4, \mathbb{C})$ with $\gamma'^\mu = A\gamma^\mu A^{-1}$.

Lorentz-invariance of the Dirac equation

Consider a Poincare-trafo (Λ, a^μ) , i.e.

$$\frac{\partial x'^\mu}{\partial x^\nu} = \Lambda_\nu^\mu \quad (6.34)$$

We want to show

$$(\gamma^\mu \nabla_\mu + m) \Psi = 0 \Leftrightarrow (\gamma'^\mu \nabla'_\mu + m) \Psi' = 0 \quad (6.35)$$

knowing that

$$\nabla'_\mu = (\Lambda^{-1})^\nu_\mu \nabla_\nu.$$

We have not yet explicitly determined Ψ' .

Remark. For $\hat{\gamma}^\mu := (\Lambda^{-1})^\mu_\nu \gamma^\nu$:

$$\hat{\gamma}^\mu \hat{\gamma}^\nu + \hat{\gamma}^\nu \hat{\gamma}^\mu = (\Lambda^{-1})^\mu_\alpha (\Lambda^{-1})^\nu_\beta (\gamma^\alpha \gamma^\beta + \gamma^\beta \gamma^\alpha) = 2 (\Lambda^{-1})^\mu_\alpha (\Lambda^{-1})^\nu_\beta \eta^{\alpha\beta} = 2\eta^{\mu\nu}$$

Thus also satisfy (6.33), and are hence equivalent to the γ 's.

$$(\Lambda^{-1})^\mu_\alpha \gamma^\alpha = D(\Lambda) \gamma^\mu D(\Lambda)^{-1} \quad (6.36)$$

Now, if we have

$$\Psi' = D(\Lambda) \Psi \quad (6.37)$$

then we get

$$\begin{aligned} (\not{\nabla} + m) \Psi' &= \left(\gamma^\mu (\Lambda^{-1})^\alpha_\mu \nabla_\alpha + m \right) D(\Lambda) \Psi = D(\Lambda) (\gamma^\mu \nabla_\mu + m) D(\Lambda)^{-1} D(\Lambda) \Psi \\ &= D(\Lambda) (\gamma^\mu \nabla_\mu + m) \Psi \end{aligned}$$

Since $D(\Lambda)$ is invertible, this shows (6.35). What remains to show is that $D(\Lambda)$ is $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$. Can check by direct calculation of generators.

Example 6.7. Rotations

$$M_a{}^\mu{}_\nu \gamma^\nu = \delta_b^\mu \epsilon_a{}^b{}_c \gamma^c = -i \delta_b^\mu \begin{pmatrix} 0 & \epsilon_a{}^b{}_c \sigma^c \\ -\epsilon_a{}^b{}_c \sigma^c & 0 \end{pmatrix} = -\frac{1}{2} \delta_b^\mu \begin{pmatrix} 0 & [\sigma_a, \sigma_b] \\ -[\sigma_a, \sigma_b] & 0 \end{pmatrix}$$

This is the ‘‘infinitesimal version’’ of LHS of (6.36). If

$$D(\Lambda(\vec{\alpha}, 0)) = \begin{pmatrix} \Pi_{\frac{1}{2}}(R(\vec{\alpha})) & 0 \\ 0 & \Pi_{\frac{1}{2}}(R(\vec{\alpha})) \end{pmatrix} \quad (6.38)$$

then

$$\begin{aligned} \frac{d}{d\alpha^b} \Big|_{\vec{\alpha}=0} D(\Lambda(\vec{\alpha})^{-1}) \gamma^a D(\Lambda(\vec{\alpha})) &= \left[\gamma^a, \frac{d}{d\alpha^b} \Big|_{\vec{\alpha}=0} D(\Lambda(\vec{\alpha})) \right] = -\frac{1}{2} \left[\begin{pmatrix} 0 & \sigma^a \\ -\sigma^a & 0 \end{pmatrix}, \begin{pmatrix} \sigma^b & 0 \\ 0 & \sigma^b \end{pmatrix} \right] \\ &= -\frac{1}{2} \begin{pmatrix} 0 & [\sigma^a, \sigma^b] \\ -[\sigma^a, \sigma^b] & 0 \end{pmatrix} \end{aligned}$$

We can get compact formulars by going back to (6.7). For

$$\Lambda_\nu^\mu = (e^\omega)_\nu^\mu$$

with ω_ν^μ a generator (i.e. $\omega_{\mu\nu} = -\omega_{\nu\mu}$) one finds

$$D(\Lambda) = e^{\frac{1}{2} \omega_{\mu\nu} J^{\mu\nu}} \quad (6.39)$$

with

$$J^{\mu\nu} = \frac{1}{4} [\gamma^\mu, \gamma^\nu] \quad (6.40)$$

Remark. One can check that (6.33) generates a rep. of the Lie alg. of the invariance group of η , no matter what dimension or signature one has.

Moreover:

$$[J^{\mu\nu}, \gamma^\alpha] = \gamma^\mu \eta^{\nu\alpha} - \gamma^\nu \eta^{\mu\alpha} \quad (6.41)$$

This is the infinitesimal version of (6.36) in general. The explicit form of generators works out to be

$$J^{kl} = -\frac{i}{2} \epsilon^{klm} \begin{pmatrix} \sigma_m & 0 \\ 0 & \sigma_m \end{pmatrix} \quad J^{k0} = \frac{1}{2} \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix} \quad (6.42)$$

Remark. • can see “block structure” of $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$

- Rotations are unitarily represented, boosts not
- (6.39) will give projective rep. of \mathcal{L}_+^\uparrow (Extension to $O(3, 1)$ will maybe done later)

Adjoint and current

For spinor $\Psi = \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_4 \end{pmatrix}$, define

$$\Psi^\dagger = (\Psi_1^*, \dots, \Psi_4^*)$$

and note that

$$\Psi^\dagger \Psi = \sum_{k=1}^4 |\Psi_k|^2 \geq 0 \quad (6.43)$$

but this is not a Lorentz-scalar (but turns out to be a density):

$$\Psi(x) \rightarrow D(\Lambda)\Psi(\Lambda^{-1}x), \quad \Psi^\dagger \rightarrow \Psi^\dagger(\Lambda^{-1}x)D(\Lambda)^\dagger$$

and hence

$$\Psi'^\dagger \Psi' = \Psi^\dagger D(\Lambda)^\dagger D(\Lambda)\Psi \neq \Psi^\dagger \Psi$$

But there is a workaround, we take from (6.33) for $\beta = i\gamma^0$ (Note: $\beta^2 = \mathbb{1}$)

$$\beta\gamma^i\beta^{-1} = -\gamma^i, \quad \beta\gamma\beta^{-1} = \gamma^0$$

and then

$$\beta\gamma^{\mu\dagger}\beta = -\gamma^\mu \quad (6.44)$$

wich finally gives

$$\beta D(\Lambda)^\dagger \beta = D(\Lambda^{-1}) \quad (6.45)$$

and further

$$\beta J^{\mu\nu\dagger} \beta = -J^{\mu\nu}$$

Hence we define adjoint spinor

$$\bar{\Psi} = \Psi^\dagger \beta \quad (6.46)$$

and then $\bar{\Psi}\Psi$ is a Lorentz scalar and

$$j^\mu := i\bar{\Psi}\gamma^\mu\Psi \quad (6.47)$$

transforms as a 4-vector and is a conserved current.

The density of this current is

$$j^0 = \Psi^\dagger \Psi \geq 0.$$

We can define the hilbert space

$$\mathcal{H} = \mathcal{L}(\mathbb{R}^3, d^3x) \otimes \mathbb{C}^4 = \bigoplus_{k=1}^4 \mathcal{L}(\mathbb{R}^3, d^3x)$$

with inner product

$$\langle \phi | \Psi \rangle := \int d^3x (\phi^\dagger \Psi)(x) \quad (6.48)$$

Observables

We get the position operator from the interpretation of $\Psi^\dagger\Psi$ as a probability density

$$x^i : \Psi \rightarrow x^i \Psi = \begin{pmatrix} x^i \Psi_1 \\ \vdots \\ x^i \Psi_4 \end{pmatrix} \text{ with } i = 1, 2, 3 \quad (6.49)$$

More observables from the generators of Poincaré-trafos: From translations we get the (canonical) momentum, without electromagnetic fields

$$p_a = -i \mathbb{1}_{4 \times 4} \partial_a \quad (6.50)$$

while in the presence of electromagnetic fields we get a different kinematic momentum

$$\vec{p}_{\text{kin}} = \left(-i \vec{\nabla} - q \vec{A} \right) \mathbb{1}_{4 \times 4}$$

(Here the normal $(\vec{\nabla})_a = \partial_a$ is meant) Rotations that do not mix components (only act on the arguments of the wavefunction) give us the orbital angular momentum

$$\vec{L} = \vec{x} \times \vec{p}$$

while the other rotations give us the spin. In the chiral rep. (the star above the equal sign denotes that we are in a certain basis):

$$\vec{S}^* = \frac{1}{2} \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \quad (6.51)$$

Now we can see explicitly

$$\vec{S}^2 = \frac{1}{2} \left(\frac{1}{2} + 1 \right) \mathbb{1}_{4 \times 4}$$

Energy can be seen as the 0-component of p_μ , where

$$p_\mu = -i \mathbb{1}_{4 \times 4} \partial_\mu.$$

We can give a direct expression via the Dirac equation

$$i\partial_t \Psi = H \Psi$$

for solutions Ψ , with

$$H = -i\vec{\alpha}\vec{\nabla} + \beta m, \quad \alpha^a = i\beta\gamma^a \quad (6.52)$$

the *Dirac Hamiltonian*. In the Dirac Basis it is given as

$$H^* = \begin{pmatrix} m \mathbb{1}_{2 \times 2} & \vec{\sigma}\vec{p} \\ \vec{\sigma}\vec{p} & -m \mathbb{1}_{2 \times 2} \end{pmatrix}$$

Plane waves

Due to (6.33) (here $\nabla = \partial \pm iqA$ gauge invariant derivative)

$$(\not{\nabla} - m) (\not{\nabla} + m) = \square_A - m^2 \quad (6.53)$$

we have

$$(\not{\nabla} + m) \Psi = 0 \Rightarrow (\square_A - m^2) \Psi = 0. \quad (6.54)$$

Each component of Ψ fulfills the KG equation. Now for $q = 0$ or $A = 0$ we take the ansatz

$$\Psi = u_{\vec{k}} e^{ik_\mu x^\mu} \quad (6.55)$$

where in view of (6.54), we set

$$k_0 = \pm \sqrt{\vec{k}^2 + m^2}. \quad (6.56)$$

Now we want to choose $u_{\vec{k}}$ such that Ψ becomes eigenstate of H :

$$H\Psi_{\vec{k}} = E\Psi_{\vec{k}}$$

For $\Psi = \begin{pmatrix} \Psi_L \\ \Psi_S \end{pmatrix}$, in the Dirac basis, this requires (L for long (slow) and S for short (fast))

$$\begin{aligned} En_L &= mu_L + \vec{p}\vec{\sigma}u_S \\ En_S &= -mu_S + \vec{p}\vec{\sigma}u_L \end{aligned}$$

Combining the equations one finds $(E - m)(E + m)u_L = (\vec{p}\vec{\sigma})^2 u_L$ and using

$$(\vec{a}\vec{\sigma})(\vec{b}\vec{\sigma}) = (\vec{a}\vec{b}) \mathbb{1}_{2 \times 2} + i(\vec{a} \times \vec{b}) \vec{\sigma} \quad (6.57)$$

one finds

$$E^2 - m^2 = \vec{p}^2$$

Consistent with (6.56) and , fixing u_L , we get

$$u_S = \frac{\vec{p}\vec{\sigma}}{E + m} u_L. \quad (6.58)$$

Without further conditions, so fixing $\vec{p}(=\vec{k})$, solution space is 4-dimensional (\mathbb{C}), 2-dim. corresponding to positive and 2-dim. to negative energy

$$E = \pm \sqrt{\vec{p}^2 + m^2}$$

Example 6.8. $\vec{p} = 0$, then for $E = +m$, $\Psi = \begin{pmatrix} u \\ 0 \end{pmatrix} e^{-imt}$. What is the meaning of u ?

Remark. $\vec{S}\Psi = \begin{pmatrix} \frac{1}{2}\vec{\sigma}u \\ 0 \end{pmatrix} e^{-imt}$

So u is giving the spin-state of the particle at rest. Also note that for $\vec{p} = 0, E > 0$ we get $u_S = 0$. Seems to give right non-relativistic limit. More to this later. For $\vec{p} = 0, E = -m$ (6.58) is not useful, therefore rather fix u_S and then determine u_L :

$$u_L = \frac{\vec{p}\vec{\sigma}}{E - m} u_S = 0$$

and thus

$$\Psi = \begin{pmatrix} 0 \\ u \end{pmatrix} e^{+imt}$$

Apparently we have the same problem with negative energy as for KG equation.

Dirac Hypothesis

Dirac equation describes Fermions. If all negative energy states are occupied: No decay and no instability possible.

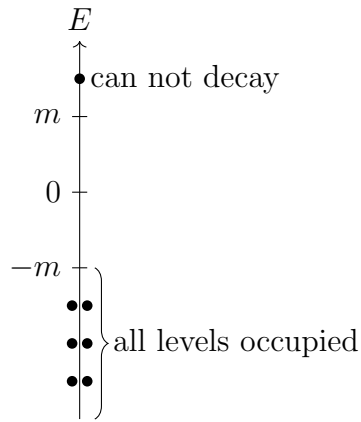


Figure 18: Energy level occupation

Remark. We need to “renormalize” charges of vacuum. Additional benefit, we can describe *positron* in this picture:

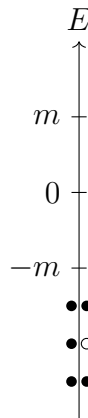


Figure 19: Missing energy level

Unoccupied negative energy state

- effective charge $-q$
- effective positive energy

We can even describe pair creation and annihilation

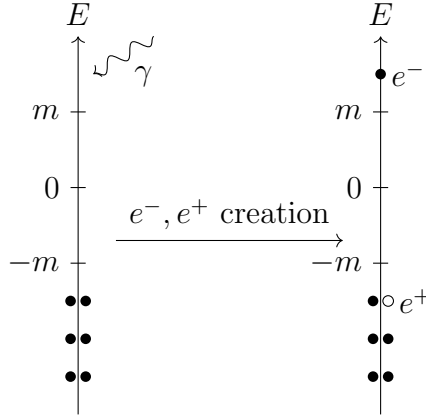


Figure 20: Electron, positron pair creation

Still the even more convincing description is in terms of quantum field theory!

Non-relativistic limit

Hamiltonian of non-rel., spin $\frac{1}{2}$ particle in a magnetic field:

$$H = \frac{\vec{p}_{kin}^2}{2m} - \vec{B}(\vec{x}) \cdot \vec{M}$$

where \vec{M} is the magnetic dipole moment of the particle. For elementary particles:

$$\vec{M} = g \frac{q}{2m} \vec{S} \quad (6.59)$$

where g is the gyromagnetic ratio (or g-factor).

For extended charged rotating object:

$$\vec{M} = \int \vec{x} \times (\vec{\omega} \times \vec{x}) \frac{\rho}{2}(\vec{x}) d^3x$$

If charge-density ρ and mass-density ρ_m have constant ratio, then (6.59) holds, with g depending on $\frac{\rho}{\rho_m}$, with $g = 1$. Measurements show that $g_e \approx 2.002$, not easily explained by the above formula. Consider the non-relativistic limit of the Dirac equation, with $A(x) = (0, \vec{A}(\vec{x}))$ (Details \rightarrow tutorial).

State with energy $E = m + E_{NR}$. In Dirac basis, to leading order in E_{NR} :

$$E_{NR}\psi_L - \vec{\sigma}\vec{p}_{kin}\psi_S = 0 \quad (6.60)$$

$$2m\psi_S - \vec{\sigma}\vec{p}_{kin}\psi_L = 0 \quad (6.61)$$

with $\vec{p}_{kin} = (-i\vec{\partial} - q\vec{A}(\vec{x}))$. (6.61) gives

$$\psi_S = \frac{1}{2m}\vec{\sigma}\vec{p}_{kin}\psi_L \quad (6.62)$$

shows that ψ_S is suppressed by factor $\frac{p_{kin}}{2m} \approx \sqrt{\frac{E_{NR}}{2m}}$. This relation in (6.60)

$$\left(\frac{\vec{p}_{kin}^2}{2m} - 2\frac{q}{2m}\vec{S} \cdot \vec{B}(x) \right) \psi_L = E_{NR}\psi_L \quad (6.63)$$

where we have used that:

$$(\vec{\sigma} \cdot \vec{p}_{kin})^2 = \vec{p}_{kin}^2 \mathbb{1}_{2 \times 2} - q\vec{\sigma} \cdot \vec{B}(x)$$

Comparison (6.63) with non-relativistic Hamiltonian shows and Dirac equation predicts:

$$g_e = 2$$

Remark. Could have started with $E = -mE_{NR}$. Obtained (6.62), (6.63) with $\psi_S \leftrightarrow \psi_L$. Negative energy solutions also present in non-relativistic limit.

Chiral-projector: Decomposition of Dirac spinor into Weyl spinors is manifest in chiral gauge:

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} \quad \gamma^\mu = -i \begin{pmatrix} 0 & \sigma^\mu \\ \bar{\sigma}^\mu & 0 \end{pmatrix}$$

it has

$$(\gamma^5)^2 = \mathbb{1}_{4 \times 4}, \quad \{\gamma^5, \gamma^\mu\} = 0 \quad (6.64)$$

where

$$\begin{pmatrix} \psi_L \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \psi_R \end{pmatrix}$$

span the eigenvalues. Projector on the eigenspaces:

$$P_\pm = \frac{1}{2} (\mathbb{1} \pm \gamma^5) \quad (6.65)$$

Basis independent det.:

$$\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3 \quad (6.66)$$

Why the name γ^5 ? (6.64) shows that (γ^μ, γ^5) is a representation of $\text{Cl}_{4+1}(\mathbb{C})$. In former times, indices run from 1, ...

Connection to parity: What is action of P on spinors? Have:

$$\begin{aligned} P\Lambda(\vec{\alpha}, 0) &= \Lambda(\vec{\alpha}, 0)P \\ P\Lambda(0, \vec{v}) &= \Lambda(0, -\vec{v})P \end{aligned}$$

Which implies for the generators

$$P\vec{N}P^{-1} = -\vec{N}, \quad P\vec{M}P^{-1} = \vec{M}$$

and hence:

$$PL^{\pm}P^{-1} = L^{\pm} \tag{6.67}$$

Thus natural action of P on spinors:

$$\Pi(P)P_{\pm}\psi(\vec{x}, t) = P_{\pm}\psi(-\vec{x}, t)$$

Can see from considering chiral basis

$$\Pi(P) = \gamma^0 \tag{6.68}$$

Physical Significance: Parity relation in standard model (experiments by Wu et al.). Result from asymmetric coupling of the gauge-fields to ψ_L, ψ_R (electroweak interaction). Sketch: Kinematic forms

$$\overline{\psi}_L(\not{\partial} - q\not{A})\psi_L + \overline{\psi}_R\not{\partial}\psi_R$$

6.5 Connection to QFT

Idea: KG equation.

1. Define Hilbert space by restricting to subset of wave functions.
2. Going to many particle picture (Fock space)

will get QFT. Define: For f, g solutions to KG equation

$$\langle f, g \rangle_{KG} := i \int (\overline{f}\partial^0 g - f\partial^0 \overline{g})|_{t=0} d^3x$$

Look at:

$$e_{\vec{k}}^{\pm} = \frac{1}{(2\pi)^{\frac{3}{2}}} \frac{1}{\sqrt{2\omega_{\vec{k}}}} e^{\pm i\omega_{\vec{k}}t + i\vec{k}\vec{x}}$$

Restrict to solution such that $\langle \cdot, \cdot \rangle_{KG}$ positive

$$h = \left\{ f = \tilde{f}(\vec{k}\vec{e}_k^+), \langle f, f \rangle_{KG} < \infty \right\}$$

Many particles:

$$\mathcal{H} = \overline{f_S}(h)$$

Many particle Hamiltonian:

$$H = d\Gamma(h) , h = \sqrt{\vec{p}^2 + m^2}$$

Annihilation and creation operators: For $e_{\vec{k}}^{\pm}$ “basis”

$$[a_{\vec{k}}, a_{\vec{k}'}^{\dagger}] = \delta^{(3)}(\vec{k} - \vec{k}')$$

Then:

$$H = \int d^3k \sqrt{\vec{k}^2 + m^2} a_{\vec{k}}^{\dagger} a_{\vec{k}}$$

positive spectrum.

$$a(\vec{x}, t) = \int d^3k \underbrace{\langle \vec{x} | e_{\vec{k}}^+ \rangle}_{e_{\vec{k}}^+(x)} a_{\vec{k}}(x)$$
$$(\square - m^2) a = 0$$

Define $\Phi(x) = a(x) + a^{\dagger}(x)$ Can obtain Φ from quantifying *field theory* with action

$$S = \int d^4x \frac{1}{2} [\partial^{\mu} \phi \partial^{\mu} \phi + m^2 \phi^2]$$