Integrated Course Ib
Theoretical quantum mechanics

lecture by
Dr. Juan-Diego Urbina
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revision and layout in LyX by
Andreas Völklein

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ATTENTION

This script does *not* replace the lecture.

Therefore it is recommended *strongly* to attend the lecture.

These notes are under constant revision, and the level of rigor is not uniform.

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Literature

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  ISBN: 0-321-50336-8

- Leonard I. Schiff: *Quantum mechanics*, McGraw-Hill, 1968
  ISBN: 0-07-085643-5

- Any introductory book on quantum mechanics.

- Richard P. Feynman, Robert B. Leighton, Matthew L. Sands: *Lectures on physics*

Contents

1 The Formalism and its interpretation

As any theory about physical phenomenons, quantum mechanics requires

i) kinematical aspects: The (mathematical) space where physical states are represented.

   Example from classical mechanics: points in phase space

ii) the definition of observables: Which quantities can be measured and how to represent them in the space of states?

   Example from classical mechanics: any function $f(\vec{r},\vec{p})$

   (This is more complicated in quantum mechanics.)

iii) an dynamical law: How do states evolve in "time"?

   Example from classical mechanics: Hamilton's equations determine $(\vec{q}(t),\vec{p}(t))$ depending on $(\vec{q}(t_0),\vec{p}(t_0))$.

1.1 The kinematical aspects of quantum mechanics

The FIRST POSTULATE says:

> "The state of a quantum mechanical system is represented as a normalized vector in a (complex) Hilbert space.
> Vectors, which differ only by a phase, represent the same state."

To understand what this means, we introduce some concepts:

a) *Hilbert space*: A (finite or infinite dimensional) complete vector space with a positive definite scalar product. Following Dirac, elements in the Hilbert space $\mathcal{H}$ are called *kets* and we represent them by $|\psi\rangle, |\phi\rangle \in \mathcal{H}$.

   For complex numbers $a,b \in \mathbb{C}$ also $a|\psi\rangle + b|\phi\rangle \in \mathcal{H}$ is a element of the Hilbert space.

   The sum is associative and the product by scalars is distributive.

b) *Scalar product*: The operation associating a complex number to each pair of states

$$\begin{aligned}\langle .,. \rangle : \mathcal{H} \times \mathcal{H} &\to \mathbb{C} \\ (|\psi\rangle, |\phi\rangle) &\mapsto \langle \psi,\phi \rangle\end{aligned}$$

   with the properties

$$\begin{aligned}\langle \eta, a\phi + b\psi \rangle &= a\langle \eta,\phi\rangle + b\langle \eta,\psi\rangle \qquad & \langle \psi,\phi\rangle &= \langle \phi,\psi\rangle^* \\ \langle \psi,\psi\rangle &\geq 0 & \langle \psi,\psi\rangle = 0 \quad &\Leftrightarrow \quad |\psi\rangle = 0\end{aligned}$$

for $a,b \in \mathbb{C}$ and $|\phi\rangle, |\psi\rangle, |\eta\rangle \in \mathcal{H}$ is called the scalar product.

The *norm* of a state $|\psi\rangle$ is then defined as:

$$\|\psi\| := \||\psi\rangle\| := \sqrt{\langle\psi,\psi\rangle}$$

If $\||\psi\rangle\| = 1$, then $|\psi\rangle$ is said to be *normalized.*

c) *Phase*: A Complex number $z \in \mathbb{C}$ with unit norm, that means $zz^* = 1$. It can be represented via a real number $\alpha \in \mathbb{R}$ as $z = e^{\mathbf{i}\alpha}$.

The physical state associated with $|\psi\rangle$ and $e^{\mathbf{i}\alpha}|\psi\rangle$ is THE SAME.

d) C*omplete basis*: A family of kets $(|\phi_i\rangle)_{i\in I\subseteq\mathbb{N}}$ such that for ALL states $|\psi\rangle \in \mathcal{H}$, there is a family of complex numbers $(c_i)_{i\in I\subseteq\mathbb{N}}$ (depending on $|\psi\rangle$) with:

$$|\psi\rangle = \sum_{i\in I} c_i |\phi_i\rangle$$

If $\langle\phi_i,\phi_j\rangle = \delta_{ij}$, then the basis is *complete* and *orthonormal.*

In the case of an uncountably infinite vector space the basis $(|q\rangle)_{q\in\mathbb{R}}$ can be written as a function of a real variable. The representation of $|\psi\rangle$ then is an infinite sum, that is an integral

$$|\psi\rangle = \int \psi(q)\,|q\rangle\,\mathrm{d}q$$

and a complete and orthonormal basis is characterized by $\langle q,q'\rangle = \delta(q-q')$.

e) *Adjoint*: For each Hilbert space $\mathcal{H}$ there is another Hilbert space $\mathcal{H}^*$ called *dual*, with elements $\langle f| \in \mathcal{H}^*$, which are LINEAR FUNCTIONALS acting on $\mathcal{H}$:

$$\begin{aligned}\langle f| : \mathcal{H} &\to \mathbb{C}\\ |\psi\rangle &\mapsto \langle f\,|\,\psi\rangle\end{aligned}$$

$\langle\psi\,|\,\phi\rangle$ is called *bracket.* Riesz theorem says, that there is a ONE TO ONE correspondence between $\mathcal{H}$ and $\mathcal{H}^*$:

$$\underset{|\psi\rangle\in\mathcal{H}}{\forall}\ \underset{\langle\psi|\in\mathcal{H}^*}{\exists}\ \underset{|\phi\rangle\in\mathcal{H}}{\forall}\ :\ \langle\psi\,|\,\phi\rangle = \langle\psi,\phi\rangle, \|\langle\psi|\| = \||\psi\rangle\|$$

The so associated $\langle\psi|$ is the *adjoint* of $|\psi\rangle$, called *bra*, and we write:

$$\begin{aligned}{}^\dagger : \mathcal{H} &\to \mathcal{H}^*\\ |\psi\rangle &\mapsto (|\psi\rangle)^\dagger = \langle\psi|\end{aligned}$$

The function † is semilinear, that means for $a,b \in \mathbb{C}$ and $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ is:

$$(a|\psi\rangle + b|\phi\rangle)^\dagger = a^*\langle\psi| + b^*\langle\phi|$$

f) *Representation*: Assume that $(|\phi_i\rangle)_{i\in I\subseteq\mathbb{N}}$ (respectively $(|q\rangle)_{q\in\mathbb{R}}$) is a complete orthonormal basis. The ket $|\psi\rangle$ is said to "be represented" in that basis by associating:

discrete case | continous case

$$\langle\psi| \mapsto \begin{pmatrix} \langle\phi_1\,|\,\psi\rangle \\ \langle\phi_2\,|\,\psi\rangle \\ \vdots \end{pmatrix} \in \mathbb{C}^{|I|} \qquad |\psi\rangle \mapsto \langle q\,|\,\psi\rangle =: \psi(q)$$

$$\langle\psi| \mapsto \begin{pmatrix} \langle\phi_1\,|\,\psi\rangle^* \\ \langle\phi_2\,|\,\psi\rangle^* \\ \vdots \end{pmatrix} \in \mathbb{C}^{|I|} \qquad \langle\psi| \mapsto \langle q\,|\,\psi\rangle^* = \psi(q)^*$$

This $\psi(q)$ is the wave function.

g) *Exterior product*: The object $|\phi\rangle\langle\psi| : \mathcal{H} \to \mathcal{H}$ is a linear operator acting on $|\eta\rangle \in \mathcal{H}$ defined by

$$(|\phi\rangle\langle\psi|)\,|\eta\rangle := \underbrace{\langle\psi\eta\rangle}_{\in\mathbb{C}}|\phi\rangle$$

with the adjoint:

$$(|\phi\rangle\langle\psi|)^\dagger := |\psi\rangle\langle\phi|$$

Example from linear algebra:

$$\vec{v} = (v_1,\ldots,v_n)^T \qquad \vec{u} = (u_1,\ldots,u_n)^T$$

$$\vec{v}^T\vec{u} = \sum_{i=1}^{n} v_i u_i$$

$$\vec{u}\vec{v}^T = \begin{pmatrix} u_1v_1 & \ldots & u_1v_n \\ \vdots & \ddots & \vdots \\ u_nv_1 & \ldots & u_nv_n \end{pmatrix}$$

1.2 Observables and measurements in quantum mechanics

What can be observed and how measurements affect quantum states is encoded into the following two POSTULATES:

> "Observables in quantum mechanics are represented by LINEAR HERMITIAN OPERATORS on $\mathcal{H}$."
>
> "The results of a measurement of the physical quantity represented by an observable can only take values belonging to the SPECTRUM of the observable. Just after measurement, that gives one of the eigenvalues of the observable, the state belongs to corresponding eigenspace."

a) $\hat{A} : \mathcal{H} \to \mathcal{H}$ is a *linear* operator if and only if:

$$\hat{A}\left(a\left|\psi\right\rangle + b\left|\phi\right\rangle\right) = a\hat{A}\left|\psi\right\rangle + b\hat{A}\left|\phi\right\rangle$$

For every linear operator $\hat{A}$ there is the identity:

$$\left\langle \psi \,\middle|\, \hat{A}\phi \right\rangle = \left\langle \phi \,\middle|\, \hat{A}^\dagger \psi \right\rangle^*$$

$\hat{A}^\dagger$ is called the *adjoint* of $\hat{A}$. If and only if $\hat{A} = \hat{A}^\dagger$ then $\hat{A}$ is called HERMITIAN.

b) The *spectrum* of an operator $\hat{Q}$ is defined by a set of numbers Q_i, called *eigenvalues*, that fulfill the equation:

$$\hat{Q}\left|Q_i\right\rangle = Q_i\left|Q_i\right\rangle$$

The $\left|Q_i\right\rangle$ are the corresponding eigenvectors. If there is more than one eigenvector for the same eigenvalue then the spectrum is called *degenerated* and the different eigenvectors are denoted by $\left|Q_i^{(d)}\right\rangle$ with $d \in D \subseteq \mathbb{N}$.

Hermitian operators have REAL eigenvalues and ORTHOGONAL eigenvectors.

That means, if $\hat{A} = \hat{A}^\dagger$, $\hat{A}\left|a_i\right\rangle = a_i\left|a_i\right\rangle$, then $a_i = a_i^*$ and $\left\langle a_i \,\middle|\, a_j\right\rangle = 0$ if $i \neq j$.

If the eigenvectors are normalized, then we can write $\left\langle a_i \,\middle|\, a_j\right\rangle = \delta_{ij}$.

c) The *spectrum decomposition* of a Hermitian operator ($\hat{A} = \hat{A}^\dagger$) with

discrete case	continous case
$\hat{A}\left\|a_i\right\rangle = a_i\left\|a_i\right\rangle$	$\hat{A}\left\|a\right\rangle = a\left\|a\right\rangle$

is given by:

$$\hat{A} = \sum_{i\in I} a_i \left|a_i\right\rangle\left\langle a_i\right| \qquad\qquad \hat{A} = \int a\left|a\right\rangle\left\langle a\right| \mathrm{d}a$$

In linear algebra a symmetric matrix $M = M^T$ with eigenvalues m_i for $i \in \{1, \ldots, n\}$ can be written as:

$$M = \begin{pmatrix} m_1 & 0 & \ldots & 0 \\ 0 & m_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & m_n \end{pmatrix} = m_1 \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & 0 \end{pmatrix} + \ldots + m_n \begin{pmatrix} 0 & 0 & \ldots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & 0 \\ 0 & \ldots & 0 & 1 \end{pmatrix}$$

d) The *unit operator* $\hat{I}$ defined by

$$\underset{\left|\phi\right\rangle\in\mathcal{H}}{\forall} \;:\; \hat{I}\left|\phi\right\rangle = \left|\phi\right\rangle$$

can be written as

discrete case	continous case
$\hat{I} = \sum_{i\in I} \left\|a_i\right\rangle\left\langle a_i\right\|$	$\hat{I} = \int \left\|a\right\rangle\left\langle a\right\| \mathrm{d}a$

where $\left(\left|a_i\right\rangle\right)_{i\in I\subseteq\mathbb{N}}$ (respectively $\left(\left|a\right\rangle\right)_{a\in\mathbb{R}}$) is a complete orthonormal basis.

e) The *projection* of $|\psi\rangle$ along a basis vector $|a_i\rangle$ (respectively $|a\rangle$) is:

discrete case	continous case
$(\lvert a_i\rangle\langle a_i\rvert)\lvert\psi\rangle = \langle a_i \mid \psi\rangle \lvert a_i\rangle$	$(\lvert a\rangle\langle a\rvert)\lvert\psi\rangle = \langle a \mid \psi\rangle \lvert a\rangle$

f) The *algebra* of the operators $\hat{Q}_1$ and $\hat{Q}_2$ is:

$$\begin{aligned}\left(\hat{Q}_1\hat{Q}_2\right)|\psi\rangle &:= \hat{Q}_1\left(\hat{Q}_2|\psi\rangle\right) \neq \left(\hat{Q}_2\hat{Q}_1\right)|\psi\rangle \\ \left(\hat{Q}_1\hat{Q}_2\right)^\dagger &:= \hat{Q}_2^\dagger\hat{Q}_1^\dagger\end{aligned}$$

The *commutator* is defined by:

$$\left[\hat{Q}_1,\hat{Q}_2\right] := \hat{Q}_1\hat{Q}_2 - \hat{Q}_2\hat{Q}_1$$

It is bilinear and has the properties:

i) It is antisymmetric:

$$\left[\hat{Q}_1,\hat{Q}_2\right] = -\left[\hat{Q}_2,\hat{Q}_1\right]$$

ii) Jacobi identity:

$$\left[\hat{Q}_1,\left[\hat{Q}_2,\hat{Q}_3\right]\right] + \left[\hat{Q}_2,\left[\hat{Q}_3,\hat{Q}_1\right]\right] + \left[\hat{Q}_3,\left[\hat{Q}_1,\hat{Q}_2\right]\right] = 0$$

iii) Leibniz identity:

$$\left[\hat{Q}_1,\hat{Q}_2\hat{Q}_3\right] = \hat{Q}_2\left[\hat{Q}_1,\hat{Q}_3\right] + \left[\hat{Q}_1,\hat{Q}_2\right]\hat{Q}_3$$

Due to these identities the commutator is analogous to the classical Poisson bracket.
Two observables $\left(\hat{A} = \hat{A}^\dagger, \hat{B} = \hat{B}^\dagger\right)$ are called *compatible* if and only if $\left[\hat{A},\hat{B}\right] = 0$.
Theorem: If $\hat{A}$ and $\hat{B}$ are compatible then there exists a basis $(|k_i\rangle)_{i\in I\subseteq\mathbb{N}}$ such that:

$$\begin{aligned}\hat{A}|k_i\rangle &= a_i|k_i\rangle \\ \hat{B}|k_i\rangle &= b_i|k_i\rangle\end{aligned}$$

Therefore the states $|k_i\rangle$ have well defined properties (a_i,b_i).

g) i) The *matrix representation* of an operator WITH RESPECT TO THE BASIS $(|a_i\rangle)_{i\in\{1,\dots,n\}}$ (respectively $(|q\rangle)_{q\in\mathbb{R}}$) is:

discrete case / continuous case

$$\hat{Q} \to \begin{pmatrix} \left\langle a_1 \middle| \hat{Q} \middle| a_1\right\rangle & \dots & \left\langle a_1 \middle| \hat{Q} \middle| a_n\right\rangle \\ \vdots & \ddots & \vdots \\ \left\langle a_n \middle| \hat{Q} \middle| a_1\right\rangle & \dots & \left\langle a_n \middle| \hat{Q} \middle| a_n\right\rangle \end{pmatrix} = \qquad \hat{Q} \to \left\langle q \middle| \hat{Q} \middle| q'\right\rangle = Q\left(q,q'\right)$$

$$= \left(\left\langle a_i \middle| \hat{Q} \middle| a_j\right\rangle\right)_{ij} =: Q_{ij}$$

ii) The *trace* of $\hat{Q}$ is defined by

discrete case	continuous case
$\operatorname{Tr}\left(\hat{Q}\right) = \sum_{i=1}^{n} \left\langle a_i \middle| \hat{Q} \middle| a_i \right\rangle$	$\operatorname{Tr}\left(\hat{Q}\right) = \int Q\left(q,q\right) \mathrm{d}q$

ans is independent of the basis.

Therefore the equation

$$\hat{Q} \left|\psi\right\rangle = \left|\phi\right\rangle$$

can be written in this basis by:

i) Multiplying $\left\langle a_i \right|$ from the left: $\left\langle a_i \middle| \hat{Q} \middle| \phi \right\rangle = \left\langle a_i \mid \phi \right\rangle$

ii) Insert an unit operator after $\hat{Q}$:

$$\left\langle a_i \middle| \hat{Q}\hat{I} \middle| \phi \right\rangle = \left\langle a_i \middle| \hat{Q} \left(\sum_{j=1}^{n} \left|a_j\right\rangle \left\langle a_j\right| \right) \middle| \phi \right\rangle = \sum_{j=1}^{n} \left\langle a_i \middle| \hat{Q} \middle| a_j \right\rangle \left\langle a_j \mid \phi \right\rangle = \left\langle a_i \mid \phi \right\rangle$$

This is the component form of the vector equation:

$$\begin{pmatrix} Q_{11} & \dots & Q_{1n} \\ \vdots & & \vdots \\ Q_{n1} & \dots & Q_{nn} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_n \end{pmatrix}$$

The continuous version is

$$\int Q\left(q,q'\right) \psi\left(q'\right) \mathrm{d}q' = \phi\left(q\right)$$

with $Q\left(q,q'\right) := \left\langle q \middle| \hat{Q} \middle| q \right\rangle$, $\psi\left(q'\right) = \left\langle q' \mid \psi \right\rangle$ and $\phi\left(q\right) = \left\langle q \mid \phi \right\rangle$.

h) Change of basis and unitary transformations.

i) An operator $\hat{U}$ is called *unitary* if and only if $\hat{U}^T = \hat{U}^{-1}$.

ii) Unitary transformations ("transformation" is the same as "operator") preserve scalar products. For $\left|\psi\right\rangle, \left|\phi\right\rangle \in \mathcal{H}$ we define:

$$\left|\psi'\right\rangle := \hat{U} \left|\psi\right\rangle \qquad \left|\phi'\right\rangle := \hat{U} \left|\phi\right\rangle$$

Then the scalar product is the same:

$$\left\langle \psi' \mid \phi' \right\rangle = \left\langle \psi \mid \phi \right\rangle$$

iii) Unitary transformations represent changes of the basis.

$$\left|\psi\right\rangle = \hat{I} \left|\psi\right\rangle = \left(\sum_i \left|a_i\right\rangle \left\langle a_i\right| \right) \left|\psi\right\rangle = \sum_{i \in I} \left\langle a_i \mid \psi \right\rangle \left|a_i\right\rangle$$

$$\left\langle b_i \mid \psi \right\rangle = \sum_{j \in I} \left\langle b_i \mid a_j \right\rangle \left\langle a_j \mid \psi \right\rangle$$

$$\begin{pmatrix} \psi_1^{(b)} \\ \vdots \\ \psi_N^{(b)} \end{pmatrix} = \mathbb{U} \cdot \begin{pmatrix} \psi_1^{(a)} \\ \vdots \\ \psi_N^{(a)} \end{pmatrix}$$
$$[\mathbb{U}]_{ij} = U_{ij} = \langle b_i \mid a_j \rangle$$

iv) For operators the transformations are:

$$\begin{aligned} Q_{ij}^{(b)} &= \left\langle b_i \middle| \hat{Q} \middle| b_j \right\rangle = \left\langle b_i \middle| \hat{I}\hat{Q}\hat{I} \middle| b_j \right\rangle = \sum_{l,m \in I} \langle b_i \mid a_l \rangle \left\langle a_l \middle| \hat{Q} \middle| a_m \right\rangle \langle a_m \mid b_j \rangle = \\ &= \sum_{l,m \in I} U_{il} Q_{lm}^{(a)} U_{mj} = \sum_{l,m} U_{il} Q_{lm}^{(a)} \left(U_{jm}\right)^* \\ \mathbb{Q}^{(b)} &= \mathbb{U}\mathbb{Q}^{(a)}\mathbb{U}^\dagger \end{aligned}$$

i) One can describe functions mapping one operator to another by their Taylor series:

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} c_n x^n \\ c_n &= \frac{1}{n!} \partial_x^n f(x) \big|_{x=0} \\ f\left(\hat{Q}\right) &:= \sum_{n=0}^{\infty} c_n \hat{Q}^n \end{aligned}$$

This is very nice. But this does not work for more than one operator, if they do not commute.

$$\begin{aligned} f(x,y) &= \sum_{n,m} c_{n,m} x^n y^m \\ f\left(\hat{Q}_1,\hat{Q}_2\right) &\neq \sum_{n,m} c_{n,m} \hat{Q}_1^n \hat{Q}_2^m \\ xy &\overset{?}{\rightarrow} \begin{cases} \hat{Q}_1\hat{Q}_2 \\ \hat{Q}_2\hat{Q}_1 \\ \frac{1}{2}\left(\hat{Q}_1\hat{Q}_2 + \hat{Q}_2\hat{Q}_1\right) \end{cases} \end{aligned}$$

In a basis of eigenvectors $|q_i\rangle$, that means $\hat{Q}|q_i\rangle = q_i |q_i\rangle$, one can write:

discrete case	continuous case
$f\left(\hat{Q}\right) = \sum_i f(q_i) \lvert q_i\rangle \langle q_i\rvert$	$f\left(\hat{Q}\right) = \int f(q) \lvert q\rangle \langle q\rvert \,\mathrm{d}q$

j) An operator can also depend on parameters:

$$\mathbb{R} \ni t \mapsto \hat{A}(t) \in \mathrm{End}_{\mathbb{C}}(\mathcal{H})$$

It has all the nice properties, but one has to be careful not to change the ordering of the operators, if they do not commute:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{A}(t)\,\hat{B}(t)\right) = \left(\frac{\mathrm{d}\hat{A}(t)}{\mathrm{d}t}\right)\hat{B}(t) + \hat{A}(t)\left(\frac{\mathrm{d}\hat{B}(t)}{\mathrm{d}t}\right)$$

$$\frac{\mathrm{d}\hat{A}(t)}{\mathrm{d}t} = \hat{B}(t) \quad \Rightarrow \quad \hat{A}(t) = \int_0^t \hat{B}(t')\,\mathrm{d}t' + \hat{A}_0$$

Extra property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\langle\psi(t)\,|\,\phi(t)\rangle\right) = \left(\frac{\mathrm{d}\langle\psi(t)|}{\mathrm{d}t}\right)|\phi(t)\rangle + \langle\psi(t)|\left(\frac{\mathrm{d}|\phi(t)\rangle}{\mathrm{d}t}\right)$$

As norm one usually uses:

$$\left\|\hat{A}\right\|^2 = \mathrm{Tr}\left(\hat{A}\hat{A}^\dagger\right)$$

1.3 What does quantum actually predict?

Think about classical mechanics:

$$(x(0),p(0)) \xrightarrow{\text{evolution}} (x(t),p(t)) \to f(x(t),p(t)) \text{ is known}$$

So classical mechanics is DETERMINISTIC (the state of a system is determined by the initial conditions) and REALISTIC (the value you are going to measure already exists before the actual measurement).

Back to quantum mechanics:

The full dynamics is encoded in the postulate:

> "In each quantum mechanical system there exists an observable $\hat{H}(t)$, called *Hamiltonian* which is assumed to be BOUNDED from below (and it is a nice operator). The solution of the equation
>
> $$\mathbf{i}\hbar\partial_t\hat{U}(t,t_0) = \hat{H}(t)\,\hat{U}(t,t_0) \qquad \hat{U}(t_0,t_0) = \hat{I} \qquad \text{for } t > t_0$$
>
> is an unitary operator $\hat{U}$, called TIME EVOLUTION OPERATOR. The time evolution of an initial state $|\psi(t_0)\rangle$ is given by $|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle$."

Comments:

a) If $\partial_t\hat{H}(t) = 0$, the one can directly solve the Schrödinger equation:

$$\hat{U}(t,t_0) = e^{\frac{-\mathbf{i}}{\hbar}\hat{H}\cdot(t-t_0)} \qquad \text{for } t > t_0 \tag{1.1}$$

b) $\hat{U}$ has a SEMIGROUP property:

$$\hat{U}(t,t')\,\hat{U}(t',t_0) = \hat{U}(t,t_0) \qquad t > t' > t_0$$

Semigroup means:

$$\hat{U}(t,t_0)^{-1} = \hat{U}(t,t_0)^\dagger \neq \hat{U}(t_0,t)$$

c) Constructing $\hat{H}(t)$ is the main step to define a quantum mechanical system, at the end it relies on experimental verification.

d) The formal solution of (1.1) is found by iteration:

$$
\begin{aligned}
\hat{U}(t,t_0) &= \hat{I} - \frac{\mathbf{i}}{\hbar}\int_{t_0}^{t} \hat{H}(t')\,\hat{U}(t',t_0)\,\mathrm{d}t' \qquad\qquad t > t' \\
&= \hat{I} - \frac{\mathbf{i}}{\hbar}\int_{t_0}^{t} \hat{H}(t')\left(\hat{I} - \frac{\mathbf{i}}{\hbar}\int_{t_0}^{t} \hat{H}(t'')\,\hat{U}(t'',t_0)\,\mathrm{d}t''\right)\mathrm{d}t' = \\
&= \hat{I} - \frac{\mathbf{i}}{\hbar}\int_{t_0}^{t} \hat{H}(t')\,\mathrm{d}t' + \left(\frac{\text{-}\mathbf{i}}{\hbar}\right)^2 \int_{t_0}^{t}\int_{t_0}^{t'} \hat{H}(t')\,\hat{H}(t'')\,\hat{U}(t'',t_0)\,\mathrm{d}t''\mathrm{d}t' = \\
&= \tau e^{\frac{\text{-}\mathbf{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t')\mathrm{d}t'}
\end{aligned}
$$

τ is the TIME ORDERING OPERATOR.

$$
\tau\left(\hat{H}(t)\,\hat{H}(t')\right) = \begin{cases} \hat{H}(t)\,\hat{H}(t') & t > t' \\ \hat{H}(t')\,\hat{H}(t) & t < t' \end{cases}
$$

e) Stationary states: Assume $\partial_t \hat{H}(t) = 0$, then the eigenstates of $\hat{H}$ are defined by the time-independent Schrödinger equation:

$$
\hat{H}\left|e_n\right\rangle = e_n\left|e_n\right\rangle
$$

Their time evolution is:

$$
\left|e_n(t)\right\rangle = e^{\text{-}\frac{\mathbf{i}}{\hbar}\hat{H}t}\left|e_n\right\rangle = \underbrace{e^{\text{-}\frac{\mathbf{i}e_n}{\hbar}t}}_{\text{phase}}\left|e_n\right\rangle = e^{\text{-}\mathbf{i}\omega_n t}\left|e_n\right\rangle
$$

For an arbitrary initial state $\left|\psi(t_0)\right\rangle$ we can calculate the final state:

$$
\begin{aligned}
\left|\psi(t)\right\rangle &= e^{\text{-}\frac{\mathbf{i}}{\hbar}\hat{H}\cdot(t-t_0)}\left|\psi(t_0)\right\rangle = e^{\text{-}\frac{\mathbf{i}}{\hbar}\hat{H}\cdot(t-t_0)}\hat{I}\left|\psi(t_0)\right\rangle = \\
&= \sum_{n=0}^{\infty}\left\langle e_n \,|\, \psi(t_0)\right\rangle e^{\text{-}\mathbf{i}\omega_n\cdot(t-t_0)}\left|e_n\right\rangle
\end{aligned}
$$

f) Instead of finding $\hat{U}$ we can solve the SCHRÖDINGER EQUATION directly for $\left|\psi(t)\right\rangle$:

$$
\begin{aligned}
\mathbf{i}\hbar\partial_t\left|\psi(t)\right\rangle &= \hat{H}(t)\left|\psi(t)\right\rangle \\
\left|\psi(t=t_0)\right\rangle &= \left|\psi(t_0)\right\rangle
\end{aligned}
$$

1.4 The probabilistic interpretation of quantum mechanics (Born's rule)

"If the states of a system at time t is given by the normalized state $\left|\psi(t)\right\rangle$, then the PROBABILITY to get the outcome a_i when the observable $\hat{A}$ is measured is given by:"

discrete case	continuous case
$P(a_i,t) = \left|\left\langle a_i \,|\, \psi(t)\right\rangle\right|^2$	$P(q,t) = \left|\left\langle q \,|\, \psi(t)\right\rangle\right|^2 \mathrm{d}q$

a)

discrete case	continuous case
$\sum_i P(a_i,t) = 1$	$\int P(q,t)\,\mathrm{d}q = 1$

$\langle a_i \,|\, \psi(t)\rangle$ is called probability Amplitude, $P(q,t)$ is the density of probability and the probability to obtain an outcome between q and $q + \mathrm{d}q$ is $|\langle q \,|\, \psi(t)\rangle|^2$.

b) The expectation value is given by:

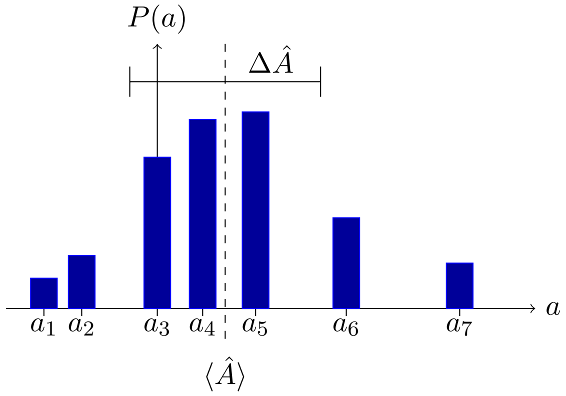
$$\begin{aligned}\overline{A} &:= \sum_i a_i P(a_i,t) = \sum_i a_i |\langle a_i \,|\, \psi(t)\rangle|^2 = \sum_i a_i \langle a_i \,|\, \psi(t)\rangle \cdot \langle a_i \,|\, \psi(t)\rangle^* = \\ &= \sum_i a_i \langle \psi(t) \,|\, a_i\rangle \cdot \langle a_i \,|\, \psi(t)\rangle = \langle \psi(t)| \left(\sum_i a_i |a_i\rangle \cdot \langle a_i|\right) |\psi(t)\rangle = \\ &= \left\langle \psi(t) \middle| \hat{A} \middle| \psi(t)\right\rangle =: \left\langle \hat{A}\right\rangle\end{aligned}$$

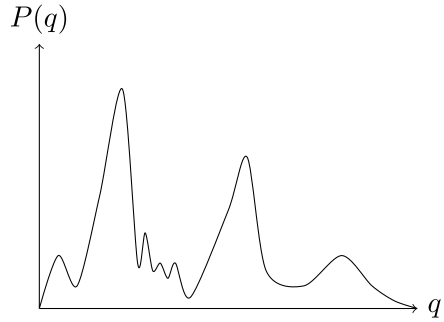
$$\begin{aligned}\mathrm{Var}\hat{A} &= \left\langle \hat{A}^2 \right\rangle - \left(\left\langle \hat{A}\right\rangle\right)^2 = \left\langle \psi(t) \middle| \hat{A}^2 \middle| \psi\right\rangle - \left\langle \psi(t) \middle| \hat{A} \middle| \psi(t)\right\rangle^2 = \\ &= \left\langle \left(\hat{A} - \hat{I}\left\langle \hat{A}\right\rangle\right)^2 \right\rangle = \sum (a_i - \overline{a}_i)^2 P(a_i,t) = \left(\Delta \hat{A}\right)^2\end{aligned}$$

The only case, one gets

$$\left\langle \left(\hat{A} - \left\langle \hat{A}\right\rangle\right)^2 \right\rangle = 0$$

is, if $|\psi(t)\rangle = |a_i\rangle$.





c) Consider the eigenstates of the Hamiltonian:

$$\hat{H}\,|e_n\rangle = e_n\,|e_n\rangle$$

If at $t = 0$ the state is $|e_n\rangle$, then the time evolution is very simple:

$$\begin{aligned}|e_n(t)\rangle &= e^{-\mathbf{i}\omega_n t}\,|e_n\rangle \\ \Rightarrow \quad \left\langle e_n(t) \middle| \hat{A} \middle| e_n(t)\right\rangle &= \left\langle e_n \middle| \hat{A} \middle| e_n\right\rangle \\ \partial_t \left\langle \hat{A}\right\rangle &= 0\end{aligned}$$

d) Define $|\eta\rangle = N\left(|\psi\rangle + |\phi\rangle\right)$. What is the probability $P_\eta\left(a_i\right)$?

$$\begin{aligned}\left|\langle a_i \,|\, \eta\rangle\right|^2 &= N^2 \left|\langle a_i \,|\, \psi\rangle + \langle a_i \,|\, \phi\rangle\right|^2 = \\ &= N^2 \left(\left|\langle a_i \,|\, \psi\rangle\right|^2 + \left|\langle a_i \,|\, \phi\rangle\right|^2 + 2\mathrm{Re}\left(\langle a_i \,|\, \psi\rangle \langle a_i \,|\, \phi\rangle^*\right)\right) = \\ &= N^2 \left(P_\psi\left(a_i\right) + P_\phi\left(a_i\right) + \text{something}\right)\end{aligned}$$

Therefore it is not enough to know the probabilities, one also has to know the phase of the states.

1.5 “Quantization”: Introducing the “fundamental” or basic observables

1.5.1 General approach

Historically, it all started with the Hydrogen atom. (In this system the Hilbert space $\mathcal{H}$ is infinite-dimensional.) It is called “canonical” quantization.

i) $\dim \mathcal{H} = \infty$ means, there can be discrete as well as continuous eigenvalues.

ii) Every quantum mechanical observable is a function of two basic observables, the position operator $\hat{q}_\alpha$ and the momentum operator $\hat{p}_\alpha$, satisfying:

$$[\hat{q}_\alpha,\hat{p}_\beta] = \mathbf{i}\hbar\delta_{\alpha\beta}\hat{I} \qquad\qquad [\hat{q}_\alpha,\hat{q}_\beta] = 0 = [\hat{p}_\alpha,\hat{p}_\beta]$$

Therefore you can define an eigenbasis $|\vec{q}\rangle$ with:

$$\hat{q}_\alpha\,|\vec{q}\rangle = q_\alpha\,|\vec{q}\rangle \qquad \hat{p}_\alpha\,|\vec{p}\rangle = p_\alpha\,|\vec{p}\rangle \qquad q_\alpha, p_\alpha \in \mathbb{R}$$

$$\left\langle \vec{q} \,\middle|\, \vec{q}\,' \right\rangle = \delta\left(\vec{q} - \vec{q}\,'\right) \qquad\qquad \left\langle \vec{p} \,\middle|\, \vec{p}\,' \right\rangle = \delta\left(\vec{p} - \vec{p}\,'\right)$$

iii) The Hamiltonian operator is given in terms of the classical Hamiltonian

$$H\left(\vec{q},\vec{p}\right) = \left(\frac{1}{2m}\sum_\alpha p_\alpha^2\right) + V\left(\vec{q}\right)$$

as:

$$\hat{H} = H\left(\hat{q}_\alpha,\hat{p}_\alpha\right) = \left(\frac{1}{2m}\sum_\alpha \hat{p}_\alpha^2\right) + V\left(\hat{q}_\alpha\right)$$

This works ONLY in Cartesian coordinates! In other coordinates the product pq occurs in H, but how to quantize qp? The operators do not commute: $\hat{q}\hat{p} \neq \hat{p}\hat{q}$

For a magnetic field with vector potential $\vec{A}\left(\vec{q}\right)$ the Hamiltonian is

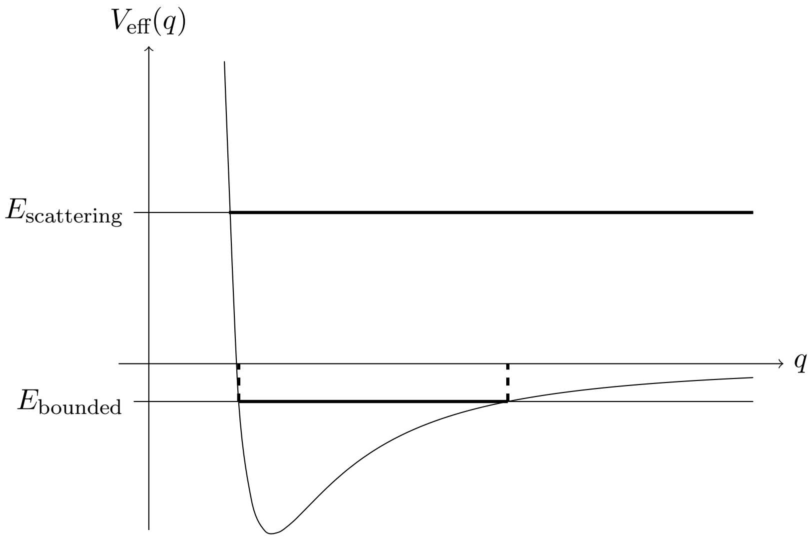
$$H = \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\left(\vec{q}\right)\right)^2$$

and also depends on products of $\vec{p}$ and $\vec{q}$.

$$\hat{H} = \sum_n e_n\,|e_n\rangle\,\langle e_n| + \int_\Omega e\left(\kappa\right)|e\left(\kappa\right)\rangle\,\langle e\left(\kappa\right)|\,\mathrm{d}k$$

$$\langle e_n \,|\, e_{n'} \rangle = \delta_{n,n'} \qquad \text{bounded}$$
$$\left\langle e\left(\kappa\right) \,\middle|\, e\left(\kappa'\right) \right\rangle = \delta\left(\kappa - \kappa'\right) \qquad \text{scattering}$$

A typical effective potential is:



iv) The representations of a state $|\psi\rangle$ in the position or momentum eigenstates are called WAVEFUNCTIONS. This means:

$$|\psi\rangle = \int \underbrace{\langle \vec{q} \,|\, \psi \rangle}_{=\psi(\vec{q})} |\vec{q}\rangle \,\mathrm{d}\vec{q} \qquad\qquad |\psi\rangle = \int \underbrace{\langle \vec{p} \,|\, \psi \rangle}_{=\tilde{\psi}(\vec{p})} |\vec{p}\rangle \,\mathrm{d}\vec{p}$$

Born's rule says, that $\left|\psi\left(\vec{q}\right)\right|^2 \mathrm{d}\vec{q}$ is the probability to find the particle between $\vec{q}$ and $\vec{q} + (\mathrm{d}q_1, \mathrm{d}q_2, \ldots)$ and $\left|\tilde{\psi}\left(\vec{p}\right)\right|^2 \mathrm{d}\vec{p}$ is the probability to find the particle between $\vec{p}$ and $\vec{p} + (\mathrm{d}p_1, \mathrm{d}p_2, \ldots)$.

1.5.2 Algebraic properties of $\hat{q}$ and $\hat{p}$

Consider the following commutators:

$$\begin{aligned}
\left[\hat{q}_\alpha, \hat{p}_\beta^2\right] &= \hat{p}_\beta \left[\hat{q}_\alpha, \hat{p}_\beta\right] + \left[\hat{q}_\alpha, \hat{p}_\beta\right] \hat{p}_\beta = 2\mathbf{i}\hbar\delta_{\alpha\beta}\hat{p}_\beta \\
\left[\hat{q}_\alpha, \hat{p}_\beta^3\right] &= \hat{p}_\beta^2 \left[\hat{q}_\alpha, \hat{p}_\beta\right] + \hat{p}_\beta \left[\hat{q}_\alpha, \hat{p}_\beta\right] \hat{p}_\beta + \left[\hat{q}_\alpha, \hat{p}_\beta\right] \hat{p}_\beta^2 = 3\mathbf{i}\hbar\delta_{\alpha\beta}\hat{p}_\beta^2 \\
&\vdots \\
\left[\hat{q}_\alpha, \hat{p}_\beta^n\right] &= \sum_{k=1}^{n} \hat{p}_\beta^{n-k} \left[\hat{q}_\alpha, \hat{p}_\beta\right] \hat{p}_\beta^{k-1} = n\mathbf{i}\hbar\delta_{\alpha\beta}\hat{p}_\beta^{n-1}
\end{aligned}$$

Since every analytic function can be represented by its Taylor series, one gets:

$$\begin{aligned}
\left[\hat{q}_\alpha, f\left(\hat{p}_\beta\right)\right] &= \mathbf{i}\hbar\delta_{\alpha\beta}\partial_x f\left(x\right)\Big|_{x=\hat{p}_\beta} =: \mathbf{i}\hbar\delta_{\alpha\beta}\partial_{\hat{p}_\beta} f\left(\hat{p}_\beta\right) \\
\left[\hat{p}_\alpha, f\left(\hat{q}_\beta\right)\right] &= -\mathbf{i}\hbar\delta_{\alpha\beta}\partial_{\hat{q}_\beta} f\left(\hat{q}_\beta\right)
\end{aligned}$$

One can show:

$$\hat{q}e^{-\frac{\mathbf{i}}{\hbar}\hat{p}q_0}\left|q\right\rangle = \left(q+q_0\right)\left|q+q_0\right\rangle$$

This follows, because $e^{-\frac{\mathbf{i}}{\hbar}\hat{p}q_0}\left|q\right\rangle$ is an eigenstate of $\hat{q}$ with eigenvalue $q+q_0$ and therefore:

$$e^{-\frac{\mathbf{i}}{\hbar}\hat{p}q_0}\left|q\right\rangle = \left|q+q_0\right\rangle$$

One can also show:

$$e^{\frac{\mathbf{i}}{\hbar}\hat{q}p_0}\left|p\right\rangle = \left|p+p_0\right\rangle$$

This is similar to:

$$e^{-\frac{\mathbf{i}}{\hbar}\hat{H}t}\left|\psi\left(t_0\right)\right\rangle = \left|\psi\left(t_0+t\right)\right\rangle$$

1.5.3 The Schrödinger equation in position and momentum representation

Consider the Hamiltonian:

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V\left(\hat{q}\right)$$

I want to "represent":

$$\begin{aligned}\hat{H}\left|e_n\right\rangle &= e_n\left|e_n\right\rangle \\ \hat{H}\left|e\right\rangle &= e\left|e\right\rangle\end{aligned}$$

For position representation, we apply $\left\langle q\right|$ to the equation, use the definitions $\psi_n\left(q\right) := \left\langle q \,\middle|\, e_n\right\rangle$ and $\tilde{\psi}_n\left(p\right) := \left\langle p \,\middle|\, e_n\right\rangle$, and multiply with the unit operator $\hat{I} = \int \left|p\right\rangle\left\langle p\right| \mathrm{d}p$ to get:

$$\begin{aligned}\frac{1}{2m}\left\langle q \,\middle|\, \hat{p}^2\cdot\hat{I} \,\middle|\, e_n\right\rangle + V\left(q\right)\left\langle q \,\middle|\, e_n\right\rangle &= e_n\left\langle q \,\middle|\, e_n\right\rangle \\ \frac{1}{2m}\int p^2\left\langle q \,\middle|\, p\right\rangle\tilde{\psi}_n\left(p\right)\mathrm{d}p + V\left(q\right)\psi_n\left(q\right) &= e_n\psi_n\left(q\right)\end{aligned}$$

In general one gets:

$$\left\langle q \,\middle|\, f\left(\hat{p}\right) \,\middle|\, \psi\right\rangle = f\left(-\hbar\partial_q\right)\psi\left(q\right)$$

The recipe is:

$$\begin{aligned}\hat{p} &\mapsto -\mathbf{i}\hbar\partial_q && \text{one dimension} \\ \hat{p} &\mapsto -\mathbf{i}\hbar\vec{\nabla} && \text{three dimensions}\end{aligned}$$

In three dimensions this is:

discrete case	continuous case
$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{q}\right)\right)\psi_n\left(\vec{q}\right) = e_n\psi_n\left(\vec{q}\right)$	$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{q}\right)\right)\psi_k\left(\vec{q}\right) = e\left(k\right)\psi_k\left(\vec{q}\right)$

The state is only in the discrete case normalizable:

$$\left\langle e_n, e_n\right\rangle = \int \left|\psi_n\left(\vec{q}\right)\right|^2 \mathrm{d}\vec{q} < \infty \qquad\qquad \left\langle e\left(k\right), e\left(k\right)\right\rangle = \int \left|\psi_k\left(\vec{q}\right)\right|^2 \mathrm{d}\vec{q} = \infty$$

Time evolution:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{q})\right)\hat{U}\left(\vec{q},\vec{q}',t\right) = \mathbf{i}\hbar\partial_t \hat{U}\left(\vec{q},\vec{q}',t\right) \qquad \hat{U}\left(\vec{q},\vec{q}',t=0\right) = \delta\left(\vec{q}-\vec{q}'\right)$$

It is much simpler to solve the Schrödinger equation for one state:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{q})\right)\psi(\vec{q},t) = \mathbf{i}\hbar\partial_t\psi(\vec{q},t) \qquad \psi(\vec{q},t=0) = \psi_0(\vec{q})$$

1.5.4 The Heisenberg and the Schrödinger "pictures"

Consider:

$$\left\langle \hat{A}\right\rangle_t := \left\langle \psi(t) \middle| \hat{A} \middle| \psi(t)\right\rangle$$
$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$$

This quantity admits a two-folded interpretation:

$$\begin{aligned}\left\langle \hat{A}\right\rangle_t &= \left(\langle\psi(t_0)|\,\hat{U}(t,t_0)^\dagger\right)\hat{A}\left(\hat{U}(t,t_0)\,|\psi(t_0)\rangle\right) && \text{the state evolves in time (Schrödinger)}\\ &= \langle\psi(t_0)|\underbrace{\left(\hat{U}(t,t_0)^\dagger\,\hat{A}\hat{U}(t,t_0)\right)}_{=:\hat{A}_H(t,t_0)}|\psi(t_0)\rangle && \text{the operator evolves in time (Heisenberg)}\end{aligned}$$

$\hat{A}_H(t,t_0)$ is the HEISENBERG OPERATOR, that is the operator $\hat{A}$ in the Heisenberg representation. If $\hat{A}=\hat{A}^\dagger$, the also $\hat{A}_H$ is Hermitian.

$$\hat{A}_H(t=t_0,t_0) = \hat{A}$$

An equation of motion for $\hat{A}$ is easy to derive:

$$\begin{aligned}\partial_t\hat{A}_H(t,t_0) &= \partial_t\left(\hat{U}(t,t_0)^\dagger\,\hat{A}(t)\,\hat{U}(t,t_0)\right) = \partial_t\left(\hat{U}^\dagger\right)\hat{A}\hat{U} + \hat{U}^\dagger\partial_t\left(\hat{A}\right)\hat{U} + \hat{U}^\dagger\hat{A}\partial_t\left(\hat{U}\right) =\\ &\overset{\hat{H}\hat{U}=\mathbf{i}\hbar\partial_t\hat{U}}{=} \left(-\frac{\mathbf{i}}{\hbar}\hat{H}\hat{U}\right)^\dagger\hat{A}\hat{U} + \hat{U}^\dagger\left(\partial_t\hat{A}\right)\hat{U} + \hat{U}^\dagger\hat{A}\left(-\frac{\mathbf{i}}{\hbar}\hat{H}\hat{U}\right) =\\ &\overset{\hat{U}\hat{U}^\dagger}{=} -\frac{\mathbf{i}}{\hbar}\left[\hat{A}_H(t,t_0),\hat{H}_H(t,t_0)\right] + \left(\partial_t\hat{A}(t)\right)_H\end{aligned}$$

Consider for example $\partial_t\hat{H}=0$, $\hat{A}_1=\hat{q}$ and $\hat{A}_2=\hat{p}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{q}_H = \frac{1}{m}\hat{p}_H \qquad \frac{\mathrm{d}}{\mathrm{d}t}\hat{p}_H = -\partial_q V(q)\big|_{q=\hat{q}_H}$$

This leads to the Ehrenfest theorem:

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\hat{q}_H(t) = -\partial_{\hat{q}_H}V(\hat{q}_H)$$
$$\hat{q}_H(t=t_0) = \hat{q}$$
$$\hat{p}_H(t=t_0) = \hat{p}$$

For $\hat{q}_H$ and $\hat{p}_H$ and the usual Hamiltonian $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{q},t)$ they satisfy "Newton's" equations. Take expectation values $\langle\psi(t_0)\,|\ldots|\,\psi(t_0)\rangle$.

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{q}\rangle_t = -\langle\psi(t_0)\,|\,\partial_{\hat{q}_H}V(\hat{q}_H)\,|\,\psi(t_0)\rangle \overset{\text{in general}}{\neq} -\partial_{\langle\hat{q}\rangle_t}V(\langle\hat{q}\rangle_t)$$

But for $V(\hat{q},t) = f_1(t)\,\hat{q}^2 + f_2(t)\,\hat{q} + f_3(t)$ the partial derivative $\partial_{\hat{q}_H} V(\hat{q}_H)$ is linear in $\hat{q}_H$ and therefore $\langle \hat{q} \rangle_t$ describes the classical trajectory with the initial conditions $\langle \psi(t_0) \,|\, \hat{q} \,|\, \psi(t_0) \rangle$ and $\langle \psi(t_0) \,|\, \hat{p} \,|\, \psi(t_0) \rangle$.

Comment: The best compromise to do quantum mechanics in a way, that looks similar (at least for short times) to classical mechanics is GAUSSIAN wavepacket.

A wavepacket is a superposition:

$$|\psi\rangle = \int \tilde{\psi}(p)\, |p\rangle \, \mathrm{d}p$$

A Gaussian wavepacket is:

$$\begin{aligned}
\left|\psi_{(q_0,p_0)}\right\rangle &= \int \psi_{(q_0,p_0)}(q)\, |q\rangle \, \mathrm{d}q \\
&= \int \tilde{\psi}_{(q_0,p_0)}(p)\, |p\rangle \, \mathrm{d}p
\end{aligned}$$

$$\psi_{(q_0,p_0)}(q) = \frac{1}{\sqrt[4]{2\pi}\sigma} \exp\left(-\frac{1}{4}\frac{(q-q_0)^2}{\sigma^2}\right) \exp\left(-\frac{\mathbf{i}}{\hbar} q p_0\right) \tag{1.2}$$

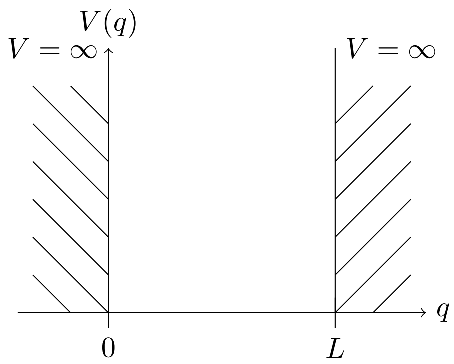
For this one gets:

$$(\Delta\hat{q})^2 (\Delta\hat{p})^2 = \frac{\hbar^2}{4}$$

$$\begin{aligned}
\left\langle \psi_{(q_0,p_0)} \,\middle|\, \hat{q} \,\middle|\, \psi_{(q_0,p_0)} \right\rangle &= q_0 \\
\left\langle \psi_{(q_0,p_0)} \,\middle|\, \hat{p} \,\middle|\, \psi_{(q_0,p_0)} \right\rangle &= p_0
\end{aligned}$$

2 Basic applications

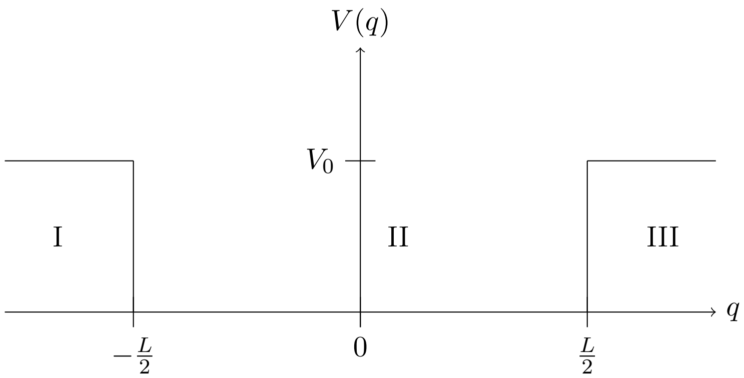
2.1 Boxes



The normalized eigenstates are:

$$\psi_n(q) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} q\right)$$
$$e_n = n^2 e_0$$

2.2 Square well



i) Energy $E < V_0$ smaller than potential wall, leads to a bound state.

Write the equation:

$$\left(-\frac{\hbar^2}{2m}\partial_q^2 + V(q)\right)\psi(q) = E\psi(q)$$
$$\partial_q^2\psi(q) = -k(E)^2\,\psi(q)$$
$$k(E) = +\sqrt{\frac{2m}{\hbar^2}(E - V(q))}$$

In the three regions I, II and III one gets:

$$k_{\mathrm{I}}(E) = \mathbf{i}\,|k_{\mathrm{I}}(E)|$$
$$k_{\mathrm{II}}(E) = |k_{\mathrm{II}}(E)|$$
$$k_{\mathrm{III}}(E) = \mathbf{i}\,|k_{\mathrm{III}}(E)|$$

ii) Write the general solution:

$$\psi_{\mathrm{I}(q)} = A_{\mathrm{I}}e^{|k_{\mathrm{I}}(E)|q} + B_{\mathrm{I}}e^{-|k_{\mathrm{I}}(E)|q}$$
$$\psi_{\mathrm{II}(q)} = A_{\mathrm{II}}e^{\mathbf{i}|k_{\mathrm{II}}(E)|q} + B_{\mathrm{II}}e^{-\mathbf{i}|k_{\mathrm{II}}(E)|q}$$
$$\psi_{\mathrm{III}(q)} = A_{\mathrm{III}}e^{|k_{\mathrm{I}}(E)|q} + B_{\mathrm{III}}e^{-|k_{\mathrm{II}}(E)|q}$$

iii) Normalization: $B_{\mathrm{I}} = A_{\mathrm{III}} = 0$

Continuity: For a finite potential ψ and $\partial_q\psi'$ are continuous.

$$\psi_{\mathrm{I}}\left(-\frac{L}{2}\right) = \psi_{\mathrm{II}}\left(-\frac{L}{2}\right) \qquad \partial_q\psi_{\mathrm{I}}\left(-\frac{L}{2}\right) = \partial_q\psi_{\mathrm{II}}\left(-\frac{L}{2}\right)$$
$$\psi_{\mathrm{II}}\left(\frac{L}{2}\right) = \psi_{\mathrm{III}}\left(\frac{L}{2}\right) \qquad \partial_q\psi_{\mathrm{II}}\left(\frac{L}{2}\right) = \partial_q\psi_{\mathrm{III}}\left(\frac{L}{2}\right)$$

Now we have four equations and four variables, but one expects infinitely many solutions.

$$\mathbb{M}\begin{pmatrix} A_{\mathrm{I}} \\ A_{\mathrm{II}} \\ B_{\mathrm{II}} \\ B_{\mathrm{III}} \end{pmatrix} = 0 \qquad \det\mathbb{M}(E) \overset{!}{=} 0$$

2.3 The harmonic oscillator (in one dimension)

The potential is:

$$V(\hat{q}) = \frac{m\omega_0^2}{2}\hat{q}^2$$

For all energies $e_n \in \mathbb{R}_{\geq 0}$ we have:

$$\hat{H}\,|e_n\rangle = e_n\,|e_n\rangle$$
$$\langle e_n\,|\,e_n\rangle = 1$$

i) The Schrödinger equation is:

$$\left(-\frac{\hbar^2}{2m}\partial_q^2 + \frac{m\omega_0^2}{2}q^2\right)\psi_n(q) = e_n\psi_n(q) \qquad \psi(q \to \pm\infty) = 0$$

ii) Use dimensionless variables:

$$q = \alpha x \qquad\qquad \phi(x) := \psi_n(\alpha x)$$

$$\left(-\frac{\hbar^2}{2m}\frac{1}{\alpha^2}\partial_q^2 + \frac{m\omega_0^2}{2}\alpha^2 q^2\right)\phi(q) = e_n\phi(x)$$
$$\left(\partial_x^2 - \frac{m^2\omega_0^2}{\hbar^2}\alpha^4 x^2\right)\phi(q) = -\frac{2m}{\hbar^2}\alpha^2 e_n\phi(x)$$

Choose:

$$\alpha := \sqrt{\frac{\hbar}{m\omega_0}} \qquad\qquad \lambda := \frac{2e_n}{\hbar\omega_0}$$

Then the problem reduces to:

$$\boxed{\left(\partial_x^2 + \left(\lambda - x^2\right)\right)\phi(x) = 0 \qquad\qquad \psi(x \to \pm\infty) = 0}$$

iii) Check the asymptotic behavior, that is, when x goes to $\pm\infty$:

$$\phi(x) \approx \exp\left(-\frac{1}{2}x^2\right)$$

Assume a solution:

$$\phi(x) = u(x)\exp\left(-\frac{1}{2}x^2\right)$$

iv) Then we get for $u(x)$ the differential equation:

$$\left(\partial_x^2 - 2x\partial_x + (\lambda - 1)\right)u(x) = 0$$

Solve this with a power series, by assuming, that $u(x)$ is analytic:

$$u(x) = \sum_{n=0}^{\infty} a_n x^n$$

This leads to the „recursion relation“:

$$a_{n+2} = \frac{(2n + 1 - \lambda)}{(n+1)(n+2)}a_n$$

Or equivalently:

$$a_{n-2} = \frac{(n-1)n}{(2n - 3 - \lambda)}a_n$$

v) Check again the asymptotic behavior, to get an idea, how $u(x)$ looks like, when $n \to \infty$:

$$\frac{a_{n+2}}{a_n} \xrightarrow{n \gg 1} \frac{2}{n}$$

But we have

$$\exp\left(-\frac{x^2}{2}\right) = \sum_{n=0}^{\infty} \underbrace{\frac{1}{n!}\left(-\frac{1}{2}\right)^n}_{=:c_n} x^{2n} = \sum_{n=0}^{\infty} c_n x^{2n}$$

with:

$$\frac{c_{n+1}}{c_n} = \frac{n!}{(n+1)!} \cdot \left(-\frac{1}{2}\right)^{n+1} \cdot (-2)^n = \frac{-1}{2\,(n+1)} \xrightarrow{n\gg 1} -\frac{1}{2n}$$

Therefore $u\,(x \to \infty)$ grows FASTER THAN $\exp\left(\frac{1}{2}x^2\right)$ and therefore:

$$\exp\left(-\frac{1}{2}x^2\right) u\,(x) \to \infty$$

If the series does not stop, $\phi\,(x)$ is *not* normalizable.

So there has to exist a „n^*“ such that:

$$\begin{aligned} 2n^* + 1 - \lambda &= 0 \\ \lambda &= 2n^* + 1 \\ e_n &= \hbar\omega_0 \left(n^* + \frac{1}{2}\right) \end{aligned}$$

This gives:

$$\psi_n\,(q) = N_n \exp\left(-\frac{1}{2}\left(\frac{q}{\alpha}\right)^2\right) H_n\left(\frac{q}{\alpha}\right)$$

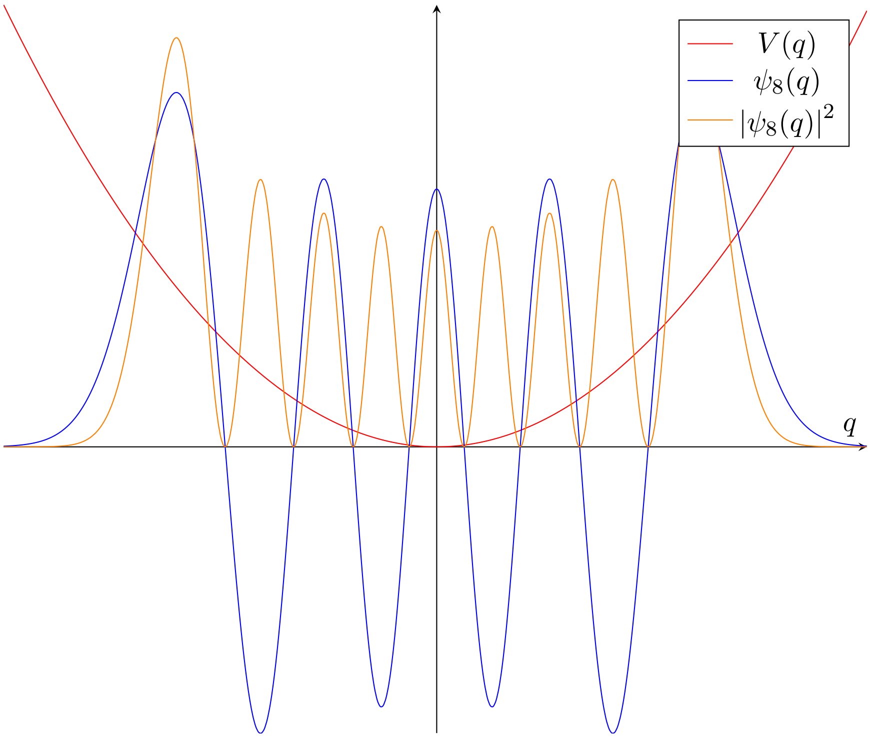
The polynomials $H_n\,(x)$ are called the HERMITE POLYNOMIALS and are explicitly:

$$H_n\,(x) = (-1)^n \sum_{k_1+2k_2=n} \frac{n!}{k_1! \cdot k_2!} (-1)^{k_1+k_2} (2x)^{k_1}$$

N_n is fixed by:

$$\int_{-\infty}^{\infty} |\psi_n\,(q)|^2 \,\mathrm{d}q = 1$$

This looks like:



Then came Dirac:

2.3.1 The number representation

Introduce two operators:

„destruction“

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{q} + \frac{\mathbf{i}}{m\omega_0} \hat{p} \right)$$

„creation“

$$\hat{a}^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{q} - \frac{\mathbf{i}}{m\omega_0} \hat{p} \right)$$

It is easy to calculate:

$$\left[\hat{a}, \hat{a}^\dagger \right] = 1$$

Introduce the „number“ operator:

$$\hat{n} := \hat{a}^\dagger \hat{a}$$

Then we can find easily:

$$\hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{m\omega_0^2}{2} \hat{q}^2 = \hbar\omega_0 \left(\hat{n} + \frac{1}{2} \right)$$

Therefore the eigenstates of $\hat{n}$ are automatically the eigenstates of $\hat{H}$.
It also satisfies:

$$[\hat{n}, \hat{a}] = \text{-}\hat{a} \qquad \left[\hat{n}, \hat{a}^\dagger \right] = \hat{a}^\dagger$$

We want to find $|\sigma\rangle$ such that:

$$\hat{n} |\sigma\rangle = \sigma |\sigma\rangle$$

We note:

$$\hat{n}\left(\hat{a}\left|\sigma\right\rangle\right) = \left(\hat{n}\hat{a}\right)\left|\sigma\right\rangle = \left(\hat{a}\hat{n} - [\hat{a},\hat{n}]\right)\left|\sigma\right\rangle = \left(\hat{a}\hat{n} - \hat{a}\right)\left|\sigma\right\rangle = \left(\sigma - 1\right)\left|\sigma\right\rangle$$

$\hat{a}\left|\sigma\right\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $\sigma - 1$, so we get:

$$\hat{a}\left|\sigma\right\rangle = N_\sigma\left|\sigma - 1\right\rangle$$

From $\left\langle\sigma\,|\,\sigma\right\rangle = \left\langle\sigma - 1\,|\,\sigma - 1\right\rangle = 1$ follows:

$$\boxed{\hat{a}\left|\sigma\right\rangle = \sqrt{\sigma}\left|\sigma - 1\right\rangle}$$

Analogously we have:

$$\boxed{\hat{a}^\dagger\left|\sigma\right\rangle = \sqrt{\sigma + 1}\left|\sigma + 1\right\rangle}$$

Take a $\sigma > 0$ and apply $\hat{a}$ to $\left|\sigma\right\rangle$ many times to get, that σ must be an integer, because otherwise the normalization constant $\sqrt{\sigma}$ would be imaginary.
There is a special state $\left|0\right\rangle$, the „vacuum“.
Let us call the states $\left|n\right\rangle$ for $n \in \mathbb{N}_0$.

$$\hat{n}\left|n\right\rangle = n\left|n\right\rangle \qquad \hat{a}\left|n\right\rangle = \sqrt{n}\left|n - 1\right\rangle \qquad \hat{a}^\dagger\left|n\right\rangle = \sqrt{n + 1}\left|n + 1\right\rangle$$

$$\hat{H}\left|n\right\rangle = e_n\left|n\right\rangle \qquad e_n = \hbar\omega_0\left(n + \frac{1}{2}\right)$$

If we know $\left|0\right\rangle$, we can construct an arbitrary $\left|n\right\rangle$:

$$\left|n\right\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n\left|0\right\rangle$$

To calculate $\left\langle q\,|\,0\right\rangle$ we use $\hat{a}\left|0\right\rangle = 0$ and represent.

$$\begin{aligned}
\left\langle q\,|\,\hat{a}\,|\,0\right\rangle &= 0\\
\left\langle q\,\middle|\,\hat{q} + \frac{\mathbf{i}}{m\omega_0}\hat{p}\,\middle|\,0\right\rangle &= 0\\
\left(q + \frac{\mathbf{i}}{m\omega_0}\left(\text{-}\mathbf{i}\hbar\partial_q\right)\right)\psi_0\left(q\right) &= 0\\
\left(\frac{\hbar}{m\omega_0}\partial_q + q\right)\psi_0\left(q\right) &= 0\\
\psi_0\left(q\right) &= N_0\exp\left(\text{-}\frac{1}{2}\left(\frac{q}{\alpha}\right)^2\right)
\end{aligned}$$

N_0 is fixed by normalization:

$$\int_{-\infty}^{\infty}\left|\psi_0\left(q\right)\right|^2\mathrm{d}q = 1$$

For example $\psi_1\left(q\right)$ is given by:

$$\begin{aligned}
\psi_1\left(q\right) = \left\langle q\,|\,1\right\rangle = \left\langle q\,\middle|\,\hat{a}^\dagger\,\middle|\,0\right\rangle &= \sqrt{\frac{m\omega_0}{2\hbar}}\left(q - \frac{\mathbf{i}}{m\omega_0}\left(-\mathbf{i}\hbar\partial_q\right)\right)\psi_0\left(q\right) =\\
&= N_0\sqrt{\frac{m\omega_0}{2\hbar}}\left(q - \frac{\hbar}{m\omega_0}\partial_q\right)\exp\left(\text{-}\frac{1}{2}\left(\frac{q}{\alpha}\right)^2\right) =\\
&= N_1\exp\left(\text{-}\frac{1}{2}\left(\frac{q}{\alpha}\right)^2\right)\cdot H_1\left(\frac{q}{\alpha}\right)
\end{aligned}$$

2.3.2 The dynamics of the harmonic oscillator

The Hamiltonian is:

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{q}^2$$

In principal we need:

$$\hat{U}(t) := \exp\left(-\frac{\mathbf{i}}{\hbar}\hat{H}t\right) = \exp\left(-\frac{\mathbf{i}}{\hbar}\left(\frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{q}^2\right)t\right)$$

Let's calculate in the position representation:

$$\left\langle q \,\middle|\, \hat{U}(t) \,\middle|\, q' \right\rangle =: U(q,q',t)$$

Remember, what $\hat{U}$ does:

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle$$

In position representation this is:

$$\psi(q,t) = \int U(q,q',t)\,\psi(q',0)\,\mathrm{d}q'$$

In some books the notation for $U(q,q',t)$ is $K(q,q',t)$.

$$\begin{aligned}
U(q,q',t) &= \sum_n \exp\left(-\frac{\mathbf{i}}{\hbar}e_n t\right)\langle q\,|\,n\rangle\langle n\,|\,q'\rangle = \\
&= \sum_n \exp\left(-\mathbf{i}\omega_0\left(n+\frac{1}{2}\right)t\right) N_n \exp\left(-\frac{1}{2}\left(\frac{q}{\alpha}\right)^2\right) H_n\left(\frac{q}{\alpha}\right)\cdot \\
&\qquad \cdot\left(N_n \exp\left(-\frac{1}{2}\left(\frac{q'}{\alpha}\right)^2\right) H_n\left(\frac{q'}{\alpha}\right)\right)^* = \\
&= \sum_n \exp\left(-\mathbf{i}\omega_0\left(n+\frac{1}{2}\right)t\right) N_n^2 \exp\left(-\frac{q^2+q'^2}{2\alpha^2}\right) H_n\left(\frac{q}{\alpha}\right) H_n\left(\frac{q'}{\alpha}\right) = \\
&= \sqrt{\frac{m\omega_0}{2\pi\mathbf{i}\hbar\sin(\omega_0 t)}}\cdot\exp\left(\frac{\mathbf{i}}{\hbar}\left(\frac{m\omega_0}{2\sin(\omega_0 t)}\right)\left(q^2+q'^2\right)\cos(\omega_0 t) - 2qq'\right)
\end{aligned}$$

To check this, consider the limes $\omega_0 \to 0$, for which we get the free particle:

$$U(q,q',t) \xrightarrow{\omega_0\to 0} \sqrt{\frac{m}{2\pi\mathbf{i}\hbar t}}\cdot\exp\left(\frac{\mathbf{i}}{\hbar}\frac{m}{2t}\left(q-q'\right)^2\right)$$

Let's try the Heisenberg picture:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\hat{q}_H(t) &= \frac{\mathbf{i}}{\hbar}\left[H(\hat{q}_H,\hat{p}_H),\hat{q}_H\right] = \frac{1}{m}\hat{p}_H \\
\frac{\mathrm{d}}{\mathrm{d}t}\hat{p}_H(t) &= \frac{\mathbf{i}}{\hbar}\left[H(\hat{q}_H,\hat{p}_H),\hat{p}_H\right] = -m\omega_0\hat{q}_H
\end{aligned}$$

The initial conditions are:

$$\hat{q}_H\left(t=0\right)=\hat{q}$$
$$\hat{p}_H\left(t=0\right)=\hat{p}$$

Remember the definition of an operator in the Heisenberg picture:

$$\hat{q}_H=\exp\left(\frac{\mathbf{i}}{\hbar}\hat{H}t\right)\hat{q}\exp\left(-\frac{\mathbf{i}}{\hbar}\hat{H}t\right)$$

Now we define the NESTED COMMUTATOR as

$$\left[\hat{B},\hat{A}\right]^{(0)}:=\hat{A}$$
$$\left[\hat{B},\hat{A}\right]^{(n+1)}:=\left[\hat{B},\left[\hat{B},\hat{A}\right]^{(n)}\right]$$

and use the operator identity for $\lambda\in\mathbb{C}$ and arbitrary operators $\hat{A}$,$\hat{B}$:

$$\exp\left(\mathbf{i}\lambda\hat{B}\right)\hat{A}\exp\left(-\mathbf{i}\lambda\hat{B}\right)=\sum_{n=0}^{\infty}\frac{(\mathbf{i}\lambda)^n}{n!}\left[\hat{B},\hat{A}\right]^{(n)}$$
$$\approx\hat{A}+\mathbf{i}\lambda\left[\hat{B},\hat{A}\right]+\frac{(\mathbf{i}\lambda)^2}{2!}\left[\hat{B},\left[\hat{B},\hat{A}\right]\right]$$

If $\left[\hat{A},\hat{B}\right]=0$, we get just $\hat{A}$.
If $\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]=\left[\hat{B},\left[\hat{A},\hat{B}\right]\right]=0$, we get $\hat{A}+\mathbf{i}\lambda\left[\hat{B},\hat{A}\right]$.
Now we come back to the problem at hand:

$$\lambda=\frac{t}{\hbar}\qquad\qquad\hat{B}=\hat{H}\qquad\qquad\hat{A}=\hat{q}$$

We know:

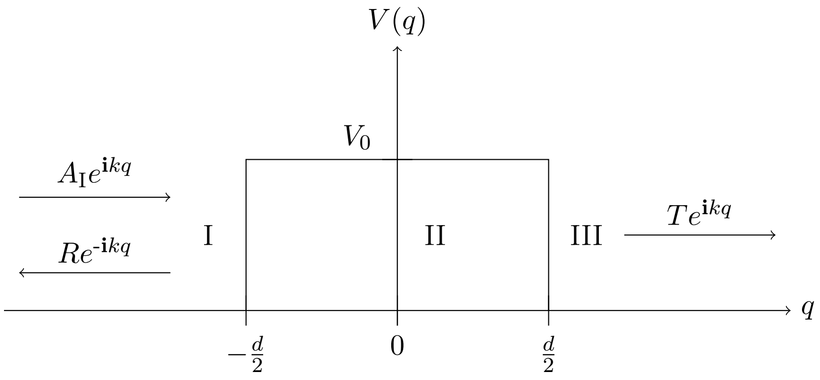
$$\left[\hat{H},\hat{q}\right]=\frac{1}{2m}\left[\hat{p}^2,\hat{q}\right]+\underbrace{\left[V\left(\hat{q}\right),\hat{q}\right]}_{=0}=\frac{1}{2m}\left(\hat{p}\left[\hat{p},\hat{q}\right]+\left[\hat{p},\hat{q}\right]\hat{p}\right)=-\frac{\mathbf{i}\hbar}{m}\hat{p}$$
$$\left[\hat{H},\hat{p}\right]=\underbrace{\frac{1}{2m}\left[\hat{p}^2,\hat{p}\right]}_{=0}+\frac{m\omega_0^2}{2}\left[\hat{q}^2,\hat{p}\right]=\mathbf{i}\hbar m\omega_0^2\hat{q}$$

Together this inductively gives:

$$\hat{q}_H\left(t\right)=\hat{q}\cos\left(\omega_0t\right)+\frac{1}{m\omega_0}\hat{p}\sin\left(\omega_0t\right)$$
$$\hat{p}_H\left(t\right)=m\omega_0\hat{q}\sin\left(\omega_0t\right)+\hat{p}\cos\left(\omega_0t\right)$$

2.4 The tunneling effect

Look at the potential:



The problem is unbounded and therefore the spectrum is continuous and every energy $E \in \mathbb{R}_{>0}$ is allowed.

Imagine that we inject the particle from the left with a certain energy E.

$$k := \frac{\sqrt{2mE}}{\hbar} \qquad k_V := \frac{\sqrt{2m\left(V_0 - E\right)}}{\hbar}$$

The goal is to find R and T as functions of the Energy E, the height V_0 and width d of the potential.

Business as usual:

The boundary condition is, that A_{I} is know and the coefficient of $e^{-\mathbf{i}kq}$ in the region III is zero. We consider only $E < V_0$.

$$\begin{aligned}
\psi_{\mathrm{I}}(q) &= A_{\mathrm{I}}e^{\mathbf{i}kq} + Re^{-\mathbf{i}kq} \\
\psi_{\mathrm{II}}(q) &= A_{\mathrm{II}}e^{k_V q} + B_{\mathrm{II}}e^{-k_V q} \\
\psi_{\mathrm{III}}(q) &= Te^{\mathbf{i}kq}
\end{aligned}$$

We have the four variables R,T,A_{II} and B_{II}. Know we impose the matching conditions:

$$\psi_{\mathrm{I}}\left(-\frac{d}{2}\right) = \psi_{\mathrm{II}}\left(-\frac{d}{2}\right) \qquad \psi'_{\mathrm{I}}\left(-\frac{d}{2}\right) = \psi'_{\mathrm{II}}\left(-\frac{d}{2}\right)$$
$$\psi_{\mathrm{I}}\left(\frac{d}{2}\right) = \psi_{\mathrm{II}}\left(\frac{d}{2}\right) \qquad \psi'_{\mathrm{I}}\left(\frac{d}{2}\right) = \psi'_{\mathrm{II}}\left(\frac{d}{2}\right)$$

This system looks like:

$$\mathbb{M} \cdot \begin{pmatrix} B \\ A_{\mathrm{II}} \\ B_{\mathrm{II}} \\ T \end{pmatrix} = A_{\mathrm{I}} \begin{pmatrix} -e^{-\mathbf{i}k\frac{d}{2}} \\ -\mathbf{i}ke^{\mathbf{i}k\frac{d}{2}} \\ 0 \\ 0 \end{pmatrix}$$

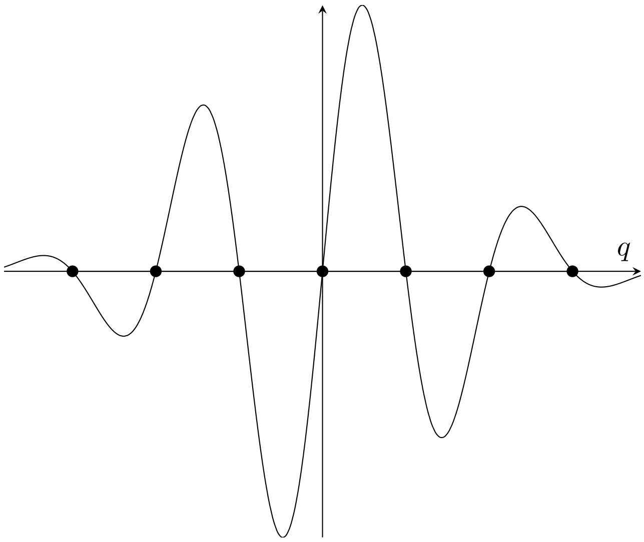
For $k_V d \gg 1$ this roughly gives:

$$\begin{aligned}
T(E) &\sim A_{\mathrm{I}}e^{-\frac{k_V(E)d}{2}} \\
\frac{T(E,d)}{T(E,d')} &\sim e^{-\frac{k_V(E)}{2}(d-d')}
\end{aligned}$$

2.5 Two formal consequences of the position representation of the Schrödinger equation

2.5.1 Oscillation theorem (1D, bounded)

If $\langle q \,|\, e_n \rangle$ has k-nodes, that means $\psi_n(q) = 0$ is k times, then $\langle q \,|\, e_{n+1} \rangle$ has $k+1$ nodes.



2.5.2 The continuity equation

Let $\psi(\vec{q},t)$ solve the Schrödinger equation for the Hamilton operator $\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V\left(\hat{\vec{q}}\right)$. Since $\hat{H}$ is Hermitian, $V(\vec{q})$ has to be real and solve:

$$\begin{aligned}
\mathbf{i}\hbar\partial_t\psi(\vec{q},t) &= \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{q})\right)\psi(\vec{q},t) \\
-\mathbf{i}\hbar\partial_t\psi^*(\vec{q},t) &= \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{q})\right)\psi^*(\vec{q},t)
\end{aligned}$$

This gives:

$$\begin{aligned}
\partial_t |\psi|^2 &= \partial_t(\psi\psi^*) = (\partial_t\psi)\psi^* + \psi(\partial_t\psi^*) = \\
&= \psi^*\left(\frac{1}{\mathbf{i}\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{q})\right)\psi\right) + \psi\left(\frac{-1}{\mathbf{i}\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{q})\right)\psi^*\right) = \\
&= \psi^*\left(-\frac{\hbar}{2m\mathbf{i}}\nabla^2\psi\right) + \psi\left(\frac{\hbar}{2m\mathbf{i}}\nabla^2\psi^*\right) = \\
&= \frac{\hbar}{2m\mathbf{i}}\left(\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right) = \\
&= \frac{\hbar}{2m\mathbf{i}}\nabla\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)
\end{aligned}$$

Therefore we have the continuity equation:

$$\partial_t |\psi|^2 - \frac{\hbar}{2m\mathbf{i}}\nabla\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) = 0$$

Define the probability density $\varrho_\psi(\vec{q},t) := |\psi(\vec{q},t)|^2$ and the probability current:

$$\vec{j}_\psi(\vec{q},t) := -\frac{\mathbf{i}\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

They are related by

$$\partial_t\varrho_\psi(\vec{q},t) + \nabla\vec{j}_\psi(\vec{q},t) = 0$$

and we can interpret them as expectation values:

$$\varrho_\psi(\vec{q},t) = |\psi(\vec{q},t)|^2 = \left|\left\langle\hat{\vec{q}}\middle|\psi(t)\right\rangle\right|^2 = \left\langle\hat{\vec{q}}\middle|\underbrace{|\psi(t)\rangle\langle\psi(t)|}_{=:\hat{\varrho}}\middle|\hat{\vec{q}}\right\rangle = \left\langle\hat{\vec{q}}\middle|\,\hat{\varrho}\,\middle|\hat{\vec{q}}\right\rangle$$

$$\begin{aligned}\vec{j}(\vec{q},t) &= \frac{-\mathbf{i}\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) = \frac{-\mathbf{i}\hbar}{2m}\left(\langle\psi|\vec{q}\rangle\,\nabla\,\langle\vec{q}|\psi\rangle - \langle\vec{q}|\psi\rangle\,\nabla\,\langle\psi|\vec{q}\rangle\right) = \\ &= \frac{-1}{2m}\left(\left\langle\vec{q}\middle|\hat{\vec{p}}\middle|\psi\right\rangle\langle\psi|\vec{q}\rangle - \langle\vec{q}|\psi\rangle\left\langle\psi\middle|\hat{\vec{p}}\middle|\vec{q}\right\rangle\right) = \\ &= \frac{-1}{2m}\langle\vec{q}|\underbrace{\left(\hat{\vec{p}}\,|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\,\hat{\vec{p}}\right)}_{=[\hat{\vec{p}},\hat{\varrho}]}|\vec{q}\rangle = \frac{-1}{2m}\langle\vec{q}|\underbrace{\left[\hat{\vec{p}},\hat{\varrho}\right]}_{=:-2m\hat{\vec{j}}}|\vec{q}\rangle = \left\langle\vec{q}\middle|\,\hat{\vec{j}}\,\middle|\vec{q}\right\rangle\end{aligned}$$

3 Symmetries, Rotations and Angular momentum

Remember from classical mechanics:
A symmetry is a physical operation that leaves the system invariant.
In classical mechanics this means we change $\vec{q}$ and $\vec{p}$.
Examples:

- For $\mathcal{R} \in \mathrm{SL}_n(\mathbb{R})$, that means $\mathcal{R}^{-1} = \mathcal{R}^T$ and $\det(\mathcal{R}) = 1$, we define:
$$\begin{aligned} \vec{q}' &= \mathcal{R}\vec{q} \\ \vec{p}' &= \mathcal{R}\vec{p} \end{aligned}$$
This leaves a Lagrangian of the Form $\mathscr{L}\left(\vec{q},\dot{\vec{q}}\right) = \frac{m}{2}\left|\dot{\vec{q}}\right|^2 - V(|\vec{q}|)$. $\Rightarrow \left\{H,\vec{L}\right\} = 0$
- The translation $\vec{q}' = \vec{q} + \vec{q}_0$ leaves the free particle with Lagrangian
$$\mathscr{L}\left(\vec{q},\dot{\vec{q}},t\right) = \frac{m}{2}\left|\dot{\vec{q}}\right|^2$$
invariant and therefore $\{H,\vec{p}\} = 0$.
- Emmy Noether: Symmetry $\Rightarrow$ Existence of a constant of motion

3.1 The tensor product in quantum mechanics

Consider two degrees of freedom (for example two particles in one dimension), described by states in $\mathcal{H}^{(1)},\mathcal{H}^{(2)}$.
A postulate of quantum mechanics says, that the composite system is described by a state in the Hilbert space $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$. This space is called TENSOR PRODUCT.
So the dimension is $\dim \mathcal{H} = \dim\left(\mathcal{H}^{(1)}\right) \cdot \dim\left(\mathcal{H}^{(2)}\right)$.
If $\left|\psi^{(1)}\right\rangle \in \mathcal{H}^{(1)}$, $\left|\psi^{(2)}\right\rangle \in \mathcal{H}^{(2)}$ then $\left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle \in \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} = \mathcal{H}$.
If $\hat{A}^{(1)}$ acts on $\mathcal{H}^{(1)}$ and $\hat{A}^{(2)}$ acts on $\mathcal{H}^{(2)}$, then $\hat{A}^{(1)} \otimes \hat{A}^{(2)}$ acts on $\mathcal{H}$ as follows:
$$\left(\hat{A}^{(1)} \otimes \hat{A}^{(2)}\right)\left(\left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle\right) = \left(\hat{A}^{(1)}\left|\psi^{(1)}\right\rangle \otimes \hat{A}^{(2)}\left|\psi^{(2)}\right\rangle\right)$$

$$\begin{aligned} \hat{A}^{(1)} &\mapsto \hat{A}^{(1)} \otimes \hat{I}^{(2)} \\ \hat{A}^{(2)} &\mapsto \hat{I}^{(1)} \otimes \hat{A}^{(2)} \\ \left[\hat{A}^{(1)},\hat{A}^{(2)}\right] &= 0 \end{aligned}$$

For $|\psi\rangle = \left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle$ and $|\varphi\rangle = \left|\varphi^{(1)}\right\rangle \otimes \left|\varphi^{(2)}\right\rangle$ we have the scalar product:

$$\langle \varphi \,|\, \psi \rangle = \left\langle \varphi^{(1)} \,\middle|\, \psi^{(1)} \right\rangle \left\langle \varphi^{(2)} \,\middle|\, \psi^{(2)} \right\rangle$$

With all this together one can write any operator $\hat{A}$ and any Ket $|\psi\rangle$:

$$\hat{A} = \sum_{n.m} c_{n,m} \hat{A}_n^{(1)} \otimes \hat{A}_m^{(2)}$$
$$|\psi\rangle = \sum_{n,m} a_{n,m} \left|\psi_n^{(1)}\right\rangle \otimes \left|\psi_m^{(2)}\right\rangle \overset{\text{i.A.}}{\neq} \left|\varphi^{(1)}\right\rangle \otimes \left|\varphi^{(2)}\right\rangle$$

A state in the form $\left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle$ is called *separable.*
If a state is not separable, it is called *entangled.*
For example:

$$\left(\hat{A}^{(1)} \otimes \hat{I}^{(2)} + \hat{I} \otimes \hat{A}^{(2)}\right)^2 = \left(\hat{A}^{(1)}\right)^2 \otimes \hat{I}^{(2)} + 2\hat{A}^{(1)} \otimes \hat{A}^{(2)} + \hat{I} \otimes \left(\hat{A}^{(2)}\right)^2$$

Now we can understand better:

$$\hat{q}_\alpha \,|\vec{q}\rangle = q_\alpha \,|\vec{q}\rangle$$

$|\vec{q}\rangle$ is just a compact way to write:

$$|\vec{q}\rangle = |q_x,q_y,q_z\rangle := |q_x\rangle \otimes |q_y\rangle \otimes |q_z\rangle$$

3.2 Rotations and angular momentum

Come back to classical mechanics. We know, that $\vec{L} = \vec{q} \times \vec{p}$ „generates“ rotations $\mathcal{R}\left(\vec{n},\mathrm{d}\vartheta\right)$ around an normalized axis $\vec{n}$ with the angle $\mathrm{d}\vartheta$.

$$f\left(\vec{q},\vec{p}\right) \to f\left(\vec{q}',\vec{p}'\right) = f\left(\mathcal{R}\left(\vec{n},\mathrm{d}\vartheta\right)\vec{q},\mathcal{R}\left(\vec{n},\mathrm{d}\vartheta\right)\vec{p}\right) \approx f\left(\vec{q},\vec{p}\right) + \mathrm{d}\vartheta \left\{ \underbrace{\vec{L}\cdot\vec{n}}_{\text{Generator}} ,f\left(\vec{q},\vec{p}\right) \right\} + O\left(\left(\mathrm{d}\vartheta\right)^2\right)$$

Another example:

$$f\left(\vec{q}\left(t\right),\vec{p}\left(t\right)\right) \to f\left(\vec{q}\left(t+\delta t\right),\vec{p}\left(t+\delta t\right)\right) \approx f\left(\vec{q},\vec{p}\right) + \mathrm{d}t \left\{H,f\left(\vec{q},\vec{p}\right)\right\}$$

Explicit calculation shows:

$$\left\{L_i,L_j\right\} = \varepsilon_{ijk} L_k$$

In quantum mechanics we DEFINE angular momentum $\vec{j}$ as the generator of rotations. Define:

$$\left|\psi^{\mathcal{R}}\right\rangle = \hat{D}\left(\mathcal{R}\right)|\psi\rangle = e^{-\frac{\mathrm{i}}{\hbar}\left(\vec{j}\cdot\vec{n}\right)\theta}\,|\psi\rangle$$

Check out, how an operator $\hat{A}$ changes:

$$\hat{A}^{\mathcal{R}} = \hat{D}\left(\mathcal{R}\right)^\dagger \hat{A}\hat{D}\left(\mathcal{R}\right) \xrightarrow{\theta\to\mathrm{d}\theta} \hat{A} + \frac{\mathbf{i}\mathrm{d}\theta}{\hbar}\left[\vec{j}\cdot\vec{n},\hat{A}\right] + O\left(\mathrm{d}\theta^2\right)$$

We want, that the group properties of the $\mathcal{R}$'s, which are

$$\begin{aligned}
\mathcal{R}(\vec{n},0) &= E_3 \\
\mathcal{R}(\vec{n}_1,\theta_1)\,\mathcal{R}(\vec{n}_2,\theta_2) &= \mathcal{R}(\vec{n}(\vec{n}_1,\vec{n}_2),\theta(\theta_1,\theta_2)) \quad \text{(cf. Goldstein Classical Mechanics)} \\
\mathcal{R}(\vec{n},\theta)^{-1} &= \mathcal{R}(\vec{n},-\theta) \\
(\mathcal{R}_1\mathcal{R}_2)\,\mathcal{R}_3 &= \mathcal{R}_1(\mathcal{R}_2\mathcal{R}_3)
\end{aligned}$$

go into the $\hat{D}$'s.

$$\begin{aligned}
\hat{D}(\vec{n},0) &= \hat{I} \\
\hat{D}_1(\vec{n}_1,\theta_1)\,\hat{D}_2(\vec{n}_2,\theta_2) &= \hat{D}(\vec{n}(\vec{n}_1,\vec{n}_2),\theta(\theta_1,\theta_2)) \\
\hat{D}(\vec{n},\theta)^{-1} &= \hat{D}(\vec{n},-\theta) \\
\left(\hat{D}_1\hat{D}_2\right)\hat{D}_3 &= \hat{D}_1\left(\hat{D}_2\hat{D}_3\right)
\end{aligned}$$

In particular we want the $\hat{D}$'s version of:

$$\begin{aligned}
\mathcal{R}(\vec{e}_x,\varepsilon)\,\mathcal{R}(\vec{e}_y,\varepsilon) - \mathcal{R}(\vec{e}_y,\varepsilon)\,\mathcal{R}(\vec{e}_x,\varepsilon) &\approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\varepsilon^2}{2} & -\varepsilon \\ 0 & \varepsilon & 1-\frac{\varepsilon^2}{2} \end{pmatrix} \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\frac{\varepsilon^2}{2} \end{pmatrix} - \\
&- \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\frac{\varepsilon^2}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\varepsilon^2}{2} & -\varepsilon \\ 0 & \varepsilon & 1-\frac{\varepsilon^2}{2} \end{pmatrix} = \\
&= \mathcal{R}\left(\vec{e}_z,\varepsilon^2\right) - E_3 = \begin{pmatrix} 0 & -\varepsilon^2 & 0 \\ \varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

So we want:

$$\left[\hat{D}(\vec{e}_x,\varepsilon),\hat{D}(\vec{e}_y,\varepsilon)\right] = \hat{D}\left(\vec{e}_z,\varepsilon^2\right) - \hat{I} + O\left(\varepsilon^3\right)$$

Use

$$\hat{D}(\vec{e}_i,\varepsilon) = \exp\left(-\frac{\mathbf{i}}{\hbar}\hat{J}_i\varepsilon\right) \approx 1 - \frac{\mathbf{i}}{\hbar}\hat{J}_i\varepsilon + \left(-\frac{\mathbf{i}}{\hbar}\right)^2 \frac{1}{2}\hat{J}_i^2\varepsilon^2 + \dots$$

to get:

$$\left[\hat{J}_i,J_j\right] = \mathbf{i}\hbar\varepsilon_{ijk}\hat{J}_k$$

Funny remark: Take the spin $\hat{\vec{s}}$ and calculate:

$$\exp\left(-\frac{\mathbf{i}}{\hbar}\hat{s}_z\theta\right)|+\rangle = \exp\left(-\mathbf{i}\frac{\theta}{2}\right)|+\rangle$$

For electrons you need a rotation of 4π to come back to the same state.

3.3 Eigenstates and eigenvalues of $\hat{\vec{j}}$

First (again) notice, that since $\left[\hat{J}_i,\hat{J}_k\right] \neq 0$ for $i \neq k$ there is not any common eigenstate for the $\vec{J}$'s, but we know:

$$\left[\left|\hat{\vec{J}}\right|^2,\hat{J}_i\right] := \left[\hat{\vec{J}}^2,\hat{J}_i\right] = 0$$

Therefore we can find a basis $|a,b\rangle$ with:

$$\hat{J}^2 |a,b\rangle = a |a,b\rangle$$
$$\hat{J}_z |a,b\rangle = b |a,b\rangle$$

Now we introduce:

$$\hat{J}_\pm := \hat{J}_x \pm \mathbf{i}\hat{J}_y$$
$$\hat{J}_\pm^\dagger = \hat{J}_\mp$$

Note that this gives:

$$\left[\hat{J}^2,\hat{J}_\pm\right] = 0 \qquad \left[\hat{J}_+,\hat{J}_-\right] = 2\hbar\hat{J}_z \qquad \left[\hat{J}_z,\hat{J}_\pm\right] = \pm\hbar\hat{J}_\pm$$

The trick is always the same:

$$\begin{aligned}\hat{J}_z\left(\hat{J}_\pm |a,b\rangle\right) &= \hat{J}_z\hat{J}_\pm |a,b\rangle = \left(\hat{J}_\pm\hat{J}_z + \left[\hat{J}_z,\hat{J}_\pm\right]\right)|a,b\rangle = \\ &= \hat{J}_\pm b |a,b\rangle \pm \hbar\hat{J}_\pm |a,b\rangle = (b \pm \hbar)\,\hat{J}_\pm |a,b\rangle\end{aligned}$$

Therefore $\hat{J}_\pm |a,b\rangle$ is an eigenstate of $\hat{J}_z$ with the eigenvalue $b \pm \hbar$:

$$\hat{J}_\pm |a,b\rangle = N^\pm (a,b)\, |a,b \pm \hbar\rangle$$

Now we show, that $|b|$ has an upper limit. Consider

$$\left\langle a,b|\hat{J}_+\hat{J}_+^\dagger|a,b\right\rangle + \left\langle a,b|\hat{J}_+^\dagger\hat{J}_+|a,b\right\rangle \in \mathbb{R}_{\geq 0}$$

and:

$$\hat{J}_+\hat{J}_+^\dagger + \hat{J}_+^\dagger\hat{J}_+ = \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ = 2\left(\hat{J}^2 - \hat{J}_z^2\right)$$

Then we get:

$$\begin{aligned}0 &\leq \left\langle a,b|\hat{J}^2 - \hat{J}_z^2|a,b\right\rangle = \langle a,b|a - b^2|a,b\rangle = a - b^2 \\ a &\geq b^2 \\ |b| &\leq \sqrt{a}\end{aligned}$$

This means, that there is a b_{max} defined by:

$$\hat{J}_+ |a,b_{\text{max}}\rangle = 0$$

From this equation we get

$$\hat{J}_- \hat{J}_+ \left|a,b_{\text{max}}\right\rangle = 0$$

and:

$$\hat{J}^2 - \hat{J}_z^2 - \hbar \hat{J}_z = a - b_{\text{max}}^2 - \hbar b_{\text{max}} = 0$$

This finally leads to:

$$a = b_{\text{max}} \left(b_{\text{max}} + \hbar\right)$$

Analogously we get for $\hat{J}_-$:

$$\hat{J}_- \left|a,b_{\text{min}}\right\rangle = 0$$

From this equation we get

$$\hat{J}_+ \hat{J}_- \left|a,b_{\text{min}}\right\rangle = 0$$

and:

$$\hat{J}^2 - \hat{J}_z^2 + \hbar \hat{J}_z = a - b_{\text{min}}^2 + \hbar b_{\text{min}} = 0$$

This finally leads to:

$$a = b_{\text{min}} \left(b_{\text{min}} - \hbar\right)$$

A solution is $b_{\text{max}} = -b_{\text{min}}$ and for a $n \in \mathbb{Z}$:

$$\begin{aligned} b_{\text{max}} &= b_{\text{min}} + n\hbar \\ b_{\text{max}} - b_{\text{mini}} = 2b_{\text{max}} &= n\hbar \\ b_{\text{max}} &= \frac{n}{2}\hbar \\ a &= \frac{n}{2}\hbar\left(\frac{n}{2}\hbar + \hbar\right) = \hbar^2 \underbrace{\frac{n}{2}}_{=:j} \left(\frac{n}{2} + 1\right) \end{aligned}$$

Some names:
$j \in \frac{1}{2}\mathbb{Z}$ is called *the total angular momentum quantum number* and

$$m \in \{-j, \ldots, -j+1, \ldots, j-1, j\}$$

is called *the magnetic quantum number*:

$$b = m\hbar \qquad\qquad a = \hbar^2 j\left(j+1\right)$$

$$\begin{aligned} \hat{J}^2 \left|j,m\right\rangle &= \hbar^2 j\left(j+1\right)\left|j,m\right\rangle \\ \hat{J}_z \left|j,m\right\rangle &= \hbar m \left|j,m\right\rangle \end{aligned}$$

With a bit of algebra we get:

$$\hat{J}_\pm \left|j,m\right\rangle = \hbar\sqrt{\left(j \mp m\right)\left(j \pm m + 1\right)}\left|j,m \pm 1\right\rangle$$

3.4 Irreducible representations of the rotation operators

We want to construct the matrix representations of $\hat{D}\left(\vec{n},\theta\right)$.
In particular in the eigenbasis of $\hat{J}^2$ and $\hat{J}_z$.
Remember:

$$\hat{D}\left(\vec{n},\theta\right) = e^{-\frac{\mathrm{i}}{\hbar}\hat{\vec{J}}\cdot\vec{n}\theta}$$

We want:

$$\left\langle j,m\right|\hat{D}\left(\vec{n},\theta\right)\left|j',m'\right\rangle = D_{jm}^{j'm'}\left(\vec{n},\theta\right)$$

First note:, because $\left[\hat{\vec{J}}^2,\hat{\vec{J}}\cdot\vec{n}\right] = 0$.

$$D_{jm}^{j'm'}\left(\vec{n},\theta\right) = D_{mm'}^{(j)}\left(\vec{n},\theta\right)\delta_{jj'}$$

The physical reason is, that a rotation doesn't change magnitudes like j.
$j = \dfrac{1}{2}$ gives a 2×2-Matrix for D, because the basis is $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$ and $\left|\frac{1}{2},\frac{1}{2}\right\rangle$.

$$\begin{pmatrix} \overbrace{\begin{pmatrix} \; j=\frac{1}{2} \; \end{pmatrix}}^{2}\Big\updownarrow 2 & 0 & \\ 0 & \overbrace{\begin{pmatrix} \; j=1 \; \end{pmatrix}}^{3}\Big\updownarrow 3 & \\ & & \ddots \end{pmatrix}$$

This is the matrix representation of a rotation operator $\hat{D}\left(\vec{n},\theta\right)$ in the basis $\left|j,m\right\rangle$ ordered as

$$\left|\frac{1}{2},-\frac{1}{2}\right\rangle, \left|\frac{1}{2},+\frac{1}{2}\right\rangle, \left|1,-1\right\rangle, \left|1,0\right\rangle, \left|1,1\right\rangle, \left|\frac{3}{2},-\frac{3}{2}\right\rangle, \left|\frac{3}{2},-\frac{1}{2}\right\rangle, \left|\frac{3}{2},\frac{1}{2}\right\rangle, \left|\frac{3}{2},\frac{3}{2}\right\rangle, \ldots$$

and it is BLOCK-DIAGONAL.

3.5 Orbital angular momentum

Consider now $\hat{J}_i = \hat{L}_i = \left(\hat{\vec{q}}\times\hat{\vec{p}}\right)_i$.

3.5.1 General considerations

i) $\left[\hat{L}_i,\hat{L}_j\right] = \mathbf{i}\hbar\varepsilon_{ijk}\hat{L}_k$

ii) Consider:

$$\exp\left(-\frac{\mathbf{i}}{\hbar}\hat{L}_z\theta\right)|\vec{q}\rangle =: |\vec{q}\rangle^R \overset{?}{=} \left|\vec{q}^R\right\rangle := |\mathcal{R}(\vec{e}_z,\theta)\,\vec{q}\rangle$$

Do it infinitesimal:

$$\theta \to \mathrm{d}\theta$$

$$\begin{aligned}|\vec{q}\rangle^R &\approx \left(1-\frac{\mathbf{i}}{\hbar}\hat{L}_z\mathrm{d}\theta\right)|\vec{q}\rangle = \left(1-\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta\left(\hat{q}_x\hat{p}_y-\hat{q}_y\hat{p}_x\right)\right)|\vec{q}\rangle = \\ &= \left(1-\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta\left(q_x\hat{p}_y-q_y\hat{p}_x\right)\right)|q_x\rangle\otimes|q_y\rangle\otimes|q_z\rangle\end{aligned}$$

Remember:

$$\exp\left(-\frac{\mathbf{i}}{\hbar}q^{(0)}\hat{p}_x\right)|\vec{q}\rangle = \left|q_x+q^{(0)}\right\rangle\otimes|q_y\rangle\otimes|q_z\rangle$$

Infinitesimally we get:

$$\left(1-\frac{\mathbf{i}}{\hbar}\mathrm{d}q^{(0)}\hat{p}_x\right)|\vec{q}\rangle = \left|q_x+\mathrm{d}q^{(0)}\right\rangle\otimes|q_y\rangle\otimes|q_z\rangle$$

Now consider the product of two infinitesimal changes:

$$\left(1+\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta q_y\hat{p}_x\right)\left(1-\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta q_x\hat{p}_y\right) \approx 1-\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta\left(q_x\hat{p}_y-q_y\hat{p}_x\right)$$

This gives:

$$\begin{aligned}|\vec{q}\rangle^R &\approx \left(1+\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta q_y\hat{p}_x\right)\left(1-\frac{\mathbf{i}}{\hbar}\mathrm{d}\theta q_x\hat{p}_y\right)|q_x\rangle\otimes|q_y\rangle\otimes|q_z\rangle = \\ &= |q_x-\mathrm{d}\theta q_y\rangle\otimes|q_y+\mathrm{d}\theta q_x\rangle\otimes|q_z\rangle = |q_x-\mathrm{d}\theta q_y,q_y+\mathrm{d}\theta q_x,q_z\rangle\end{aligned}$$

Compare this with the rotated eigenstate of the position:

$$\left|\vec{q}^R\right\rangle = |\mathcal{R}(\vec{e}_z,\mathrm{d}\theta)\,\vec{q}\rangle \approx \left|\begin{pmatrix}1 & -\mathrm{d}\theta & 0\\ \mathrm{d}\theta & 1 & 0\\ 0 & 0 & 1\end{pmatrix}\vec{q}\right\rangle = |q_x-\mathrm{d}\theta q_y,q_y+\mathrm{d}\theta q_x,q_z\rangle \approx |\vec{q}\rangle^R$$

In general we get:

$$\exp\left(-\frac{\mathbf{i}}{\hbar}\hat{\vec{L}}\cdot\vec{n}\eta\right)|\vec{q}\rangle = |\mathcal{R}(\vec{n},\eta)\,\vec{q}\rangle$$

3.5.2 Eigenstates in the position representation

We call the eigenstates $|l,m\rangle$.
We introduce:

$$\begin{aligned}\hat{r} &= \sqrt{\hat{q}_x^2+\hat{q}_y^2+\hat{q}_z^2}\\ \hat{q}_x &= \hat{r}\sin\hat{\theta}\cos\hat{\varphi}\\ \hat{q}_y &= \hat{r}\sin\hat{\theta}\sin\hat{\varphi}\\ \hat{q}_z &= \hat{r}\cos\theta\end{aligned}$$

$$|\vec{q}\rangle = |r\rangle \otimes |\theta,\varphi\rangle = |r\rangle \otimes |\vec{n}\rangle$$

We want to construct $\langle \theta,\varphi | l,m\rangle$. As usual we start with

$$\left\langle \theta,\varphi \,\middle|\, \hat{L}_z \,\middle|\, l,m \right\rangle = \hbar m \left\langle \theta,\varphi \,|\, l,m \right\rangle$$

and do it infinitesimally:

$$\left\langle \theta,\varphi | \hat{D}\left(\vec{e}_z,\mathrm{d}\varphi\right) | l,m \right\rangle = \left\langle \theta,\varphi | \exp\left(-\frac{\mathbf{i}}{\hbar}\hat{L}_z \mathrm{d}\varphi\right) | l,m \right\rangle = \langle \theta,\varphi - \mathrm{d}\varphi | l,m \rangle$$

We also get for $\mathrm{d}\varphi \to 0$:

$$\left\langle \theta,\varphi \,\middle|\, \left(1 - \frac{\mathbf{i}}{\hbar}\hat{L}_z \mathrm{d}\varphi\right) \,\middle|\, l,m \right\rangle = \langle \theta,\varphi \,|\, l,m\rangle - \frac{\mathbf{i}}{\hbar}\mathrm{d}\varphi \left\langle \theta,\varphi \,\middle|\, \hat{L}_z \,\middle|\, l,m \right\rangle$$

This gives:

$$m\hbar \langle \theta,\varphi \,|\, l,m\rangle = \left\langle \theta,\varphi \,\middle|\, \hat{L}_z \,\middle|\, l,m \right\rangle = -\mathbf{i}\hbar \partial_\varphi \langle \theta,\varphi \,|\, l,m\rangle$$

$$\partial_\varphi \langle \theta,\varphi \,|\, l,m\rangle = \mathbf{i}m \langle \theta,\varphi \,|\, l,m\rangle$$

$$\langle \theta,\varphi \,|\, l,m\rangle = f_l^m(\theta)\, e^{\mathbf{i}m\varphi}$$

Introduce this into

$$\left\langle \theta,\varphi | \hat{L}^2 | l,m \right\rangle = \hbar^2 l\,(l+1) \langle \theta,\varphi \,|\, l,m\rangle$$

$$-\hbar^2 \left(\frac{1}{\sin^2\theta}\partial_\varphi^2 + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\partial_\theta\right)\right) \langle \theta,\varphi \,|\, l,m\rangle = \hbar^2 l\,(l+1) \langle \theta,\varphi \,|\, l,m\rangle$$

to get for $m,l \in \mathbb{Z}$:

$$\left(\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\partial_\theta\right) - \frac{m^2}{\sin^2\theta} + l\,(l+1)\right) f_l^m(\theta) = 0$$

Transform $x = \cos\theta$ and solve this by a power series. The solutions $P_l^m(\cos\theta)$ are the *associated Legendre polynomials.*

Together we have the *spherical harmonics*:

$$\langle \theta,\varphi \,|\, l,m\rangle = Y_l^m(\theta,\varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \cdot \frac{(l-m)!}{(l+m)!}} \cdot e^{\mathbf{i}m\varphi} P_l^m(\cos\theta)$$

Of course they are normalized:

$$\left\langle l',m' \,\middle|\, l,m \right\rangle = \delta_{ll'}\delta_{mm'}$$

$$\Rightarrow \qquad \int_0^{2\pi}\int_0^{\pi} Y_{l'}^{m'}(\theta,\varphi)^* \, Y_l^m(\theta,\varphi) \sin\theta \mathrm{d}\theta = \delta_{ll'}\delta_{mm'}$$

Therefore any function of

$$\vec{n} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$$

can be expanded in terms of $Y_l^m(\theta,\varphi)$'s, because they form a complete basis:

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} |l,m\rangle\langle l,m| = \hat{I}_{\text{angular}}$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_l^m(\theta,\varphi)\,Y_l^m(\theta',\varphi') = \delta(\vec{n}-\vec{n}')$$

From the general theory we also know:

$$\hat{L}_\pm|l,m\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}\,|l,m\pm 1\rangle$$

For an arbitrary normalized state $|\alpha\rangle$ in the angular Hilbert space one gets:

$$\left\langle \theta,\varphi \middle| \hat{L}_- \middle| \alpha\right\rangle = \mathbf{i}\hbar e^{\mathbf{i}\varphi}\left[\mathbf{i}\partial_\theta - \cot\theta\right]\langle\theta,\varphi\,|\,\alpha\rangle$$

For example:

$$Y_l^{l-1}(\theta,\varphi) = -N_l^l e^{\mathbf{i}(l-1)\varphi}\left(l\cot\theta - \partial_\theta\right)P_l^l(\cos\theta)$$
$$P_l^l(\cos\theta) = \sin^l(\theta)$$

$$Y_l^{-m}(\theta,\varphi) = (-1)^m\left(Y_l^m(\theta,\varphi)\right)^*$$

3.5.3 Relation with the kinetic energy

Remember from classical mechanics:

$$H(\vec{q},\vec{p}) = \frac{1}{2m}p^2 + V(\vec{q})$$

In spherical coordinates we have the canonical transformation

$$\begin{pmatrix} q_x \\ q_y \\ q_z \end{pmatrix} \to \begin{pmatrix} r \\ \theta \\ \varphi \end{pmatrix} \qquad\qquad \Rightarrow \quad \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} \to \begin{pmatrix} p_r \\ p_\theta \\ p_\varphi \end{pmatrix}$$

with the commutators

$$\{r,p_r\} = \{\theta,p_\theta\} = \{\varphi,p_\varphi\} = 1$$

and the other commutators are zero. The Hamiltonian is then

$$H(r,\theta,\varphi,p_r,p_\theta,p_\varphi) = \frac{1}{2m}p_r^2 + \frac{1}{2mr^2}L^2 + V(r,\theta,\varphi)$$

with:

$$L^2 = \frac{1}{\sin^2\theta}p_\varphi^2 + p_\theta^2$$

To see this in quantum mechanics, we use

$$\hat{L}^2 = \hat{q}^2\hat{p}^2 - \left(\hat{\vec{q}}\cdot\hat{\vec{p}}\right)^2 + \mathbf{i}\hbar\hat{\vec{q}}\cdot\hat{\vec{p}}$$

and calculate for an arbitrary state $|\alpha\rangle$:

$$\left\langle \vec{q}\middle|\hat{L}^2\middle|\alpha\right\rangle = q^2\left\langle\vec{q}\,\middle|\,\hat{p}^2\,\middle|\,\alpha\right\rangle - \vec{q}\cdot\left(-\mathbf{i}\hbar\vec{\nabla}\right)\cdot\vec{q}\cdot\left(-\mathbf{i}\hbar\vec{\nabla}\right)\langle\vec{q}\,|\,\alpha\rangle + \mathbf{i}\hbar\vec{q}\cdot\left(-\mathbf{i}\hbar\vec{\nabla}\right)\langle\vec{q}\,|\,\alpha\rangle$$

$$\left\langle\vec{q}\middle|\frac{1}{2m}\hat{p}^2\middle|\alpha\right\rangle = -\frac{\hbar^2}{2m}\left(\frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r}\partial_r\right)\langle\vec{q}\,|\,\alpha\rangle + \frac{1}{2mr^2}\left\langle\vec{q}\middle|\hat{L}^2\middle|\alpha\right\rangle =$$
$$= -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\partial_r\left(r^2\partial_r\right)\right)\langle\vec{q}\,|\,\alpha\rangle + \frac{1}{2mr^2}\left\langle\vec{q}\middle|\hat{L}^2\middle|\alpha\right\rangle$$

3.5.4 Central forces

Definition:
A central force has a potential, that depends only on the radial coordinate:

$$V(\vec{q}) = V(\hat{r})$$

Therefore it commutes with $\hat{p}^2$ and $\hat{L}^2$ and we have a set of common eigenstates:

$$\begin{aligned} \hat{H}\,|E,l,m\rangle &= E\,|E,l,m\rangle \\ \hat{L}^2\,|E,l,m\rangle &= \hbar^2 l\,(l+1)\,|E,l,m\rangle \\ \hat{L}_z\,|E,l,m\rangle &= \hbar m\,|E,l,m\rangle \end{aligned}$$

We define

$$\psi_{Elm}(r,\theta,\varphi) := \langle r,\theta,\varphi \,|\, E,l,m\rangle = R_{Elm}(r)\,Y_l^m(\theta,\varphi)$$

and get:

$$\left(-\frac{\hbar^2}{2mr^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right) + \frac{\hbar^2 l\,(l+1)}{2mr^2} + V(r)\right) R_{Elm}(r) = E R_{Elm}(r)$$

This doesn't depend on the quantum number m, so we just write $R_{Elm}(r)$. Now we transform

$$R_{El}(r) := \frac{U_{El}(r)}{r}$$

and get:

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \underbrace{\left(V(r) + \frac{\hbar^2 l\,(l+1)}{2mr^2}\right)}_{=:V_{\text{eff}}(r)}\right) U_{El}(r) = E U_{El}(r)$$

3.6 Addition of angular momentum

Consider two particles with the same mass and momenta $\vec{p}^{\,(1)}$ and $\vec{p}^{\,(2)}$. In classical mechanics they generate translations ($k \in \{1,2\}$):

$$f\left(\vec{q}^{\,(k)} + \delta\vec{q}^{\,(k)},\vec{p}^{\,(k)}\right) \approx f\left(\vec{q}^{\,(k)},\vec{p}^{\,(k)}\right) + \left\{\vec{p}^{\,(k)}, f\left(\vec{q}^{\,(k)}\right)\right\} \cdot \delta\vec{q}^{\,(k)} + O\left(\left(\delta\vec{q}^{\,(k)}\right)^2\right)$$

$\vec{p} := \left(\vec{p}^{\,(1)},\vec{p}^{\,(2)}\right)$ generates translations of $\vec{q} := \left(\vec{q}^{\,(1)},\vec{q}^{\,(2)}\right)$:

$$f(\vec{q} + \delta\vec{q},\vec{p}) \approx f(\vec{q},\vec{p}) + \{\vec{p}, f(\vec{q})\} \cdot \delta\vec{q} + O\left((\delta\vec{q})^2\right)$$

What is the meaning (in the sense of generators) of:

$$\vec{P} := \vec{p}^{\,(1)} + \vec{p}^{\,(2)}$$

Remember that $\vec{P}$ and $\vec{Q} = \frac{1}{2}\left(\vec{q}^{\,(1)} + \vec{q}^{\,(2)}\right)$ are canonical, that means:

$$\{Q_i,P_j\} = \delta_{ij}$$

Therefore $\vec{P}$ generates translations in $\vec{Q}$.

$$f\left(\vec{q}^{\,(1)}+\delta\vec{Q},\vec{q}^{\,(2)}+\delta\vec{Q},\vec{p}^{\,(1)},\vec{p}^{\,(2)}\right)=f\left(\vec{q}^{\,(1)},\vec{q}^{\,(2)},\vec{p}^{\,(1)},\vec{p}^{\,(2)}\right)+$$
$$+\left\{\vec{P},f\left(\vec{q}^{\,(1)},\vec{q}^{\,(2)},\vec{p}^{\,(1)},\vec{p}^{\,(2)}\right)\right\}\cdot\delta\vec{Q}+O\left(\left(\delta\vec{Q}\right)^2\right)$$

In the same way $\vec{L}^{\,(1)}+\vec{L}^{\,(2)}$ generates a RIGID rotation of the total system.

3.6.1 Formal theory (2 "particles")

We start with two angular momenta $\hat{\vec{J}}^{(1)}$ and $\hat{\vec{J}}^{(2)}$ with ($n\in\{1,2\}$):

$$\left[\hat{J}_i^{(n)},\hat{J}_j^{(n)}\right]=\mathbf{i}\hbar\varepsilon_{ijk}\hat{J}_k^{(1)}$$
$$\left[\hat{J}_i^{(1)},\hat{J}_j^{(2)}\right]=0$$

The "total" angular momentum is:

$$\hat{J}_i:=\hat{J}_i^{(1)}\otimes\hat{I}^{(2)}+\hat{I}^{(1)}\otimes\hat{J}_i^{(2)}=:\hat{J}_i^{(1)}+\hat{J}_i^{(2)}$$

And a "total" rotation by $\vec{n},\theta$ is:

$$\hat{D}\left(\vec{n},\theta\right):=\hat{D}\left(\vec{n},\theta\right)^{(1)}\otimes\hat{D}\left(\vec{n},\theta\right)^{(2)}=e^{-\frac{\mathbf{i}}{\hbar}\hat{\vec{J}}^{(1)}\cdot\vec{n}\theta}\cdot e^{-\frac{\mathbf{i}}{\hbar}\hat{\vec{J}}^{(2)}\cdot\vec{n}\theta}=e^{-\frac{\mathbf{i}}{\hbar}\hat{\vec{J}}\cdot\vec{n}\theta}$$

Check whether $\hat{\vec{J}}$ is an angular momentum:

$$\left[\hat{J}_i,\hat{J}_j\right]=\mathbf{i}\hbar\varepsilon_{ijk}\hat{J}_k$$

So we have two possible sets of commuting operators:

1. DECOUPLED BASIS: Take $\left\{\left(\hat{J}^{(1)}\right)^2,\left(\hat{J}^{(2)}\right)^2,\hat{J}_z^{(1)},\hat{J}_z^{(1)}\right\}$ with the common eigenstates:

   $$\left|j_1,j_2,m_1,m_2\right\rangle:=\left|j_1,m_1\right\rangle\otimes\left|j_2,m_2\right\rangle$$

   For $k\in\{1,2\}$ we have:

   $$\left(\hat{J}^{(k)}\right)^2\left|j_1,j_2,m_1,m_2\right\rangle=\hbar^2\left(j_k+1\right)\left|j_1,j_2,m_1,m_2\right\rangle$$
   $$\hat{J}_z^{(k)}\left|j_1,j_2,m_1,m_2\right\rangle=\hbar m_k\left|j_1,j_2,m_1,m_2\right\rangle$$

2. COUPLED BASIS: Take $\left\{\left(\hat{J}^{(1)}\right)^2,\left(\hat{J}^{(2)}\right)^2,\hat{J}^2,\hat{J}_z\right\}$ – observe $\left[\hat{J}^2,\hat{J}_z^{(k)}\right]\neq 0$ – with the common eigenstates $\left|j_1,j_2,j,m\right\rangle$ with:

   $$\hat{J}^2\left|j_1,j_2,j,m\right\rangle=\hbar^2 j\left(j+1\right)\left|j_1,j_2,j,m\right\rangle$$
   $$\hat{J}_z\left|j_1,j_2,j,m\right\rangle=\hbar m\left|j_1,j_2,j,m\right\rangle$$

The two bases are related (for fixed j_1,j_2):

$$|j_1,j_2,j,m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \underbrace{\langle j_1,j_2,m_1,m_2|j_1,j_2,j,m\rangle}_{\text{Lebsch-Gordan coeffizients}} |j_1,j_2,m_1,m_2\rangle$$

Some properties of $\langle m_1,m_2|j,m\rangle := \langle j_1,j_2,m_1,m_2|j_1,j_2,j,m\rangle$:
Consider

$$\hat{J}_z - \hat{J}_z^{(1)} - \hat{J}_z^{(2)} = 0$$

and sandwich between $\langle j_1,j_2,m_1,m_2| \ldots |j_1,j_2,j,m\rangle$ to get:

$$(m - m_1 - m_2) \langle m_1,m_2|j,m\rangle = 0$$

Therefore $\langle m_1,m_2|j,m\rangle = 0$ for $m \neq m_1 + m_2$ and one can eliminate one of the sums above. One can also proof:

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

From unitarity of the matrix for the change of basis we get:

$$\sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle m_1 m_2|j,m\rangle \langle m_1 m_2|j',m'\rangle^* = \delta_{jj'}\delta_{mm'}$$

$$\sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m=-j}^{j} \langle m_1 m_2|j,m\rangle \langle m_1' m_2'|j,m\rangle^* = \delta_{m_1 m_1'}\delta_{m_2 m_2'}$$

Finally using $\hat{J}_\pm = \hat{J}_\pm^{(1)} + \hat{J}_\pm^{(2)}$ gives:

$$\begin{aligned}\sqrt{(j \mp m)(j \pm m + 1)} \langle m_1,m_2 \,|\, j,m \pm 1\rangle &= \sqrt{(j_1 \pm m_1)(j_1 \mp m_1 + 1)} \langle m_1 \mp 1,m_2 \,|\, j,m\rangle + \\ &+ \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)} \langle m_1,m_2 \pm 1 \,|\, j,m\rangle\end{aligned}$$

3.6.2 The formal theory for many particles

This is a REAL MESS!!

3.6.3 Example: Two spin $\frac{1}{2}$ particles

Here the total spin is:

$$\hat{\vec{S}} = \hat{\vec{S}}^{(1)} + \hat{\vec{S}}^{(2)} \qquad \hat{S}_z = \hat{S}_z^{(1)} + \hat{S}_z^{(2)} \qquad \hat{S}^2 = \left(\hat{S}^{(1)}\right)^2 + \left(\hat{S}^{(1)}\right)^2 + 2\hat{\vec{S}}^{(1)} \cdot \hat{\vec{S}}^{(2)}$$

And the quantum numbers are $j_1 = s_1 = \frac{1}{2}$, $j_2 = s_2 = \frac{1}{2}$. The total is $m = m_1 + m_2$ and s is restricted to:

$$\left|\frac{1}{2} - \frac{1}{2}\right| \leq s \leq \frac{1}{2} + \frac{1}{2}$$
$$0 \leq s \leq 1$$

– The decoupled basis ($|m_1,m_2\rangle$) is:

$$\left\{ \left|\frac{1}{2},\frac{1}{2}\right\rangle, \left|\frac{1}{2},-\frac{1}{2}\right\rangle, \left|-\frac{1}{2},\frac{1}{2}\right\rangle, \left|-\frac{1}{2},-\frac{1}{2}\right\rangle \right\}$$

Remember that this basis does not have a well defined $\hat{S}^2$.

– The coupled basis ($|s,m\rangle$) is:

$$\begin{aligned}\{|s=0,m=0\rangle, |s=1,m=-1\rangle, |s=1,m=0\rangle, |s=1,m=1\rangle\} &= \\ = \{ \underbrace{|0,0\rangle}_{\text{"Singlet"}}, \underbrace{|1,-1\rangle, |1,0\rangle, |1,1\rangle}_{\text{"Triplet" states}} \}\end{aligned}$$

Using $m = m_1 + m_2$ we get:

$$\begin{aligned}|s=1,m=1\rangle &= \left|\frac{1}{2},\frac{1}{2}\right\rangle := \left|\frac{1}{2}\right\rangle^{(1)} \otimes \left|\frac{1}{2}\right\rangle^{(2)} \\ |s=1,m=0\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},-\frac{1}{2}\right\rangle + \left|-\frac{1}{2},\frac{1}{2}\right\rangle\right) \\ |s=1,m=-1\rangle &= \left|-\frac{1}{2},-\frac{1}{2}\right\rangle \\ |s=0,m=0\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},-\frac{1}{2}\right\rangle - \left|-\frac{1}{2},\frac{1}{2}\right\rangle\right)\end{aligned}$$

(Take a look at: Sakurai, Section 3.10: "*Spin Correlation measurements and Bell's inequality*")

Think about the Hamiltonian for $k \in \mathbb{R}_{<0}$:

$$\hat{H} = \underbrace{\underbrace{\hbar\omega\left(\hat{S}_z^{(1)} + \hat{S}_z^{(2)}\right)}_{\hat{S}_z^{(1)},\hat{S}_z^{(2)} \text{ are conserved}} + k\hat{\vec{S}}^{(1)} \cdot \hat{\vec{S}}^{(2)}}_{\hat{S}^2,\hat{S}_z \text{ are conserved}}$$

We use:

$$\hat{\vec{S}}^{(1)} \cdot \hat{\vec{S}}^{(2)} = \frac{1}{2}\left(\hat{S}^2 - \left(\hat{S}^{(1)}\right)^2 - \left(\hat{S}^{(2)}\right)^2\right)$$

3.7 Symmetry in quantum mechanics

3.7.1 Continuous symmetries

If we have $\left[\hat{H},\hat{G}\right] = 0$, $\hat{G} = \hat{G}^\dagger$ and $\hat{G}\,|g_n\rangle = g_n\,|g_n\rangle$, then we know:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{G}_H(t) &= 0 \\ \hat{U}_\tau &:= e^{-\frac{\mathrm{i}}{\hbar}\hat{G}\tau} \\ \hat{G}\left(\hat{U}(t,t_0)\,|g_n\rangle\right) &= g_n\hat{U}(t,t_0)\,|g_n\rangle\end{aligned}$$

Example:

$$\hat{H} = \frac{1}{2m}\hat{p}^2 \qquad\qquad \left[\hat{H},\hat{p}\right] = 0$$

Therefore $\hat{U}(t)\,|\hat{p}\rangle$ is always an eigenstate of $\hat{p}$.

A new concept, a purely quantum mechanical consequence of symmetry is the concept of "degeneracies".
Consider $\left[\hat{H},\hat{G}\right] = \left[\hat{H},\hat{U}_\tau\right] = 0$, then, trivially we get:

$$\hat{H}\left(\hat{U}_\tau\,|e_n\rangle\right) = e_n\left(\hat{U}_\tau\,|e_n\rangle\right)$$

There are two possibilities:

i) $\hat{U}\,|e_n\rangle = e^{\mathbf{i}\delta}\,|e_n\rangle$ (nothing special)

ii) $\hat{U}\,|e_n\rangle \neq e^{\mathbf{i}\delta}\,|e_n\rangle$ then $|e_n\rangle$ and $\hat{U}_\tau\,|e_n\rangle$ are two degenerate eigenstates with eigenvalue e_n.

Example: $\left[\hat{U},\hat{L}_i\right] = 0$, $\hat{H}\,|n,l,m\rangle = E_{nl}\,|n,l,m\rangle$ and:

$$\langle\vec{q}\,|\,n,l,m\rangle = R_{nl}(r)\,Y_l^m(\theta,\varphi)$$

The symmetry operator is:

$$\exp\left(-\frac{\mathbf{i}}{\hbar}\hat{\vec{L}}\cdot\vec{n}\theta\right)$$

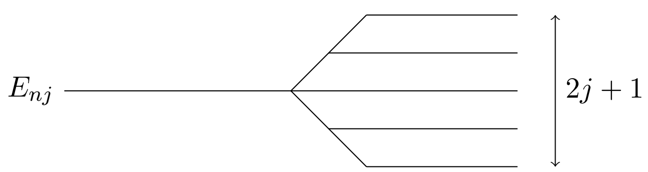
$$\exp\left(-\frac{\mathbf{i}}{\hbar}\hat{\vec{L}}\cdot\vec{n}\theta\right)|n,l,m\rangle = \sum_{m'=-l}^{l} D^{(l)}_{m,m'}(\vec{n},\theta)\,\left|n,l,m'\right\rangle$$

So the energy E_{nl} is $(2l+1)$-*fold degenerate*. The reason at the end is, that $\left[\hat{L}_i,\hat{L}_j\right] \neq 0$.

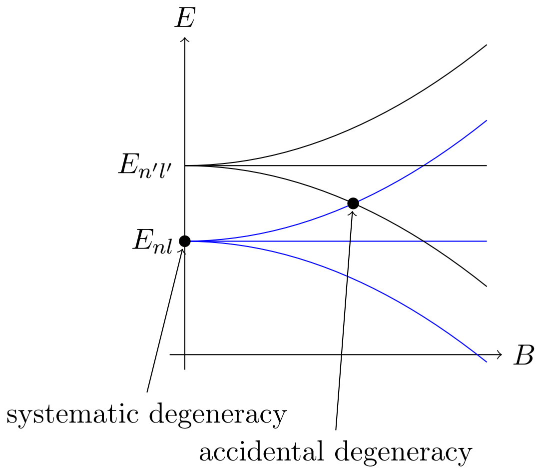
Example: $\hat{H} = \frac{1}{2m}\hat{\vec{p}}^2 + V(\hat{r}) + V_{ls}(\hat{r})\,\hat{\vec{l}}\cdot\hat{\vec{s}}$

$$\left[\hat{H},\hat{\vec{l}}\right] \neq 0 \qquad\qquad \left[\hat{H},\hat{\vec{s}}\right] \neq 0 \qquad\qquad \left[\hat{H},\hat{\vec{j}}\right] = 0$$

The eigenstates are $|n,j,m\rangle$ and therefore E_{nj} is $(2j+1)$-fold degenerate.



"Splitting" of the "multiplett".



3.7.2 Discrete symmetries

You do not see them in classical mechanics.

i) Parity inverts position and momentum vectors:

$$\hat{\pi}^{\dagger}\hat{q}_i\hat{\pi} = -\hat{q}_i$$
$$\hat{\pi}^{\dagger}\hat{p}_i\hat{\pi} = -\hat{p}_i$$

But angular momentum doesn't change:

$$\hat{\pi}^{\dagger}\hat{j}_i\hat{\pi} = \hat{j}_i$$

These are called "pseudo-vectors".
States:

$$\hat{\pi}\,|\vec{q}\rangle = |-\vec{q}\rangle$$
$$\hat{\pi}\,|\vec{p}\rangle = |-\vec{p}\rangle$$

$$\hat{\pi}^2 = \hat{I} \qquad \hat{\pi}^{\dagger} = \hat{\pi}^{-1} \qquad \hat{\pi}^{\dagger} = \hat{\pi}$$

From these properties follows, that the eigenvalues of π are ± 1.
A $+1$ eigenstate is called *even* and a -1 eigenstate is called *odd under parity.*
If we have $\hat{\pi}\,|\alpha_\pm\rangle = \pm\,|\alpha_\pm\rangle$ with $\psi_\pm(\vec{q}) = \langle\vec{q}|\alpha_\pm\rangle$ then we get:

$$\psi_\pm(\pm\vec{q}) = \pm\psi_\pm(\vec{q})$$

Example: $\hat{p}\,|p\rangle = p\,|p\rangle$

$$\langle q|p\rangle = \frac{1}{\sqrt{2m}}e^{\frac{\mathrm{i}}{\hbar}pq}$$

They are *not* eigenstates of $\hat{\pi}$.

$$|\alpha_\pm\rangle := \frac{1}{\sqrt{2}}\left(|\vec{p}\rangle \pm |-\vec{p}\rangle\right)$$

$$\langle q|\alpha_\pm\rangle = \begin{cases} \frac{1}{\sqrt{2}}\cos\left(\frac{1}{\hbar}pq\right) \\ \frac{1}{\sqrt{2}}\sin\left(\frac{1}{\hbar}pq\right) \end{cases}$$

Example: Eigenstates of a central force $|n,l,m\rangle$.

We know, $\left[\hat{\vec{L}},\hat{\pi}\right] = 0$, so automatically $|n,l,m\rangle$ has a well defined parity. This means:

$$\hat{\pi}\,|n,l,m\rangle = \pm\,|n,l,m\rangle$$

Do your job:

$$\langle\vec{q}|n,l,m\rangle = R_{nl}\,(r)\,Y_l^m\,(\theta,\varphi)$$

Change $\vec{q}\to-\vec{q}$. In spherical coordinates $(r,\theta,\varphi)\to(r,\pi-\theta,\varphi+\pi)$. Remember:

$$Y_l^m\,(\theta,\varphi) = (-1)^m\sqrt{\frac{(2l+1)\,(l-m)!}{4\pi\,(l+m)!}}\cdot P_l^m\,(\cos\theta)\,e^{\mathbf{i}m\varphi}$$
$$Y_l^m\,(\pi-\theta,\varphi+\pi) = (-1)^l\,Y_l^m\,(\theta,\varphi)$$

Tips to construct $\hat{\pi}$.

1D harmonic oscillator:

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{q}^2$$

Check as an exercise:

$$\hat{\pi} = e^{\mathbf{i}\pi\hat{n}}$$

Theorem:

If $\hat{H}\,|e_n\rangle = e_n\,|e_n\rangle$ and $\left[\hat{H},\hat{\pi}\right] = 0$. If the spectrum e_n is *not* degenerate, the eigenstates of $\hat{H}$ have well defined parity.

4 Perturbation theory (time-independent)

5 Perturbation theory (time-dependent)

6 Many-particle systems

7 Scattering theory

8 Orthogonal Polynomials

Sturm-Liouville equations:
Take $x \in [x_0,x_1]$ and $a(x) \neq 0$ and $a(x), b(x), c(x) \in C^0([x_0,x_1],\mathbb{R})$:

$$a(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}y(x) + b(x)\frac{\mathrm{d}}{\mathrm{d}x}y(x) + c(x)y(x) + \lambda y(x) = 0$$

Boundary condition:

$$\left[\alpha_1 y(x) + \alpha_2 \frac{\mathrm{d}}{\mathrm{d}x}y(x)\right]_{x=x_0} = 0$$
$$\left[\beta_1 y(x) + \beta_2 \frac{\mathrm{d}}{\mathrm{d}x}y(x)\right]_{x=x_1} = 0$$

Define

$$p(x) := \exp\left(\int_{x_0}^{x} \frac{b(s)}{a(s)}\mathrm{d}s\right)$$
$$r(x) := \frac{1}{a(x)}p(x)$$
$$q(x) := \frac{c(x)}{a(x)}p(x)$$

to get:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}y(x)\right) + (q(x) + \lambda r(x))\,y(x) = 0$$

$$\hat{\mathscr{L}} := \frac{1}{r(x)}\left(\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)\right)$$

$$\hat{\mathscr{L}}y_n(x) = -\lambda_n y_n(x)$$

This equation is solved by non-zero functions $y_n(x)$ for some λ_n.
Theorem: If $p(x) > 0, r(x) > 0$ and $q(x) \geq 0$, then the set $\{y_n(x)\}_{n=1}$ is orthogonal, that is:

$$\langle y_n | y_m \rangle := \int_{x_0}^{x_1} r(x)\,y_n(x)\,y_m(x)\,\mathrm{d}x = k_n^2 \delta_{nm}$$

$r(x)$ is called "weight". Introduce a new set of functions

$$\varphi_n(x) := y_n(x)\frac{\sqrt{r(x)}}{k_n}$$

to get:

$$\int_{x_0}^{x_1} \varphi_n(x)\,\varphi_m(x)\,\mathrm{d}x = \delta_{nm}$$

But the $\varphi_n(x)$ do not solve the differential equation, so physicist don't use them.

i) Legendre:

$$\underbrace{(1-x)^2}_{=a(x)}\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\underbrace{-2x}_{=b(x)}\frac{\mathrm{d}y}{\mathrm{d}x}+\underbrace{n(n+1)}_{=\lambda}y=0$$

Defined for $x \in [-1,1]$. We get:

$$\begin{aligned} p(x) &= \exp\left(\int_{-1}^{x}\frac{-2s}{1-s^2}\mathrm{d}s\right) = 1-x^2 \\ q(x) &= 0 \\ r(x) &= 1 \end{aligned}$$

This is the simplest value for $r(x)$.

Extra: The set $\{1,x,x^2,\ldots,\}$ is linearly independent.

$$\int_{-1}^{1} r(x)\,x^n x^m \mathrm{d}x \neq \delta_{nm}$$

Using the Gram-Schmidt-formalism to make orthogonal polynomials gives for $r=1$ the Legendre polynomials.

In the Sturm-Liouville form:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1-x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right)}_{=\hat{\mathscr{L}}}y(x) = -n(n+1)\,y(x)$$

Use power series and get normalized solutions:

$$\begin{aligned} p_0(x) &= 1 \\ p_1(x) &= x \\ p_2(x) &= \frac{1}{2}\left(3x^2-1\right) \end{aligned}$$

For each set of orthogonal polynomials there is a *Rodrigues formula*:

$$P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(x^2-1\right)^n$$

The *recursion relation* is:

$$(n+1)\,P_{n+1}(x) - (2n+1)\,xP_n(x) + nP_{n-1}(x) = 0$$

Every Sturm-Liouville equation solution satisfy a three term recursion relation, because it is a second order equation.

The *Generating function* is:

$$\frac{1}{\sqrt{1-2tz+t^2}} = \sum_{n=0}^{\infty} t^n P_n(z)$$

ii) Chebyshev:

$$\left(1-x^2\right)\frac{\mathrm{d}^2y}{\mathrm{d}x^2}-x\frac{\mathrm{d}y}{\mathrm{d}x}+\underbrace{n^2}_{=\lambda}y=0$$

for $x\in[-1,1]$.

$$p(x)=\sqrt{1-x^2}$$
$$q(x)=0$$
$$r(x)=\frac{1}{\sqrt{1-x^2}}$$

$$T_0(x)=1$$
$$T_1(x)=x$$
$$T_2(x)=2x^2-1$$

Rodrigues formula:

$$T_n(x)=\cos\left(n\cos^{-1}(x)\right)$$

What is the related potential in quantum mechanics?

$$\int_{-1}^{1}\frac{T_n(x)\,T_m(x)}{\sqrt{1-x^2}}=\begin{cases}\pi\delta_{nm} & n=0\\ \frac{\pi}{2}\delta_{nm} & n>0\end{cases}$$

Recursion:

$$T_{n+1}-2xT_n+T_{n-1}=0$$

Generating function:

$$\frac{1-t^2}{1-2tz+t^2}=T_0(x)+2\sum_{n=1}^{\infty}T_n(x)\,t^n$$

iii) Hermite:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}y-2x\frac{\mathrm{d}y}{\mathrm{d}x}+\lambda y=0$$

We can take without trouble $x\in(-\infty,\infty)$.

$$p(x)=e^{-x^2}$$
$$q(x)=0$$
$$r(x)=e^{-x^2}$$

In Storm-Liouville form:

$$e^{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(e^{-x^2}\frac{\mathrm{d}}{\mathrm{d}x}\right)y(x)\right)=-\lambda y(x)$$

$$H_0(x) = 1$$
$$H_1(x) = 2x$$
$$H_2(x) = 4x^2 - 2$$

Rodrigues formula:

$$H_n(x) = (-1)^n e^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} e^{-x^2}$$

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) \, \mathrm{d}x = 2^n n! \sqrt{\pi} \delta_{nm}$$

Recursion:

$$H_{n+1} - 2xH_n + 2nH_{n-1} = 0$$

Generating function:

$$e^{-t^2+2tx} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x)$$

Appendix

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Andreas Völklein

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