Quantum Mechanics II.

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Quantum mechanics is usually taught on four different levels:

1. Basic ideas, simple examples for a one dimensional particle, particle in spherical potential

2. More realistic, three dimensional cases with few particles

3. Several particles, relativistic effects (Quantum Field Theory)

4. Fundamental issues, challenges, paradoxes and interpretation of the quantum world

This lecture note belongs to level 2.

You should be warned when embarking level 1 to leave your expectations, intuitions behind and start more or less from scratch to build up a view of physics. There is no other discipline thought at Universities where one has to ask the students at the half of their university time to follow such a strange attitude. Now, at level 2., you should keep the experience of your first encounter with quantum mechanics, whatever confusing and unsatisfactory they were, this is the time to develop further technical know-how.

But please keep your dissatisfaction about the subject in mind and remember it later to try to improve our understanding and maneuverability in the quantum world. It is not clear how far we are from a better understanding of quantum mechanics. We may miss only few elements or we may even have to change completely our mathematics. But it is sure that we have to improve our way we look at Nature. Until this happens, in lacking of better ideas, try to understand why don't you understand quantum mechanics.

I. PERTURBATION EXPANSION

The Hamiltonian, being a Hermitian operator, can always be brought into a diagonal form by using an appropriate basis where the Schrödinger equation, and the dynamics of a quantum system is trivial. But this simplicity is naturally misleading because the basis where the dynamics is simple is usually highly non-trivial in terms of the usual observables.

A systematic approximation scheme, the perturbation expansion, is based on the assumption that the Hamiltonian can be written as a sum of two hermitian operators, $H = H_0 + gH_1$, one is stationary and easily diagonalizable and the other is assumed to be weak, a condition to be specified later. We treat g as a small parameter and organize the solution of the Schrödinger equation as a power series in g.

A. Stationary perturbations

We assume first that H_0 is non-degenerate, H_1 is time independent and seek the spectrum and the stationary states, $H|\psi_n\rangle = E_n|\psi_n\rangle$. For this end we assume that the unknown eigenvector and eigenvalues can be expanded in the small parameter,

$$\begin{aligned} |\psi_n\rangle &= |\psi_n^{(0)}\rangle + g|\psi_n^{(1)}\rangle + g^2|\psi_n^{(2)}\rangle + \cdots , \\ E_n &= E_n^{(0)} + gE_n^{(1)} + g^2E_n^{(2)} + \cdots , \end{aligned} \tag{1}$$

which gives, after inserting into the eigenvalue equation,

$$\begin{aligned} 0 \;=\; & g^0\left(H_0|\psi_n^{(0)}\rangle - E_n^{(0)}|\psi_n^{(0)}\rangle\right) \\ & +g\left(H_0|\psi_n^{(1)}\rangle + H_1|\psi_n^{(0)}\rangle - E_n^{(1)}|\psi_n^{(0)}\rangle - E_n^{(0)}|\psi_n^{(1)}\rangle\right) \\ & +g^2\left(H_0|\psi_n^{(2)}\rangle + H_1|\psi_n^{(1)}\rangle - E_n^{(2)}|\psi_n^{(0)}\rangle - E_n^{(1)}|\psi_n^{(1)}\rangle - E_n^{(0)}|\psi_n^{(2)}\rangle\right) + \cdots , \end{aligned} \tag{2}$$

written orders one-by-one as

$$\begin{aligned} \mathcal{O}\left(g^0\right): \quad & H_0|\psi_n^{(0)}\rangle && = E_n^{(0)}|\psi_n^{(0)}\rangle \\ \mathcal{O}\left(g\right): \quad & (H_0 - E_n^{(0)})|\psi_n^{(1)}\rangle && = (E_n^{(1)} - H_1)|\psi_n^{(0)}\rangle \\ \mathcal{O}\left(g^2\right): \quad & (H_0 - E_n^{(0)})|\psi_n^{(2)}\rangle && = (E_n^{(1)} - H_1)|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle \\ \mathcal{O}\left(g^k\right): \quad & (H_0 - E_n^{(0)})|\psi_n^{(k)}\rangle && = (E_n^{(1)} - H_1)|\psi_n^{(k-1)}\rangle + \cdots + E_n^{(k)}|\psi_n^{(0)}\rangle. \end{aligned} \tag{3}$$

The zeroth-order equation shows that the vectors $|\psi_n^{(0)}\rangle$, the eigenvectors of a non-degenerate Hermitian operator are orthogonal, $\langle\psi_m^{(0)}|\psi_n^{(0)}\rangle = \delta_{mn}$.

It comes as a surprise that the higher order equations can not be solved in a unique manner. In fact, to solve say the last equation for $|\psi_n^{(k)}\rangle$ one multiplies the equation by $(H_0 - E_n^{(0)})^{-1}$. However the latter operator has a non-trivial null-space (the null-space of an operator A is a linear subspace, consistsing of the vectors turned into zero by the operator in question, $A|0\rangle = 0$) where its inverse does not exist. To overcome this difficulty observe that if the vector $|\psi_n^{(k)}\rangle$ represents a solution of the k-th order eigenvalue equation then another solution can be found by adding to it a vector from the null-spaces, $|\psi_n^{(k)}\rangle + c|\psi_n^{(0)}\rangle$. We choose $c = -\langle\psi_n^{(0)}|\psi_n^{(k)}\rangle$, or equivalently we impose the condition $\langle\psi_n^{(0)}|\psi_n^{(k)}\rangle = \delta_{k,0}$, to render the solution unique and well defined.

This method of solving the equations fails if the spectrum is continuous. In that case one adds an infinitesimal imaginary term to the free Hamiltonian, $H_0 \to H_0 + i\epsilon$, with $\epsilon \to 0$, c.f. eq. (364).

We consider the first two orders in some details:

1. *First order:* One supposes the form $|\psi_n^{(1)}\rangle = \sum_k c_{n,k}|\psi_k^{(0)}\rangle$ and the projection of the second equation of (3) on $\langle\psi_k^{(0)}|$ gives

$$\begin{aligned}(E_k^{(0)} - E_n^{(0)})c_{n,k} &= E_n^{(1)}\delta_{k,n} - H_{1kn},\\ c_{n,k} &= \begin{cases}\frac{H_{1kn}}{E_n^{(0)}-E_k^{(0)}}, & k \neq n\\ 0 & k = n,\end{cases}\\ E_n^{(1)} &= H_{1nn},\end{aligned} \tag{4}$$

   where $H_{1mn} = \langle\psi_m^{(0)}|H_1|\psi_n^{(0)}\rangle$.

2. *Second order:* We now write $|\psi_n^{(2)}\rangle = \sum_k d_{n,k}|\psi_k^{(0)}\rangle$ and project the third equation of (3) on $\langle\psi_k^{(0)}|$,

$$(E_k^{(0)} - E_n^{(0)})d_{n,k} = E_n^{(1)}c_{n,k} + E_n^{(2)}\delta_{k,n} - \sum_\ell H_{1k\ell}c_{n,\ell} \tag{5}$$

   The case $k = n$, using $c_{n,n} = 0$ gives

$$E_n^{(2)} = \sum_\ell \frac{|H_{1n\ell}|^2}{E_n^{(0)} - E_\ell^{(0)}} \tag{6}$$

   and we find

$$d_{n,k} = \begin{cases}-\frac{H_{1nn}H_{1kn}}{(E_n^{(0)}-E_k^{(0)})^2} + \frac{1}{E_n^{(0)}-E_k^{(0)}}\sum_\ell \frac{H_{1k\ell}H_{1\ell n}}{E_n^{(0)}-E_\ell^{(0)}}, & k \neq n\\ 0 & k = n.\end{cases} \tag{7}$$

These corrections are small as long as

$$\begin{aligned}g\langle\psi_n^{(0)}|H_1|\psi_n^{(0)}\rangle &\ll E_n^{(0)}\\ g|\langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle| &\ll |E_n^{(0)} - E_k^{(0)}|.\end{aligned} \tag{8}$$

The first equation indicates that perturbation should be smaller than H_0 in the diagonal, a conditions which is compatible with classical expectations. But the second inequality states an upper bound for the off-diagonal matrix elements of the perturbation which, it is a genuine quantum bound.

Is the perturbation expansion convergent? Though the inequalities (8) can be satisfied for sufficiently small g the perturbation series are usually non-convergent due to the fast increasing coefficients of the power series. Consider for instance an anharmonic oscillators, defined by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 + \frac{g}{4!}x^4. \tag{9}$$

The basic assumption of perturbation expansion is that the eigenvalues and the eigenvectors are analytical at $g = 0$. But this is usually not the case because analyticity shows up on a complex plane rather than on a line. In fact, the power series (1) should be considered for complex g and their converge domain is $|g| < g_c$, g_c being the convergence radius. In other words, if a series is analytic at $g = 0$ then there is a neighborhood of $g = 0$ on the complex g-plane where it is convergent. But the Hamiltonian is unbounded form below for negative coupling constant, $g < 0$ and the physics is radically different from the positive coupling constant case, whatever close a real g is to zero. The perturbation series of quantum systems is at most asymptotic, meaning that the error of the truncation of the series at the order n can be bounded by the $n+1$-th order contribution. But a fundamental problem arises even in this case: Though the higher order contribution tend to be smaller at the beginning but the successive orders become large after the order around $1/g$. Therefore there is a maximal accuracy in perturbation expansion and it is reached around the order $1/g$.

B. Degenerate perturbation

The second condition of (8) is violated if the unperturbed Hamiltonian is degenerate. Let us now suppose that we have an N-dimensional degeneracy, $E_k^{(0)} = E_\ell^{(0)}$ for $1 \leq k, \ell \leq N$ $|\psi_k^{(0)}\rangle$. The problem is that H_0 is diagonal in any base, chosen within the degenerate subspace. But this arbitrariness is not present anymore for $g \neq 0$, in other word the eigenvectors are not continuous functions of g at $g = 0$. The continuity at $g = 0$ can be regained by using the appropriate basis where the perturbation is diagonal. However this is a useful procedure only if the degenerate subspace has low dimension.

We use therefore the unperturbed base, $|\psi_k^{(0)}\rangle$, where the perturbation is diagonal in the degenerate subspace,

$$H_1 = \begin{pmatrix} \begin{pmatrix} H_{1\ 1,1} & 0 & \cdots & 0 \\ 0 & H_{1\ 2,2} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & H_{1\ N,N} \end{pmatrix} & B \\ B^\dagger & H_1' \end{pmatrix}, \tag{10}$$

and suppose for the sake of simplicity that $H_{1\ j,j} \neq H_{1\ k,k}$ for $j \neq k$. We include the diagonal

submatrix of eq. (10) into the unperturbed Hamiltonian,

$$H_0 \to H_0 + \begin{pmatrix} \begin{pmatrix} H_{1\ 1,1} & 0 & \cdots & 0 \\ 0 & H_{1\ 2,2} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & H_{1\ N,N} \end{pmatrix} & 0 \\ 0 & 0 \end{pmatrix}, \qquad H_1 \to \begin{pmatrix} 0 & B \\ B^\dagger & H_1' \end{pmatrix}, \tag{11}$$

and the perturbation expansion is now well defined, having no degeneracy in the unperturbed Hamiltonian. The eigenvalue a of a matrix A satisfies the eigenvalue condition $A|\psi\rangle = a|\psi\rangle$ which can be writen as $(A - a\mathbb{1})|\psi\rangle = 0$ showing that the spectrum of A consists of the set of the solutions of the characteristic equation $\det(A - a\mathbb{1}) = 0$. Hence the first order shift of the eigenvalue within the degenerate subspace of the orignal H_0 are determined by the characteristic equation

$$\det[H_{1\ k\ell} - \delta_{k,\ell} E_k^{(1)}] = 0. \tag{12}$$

The solution is

$$E_k^{(1)} = H_{1\ kk} \tag{13}$$

in the basis where the perturbation is diagonal. The higher orders give the corrections

$$\begin{aligned} |\psi_k\rangle &= |\psi_k^{(0)}\rangle + \mathcal{O}(g) \\ E_k &= E_k^{(0)} + gH_{1kk} + \mathcal{O}(g^2) \end{aligned} \tag{14}$$

by the blocks B and H_1'.

The increased sensitivity of the eigenfunctions on perturbations when the unperturbed Hamiltonian becomes degenerate is a genuine quantum effect without analogy in classical physics. It shows that weak interactions are important if the unperturbed Hamiltonian is exactly or even approximately degenerate. To understand the dynamical role of the density of the excitation spectrum let us call a system rigid or soft when the typical level spacing above the ground state is large or small, compared to the characteristic energy of its environment, e.g. the thermal energy. The ground state of a soft system is easy to excite. Each excited state is orthogonal to the others thus the interaction with its environment orthogonalizes quickly the state of a soft system. The states of a rigid system change more slowly. The orthogonal states are completely different thus a system with denser excitation spectrum is brought into a completely different state easier by its interaction with the environment. Stated in terms of the observables, a soft system displays larger fluctations than a rigid one as its interacts with its environment.

Let us now consider for the sake of an example the interaction of a microscopic system with a macroscopic one, say an atom inserted into a gas in which the interaction among the gas particles is negligible. The particle of mass m, confined into an interval of size L has a typical level spacing $\Delta E \sim \hbar^2/mL^2$ in the kinetic energy. Hence am ideal gas, occupying a larger volume, is softer and a weak interaction can produce a stronger response from it. The perturbation expansion in the atom-gas interaction ceases to be applicable if the typical ratios are not small,

$$\frac{gH_{1kn}}{\frac{\hbar^2}{mL^2}} \sim 10^{54} mL^2 gH_{1kn} > 1 \tag{15}$$

in CGS units where the m and L have to be expressed in units of gram and centimeter. Therefore extremely weak couplings lead to nonperturbative interactions in macroscopic systems and the interaction between a microscopic and a macroscopic systems is never weak. This is the mechanism which generates the classical limit in quantum mechanics. The relaxation and the establishment of equilibrium, basic assumptions in statistical physics, can be seen by degenerate perturbation expansion in the interaction between blocks with local equilibrium in the thermodynamical limit, as well.

C. Time dependent perturbations

We turn to the case when the perturbation is time dependent,

$$H = H_0 + gH_1(t), \tag{16}$$

and the perturbation is localized in time as shown in Fig. 1. We furthermore assume that the initial condition is

$$|\psi(t = -\infty)\rangle = |\psi_n^{(0)}\rangle, \tag{17}$$

and seek the transition probability

$$P_{n\to k}(t) = |\langle\psi_k^{(0)}|\psi(t)\rangle|^2, \tag{18}$$

generated by the interactions between two unperturbed, asymptotic stationary state $|\psi_n^{(0)}\rangle \to |\psi_k^{(0)}\rangle$ at time t.

We write the time dependent state as

$$|\psi(t)\rangle = \sum_k c_k(t)|\psi_k^{(0)}(t)\rangle \tag{19}$$

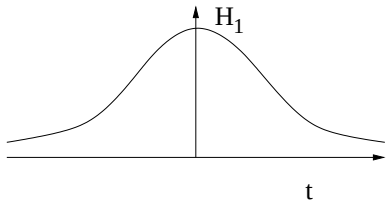


FIG. 1: Typical time dependence of the perturbation.

where the unperturbed state carries the time evolution, generated by H_0,

$$i\hbar\partial_t|\psi_k^{(0)}(t)\rangle = H_0|\psi_k^{(0)}(t)\rangle. \tag{20}$$

It is advantageous to use the eigenstate,

$$H_0|\psi_k^{(0)}(0)\rangle = E_k^{(0)}|\psi_k^{(0)}(0)\rangle, \tag{21}$$

giving rise to time evolution

$$|\psi_k^{(0)}(t)\rangle = e^{-i\frac{t}{\hbar}E_k^{(0)}}|\psi_k^{(0)}(0)\rangle. \tag{22}$$

This is sometime called interaction representation because the time dependence of the total Hamiltonian is distributed in such a manner in the state (19) that the unperturbed state evolves with H_0 and the perturbation generates the time dependence for $c_k(t)$.

The Schrödinger equation

$$i\hbar\partial_t|\psi(t)\rangle = [H_0 + gH_1(t)]|\psi(t)\rangle \tag{23}$$

now reads as

$$i\hbar\sum_k(\partial_t c_k(t)|\psi_k^{(0)}(t)\rangle + c_k(t)\partial_t|\psi_k^{(0)}(t)\rangle) = [H_0 + gH_1(t)]|\sum_k c_k(t)|\psi_k^{(0)}(t)\rangle. \tag{24}$$

Since $i\hbar\partial_t|\psi_k^{(0)}(t)\rangle = H_0|\psi_k^{(0)}(t)\rangle$ the projection of this equation on $\langle\psi_\ell^{(0)}|$ gives

$$i\hbar\partial_t c_\ell(t) = g\sum_k\langle\psi_\ell^{(0)}(t)|H_1(t)|\psi_k^{(0)}(t)\rangle c_k(t) = g\sum_k H_{1\ell k}(t)c_k(t). \tag{25}$$

We assume the power series

$$c_\ell(t) = \sum_k g^k c_\ell^{(k)}(t) \tag{26}$$

and find

$$\begin{aligned}\mathcal{O}\left(g^0\right):&\ i\hbar\partial_t c_\ell^{(0)}(t) = \ 0,\\ \mathcal{O}\left(g^m\right):&\ i\hbar\partial_t c_\ell^{(m)}(t) = \ \sum_k H_{1\ell k}(t)c_k^{(m-1)}(t).\end{aligned} \tag{27}$$

The solution, satisfying the initial condition $c_k^{(0)} = \delta_{k,n}$ is

$$c_k(t) = \underbrace{\delta_{k,n}}_{c_k^{(0)}} \underbrace{- \frac{ig}{\hbar} \int_{-\infty}^{t} dt' H_{1kn}(t')}_{c_k^{(1)}} + \mathcal{O}\left(g^2\right). \tag{28}$$

We assume for the sake of simplicity the form $H_1(t) = f(t)H'$, where $f(t)$ is a c-number function and H' is an operator,

$$H_{1\ell k}(t) = e^{i\frac{t}{\hbar}E_\ell^{(0)}} \langle \psi_\ell^{(0)}(0)|H'|\psi_k^{(0)}(0)\rangle e^{-i\frac{t}{\hbar}E_k^{(0)}} f(t) = H'_{\ell k} e^{i\omega_{\ell k}t} f(t) \tag{29}$$

with $\hbar\omega_{\ell k} = E_\ell^{(0)} - E_k^{(0)}$ and $H'_{\ell k} = \langle \psi_\ell^{(0)}(0)|H'|\psi_k^{(0)}(0)\rangle$. The leading order solution (28),

$$c_k(t) = \delta_{k,n} - \frac{igH'_{kn}}{\hbar} \int_{-\infty}^{t} dt' f(t') e^{i\omega_{k,n}t'} + \mathcal{O}\left(g^2\right), \tag{30}$$

gives the transition probability

$$P_{n(\neq k)\to k}(t) = |c_k(t)|^2 = \left|\frac{gH'_{kn}}{\hbar}\right|^2 \left|\int_{-\infty}^{t} dt' f(t') e^{i\omega_{kn}t'}\right|^2 + \mathcal{O}\left(g^3\right). \tag{31}$$

We consider now and important example, when a sinusoidal perturbation is turned on suddenly,

$$f(t) = \begin{cases} 2\cos\omega t, & \omega > 0 \quad t > 0 \\ 0 & t < 0, \end{cases}. \tag{32}$$

Such a perturbation is not of the type, shown in Fig. 1 but we can always assume that the external perturbation is turned off after observation, $f(t') = 0$ for $t' > t$ without changing the transition amplitude to justify the use of unperturbed stationary states in Eqs. (17)-(18). The expression (30) of the transition amplitude gives

$$\begin{aligned} c_k &= -\frac{igH'_{kn}}{\hbar} \int_0^t dt' e^{i\omega_{k,n}t'} \left(e^{i\omega t'} + e^{-i\omega t'}\right) \\ &= -\frac{gH'_{kn}}{\hbar} \left(\frac{e^{i(\omega_{k,n}-\omega)t} - 1}{\omega_{k,n} - \omega} + \frac{e^{i(\omega_{k,n}+\omega)t} - 1}{\omega_{k,n} + \omega}\right) \end{aligned} \tag{33}$$

for $k \neq n$. The trigonometrical identity

$$e^{i\phi} - 1 = e^{i\frac{\phi}{2}} \left(e^{i\frac{\phi}{2}} - e^{-i\frac{\phi}{2}}\right) = 2ie^{i\frac{\phi}{2}} \sin\frac{\phi}{2}, \tag{34}$$

can be used to arrive at

$$c_k = -\frac{2igH'_{k,n}}{\hbar} \left(\frac{e^{\frac{i}{2}(\omega_{kn}-\omega)t} \sin\frac{\omega_{kn}-\omega}{2}t}{\omega_{kn} - \omega} + \frac{e^{\frac{i}{2}(\omega_{kn}+\omega)t} \sin\frac{\omega_{kn}+\omega}{2}t}{\omega_{kn} + \omega}\right). \tag{35}$$

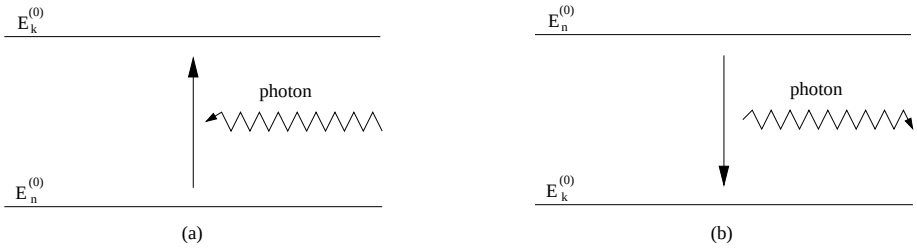


FIG. 2: (a): absorption: $P^-_{n\to k} = P(n+\gamma \to k)$, (b): emission: $P^+_{n\to k} = P(n \to k+\gamma)$

Let us now look closer at the transition amplitude in case of a perturbation whose frequency is in the vicinity of an unperturbed frequency difference, $\omega \approx |\omega_{kn}|$. The dominant part of the transition is

$$P \approx \begin{cases} P^+ & \omega_{kn} > 0 \text{ (absorption)}, \\ P^- & \omega_{kn} < 0 \text{ (emission)}, \end{cases} \tag{36}$$

c.f. Fig. 2, where

$$P^\pm_{n\to k} = \frac{4g^2|H'_{k,n}|^2}{\hbar^2(\omega_{kn} \mp \omega)^2} \sin^2 \frac{1}{2}(\omega_{kn} \mp \omega)t. \tag{37}$$

The asymptotic expressions for small and large t are

$$\begin{aligned} t \approx 0: \; P^\pm_{n\to k} &= t^2 \frac{|gH'_{kn}|^2}{\hbar^2} \\ t \to \infty: \; w^\pm_{n\to k} &= \frac{P^\pm_{n\to k}}{t} = \frac{2\pi|gH'_{kn}|^2}{\hbar^2}\delta(\omega_{kn} \mp \omega) \end{aligned} \tag{38}$$

where the representation

$$\delta(x) = \frac{2}{\pi} \lim_{\eta\to\infty} \frac{\sin^2 \frac{\eta x}{2}}{\eta x^2}. \tag{39}$$

of the Dirac-delta is used.

D. Non-exponential decay rate

One hears often that a radiactive nucleus decays with exponentially decreasing probaility in time. Let us have a closer look on the time dependence of the decay of an unstable state. We suppose that the system starts in the state $|\psi_{in}\rangle$ at $t = 0$. It is important to keep in mind that $|\psi_{in}\rangle$ is not a stationary state of the Hamiltonian H. This state evolves as

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi_{in}\rangle \tag{40}$$

hence the probability to preserve the initial state at time t is

$$P_0(t) = |A(t)|^2 \tag{41}$$

where the initial state persistence amplitude is

$$A(t) = \langle\psi_{in}|e^{-\frac{i}{\hbar}Ht}|\psi_{in}\rangle. \tag{42}$$

The decay of the probability is usually not exponential and display short, intermediate and long time regimes.

Short time regime: The expansion of the persistence amplitude for short time gives

$$A(t) = 1 - \frac{it}{\hbar}\langle\psi_{in}|H|\psi_{in}\rangle - \frac{t^2}{2\hbar^2}\langle\psi_{in}|H^2|\psi_{in}\rangle + \mathcal{O}\left(t^3\right) \tag{43}$$

and

$$\begin{aligned} P_0(t) &= 1 + \frac{t^2}{\hbar^2}\langle\psi_{in}|H|\psi_{in}\rangle^2 - \frac{t^2}{\hbar^2}\langle\psi_{in}|H^2|\psi_{in}\rangle + \mathcal{O}\left(t^3\right) \\ &= 1 - \frac{t^2}{t_Z^2} + \mathcal{O}\left(t^3\right), \end{aligned} \tag{44}$$

cf. the first equation in (38), where the Zeno time is defined by

$$t_Z = \frac{\hbar}{\sqrt{\langle\psi_{in}|(H - \langle\psi_{in}|H|\psi_{in}\rangle)^2|\psi_{in}\rangle}}. \tag{45}$$

Therefore the decay probability is parabolic for short time.

Intermediate time regime: One can easily find the source of the deviation from the expected exponential decay law. For this end we introduce the projection operator on the initial state, $L = |\psi_{in}\rangle\langle\psi_{in}|$ with $\langle\psi_{in}|\psi_{in}\rangle = 1$, and on its transverse subspace, $T = \mathbb{1} - L$, and write the state at time t as

$$\begin{aligned} |\psi(t)\rangle &= (\underbrace{L + T}_{\mathbb{1}})e^{-\frac{i}{\hbar}Ht}|\psi_{in}\rangle \\ &= |\psi_{in}\rangle A(t) + |\phi(t)\rangle, \end{aligned} \tag{46}$$

where the orthogonality

$$\langle\psi_{in}|\phi(t)\rangle = 0 \tag{47}$$

holds by construction. The vector $|\phi(t)\rangle$ stands clearly for the decay product. Applying the time evolution operator $e^{-\frac{i}{\hbar}Ht'}$ on eq. (46) and projecting it onto $\langle\psi_{in}|$ we find

$$A(t + t') = A(t)A(t') + \langle\psi_{in}|e^{-\frac{i}{\hbar}Ht'}|\phi(t)\rangle. \tag{48}$$

The last term is non-vanishing if the decay product at time t does not remain orthogonal to the initial state, in other words when the decay product, $\phi(t)\rangle$, evolves back to the undecayed state. Eq. (48) displays an interference pattern in the persistence amplitude: The system is in the undecayed state at time $t+t'$ either when it is undecayed at time t or when it has already decayed at time t but gets re-exited. In the absence of the latter process the functional equation $A(t+t') = A(t)A(t')$ has only a two-parameter family of solution within the set of continuous functions, $A(t) = A(0)e^{-t/\tau}$, and the decay is exponential. The evolution of the decay product back to the undecayed state is responsible for the deviation from the exponential decay. The perturbative result, Eqs. (38) are consistent with these features.

It it worthwhile noting that the time evolution, generated by a Hermitian Hamiltonian always regenerates the undecayed state at least partially. In fact, the relation $H^\dagger = H$ shows that the leading order contribution to the transition probability, (37), is symmetric with respect to $n \leftrightarrow k$ and $P^+ \leftrightarrow P^-$, the exchanges of the initial and final states. Genuine irreversibility, non-unitary time evolution is needed to recover the experimentally well established exponential decays. For this end one has to take into account the environment of the quantum systems, a complication not addressed here.

We may gain another view of this problem by inspecting the dependence of the decay on the structure of the initial state, in particular the spread of its energy. Let us write the initial state as

$$|\psi_{in}\rangle = \sum_n |n\rangle\langle n|\psi_{in}\rangle, \tag{49}$$

where $H|n\rangle = E_n|n\rangle$. The persistence amplitude is of the form

$$A(t) = \sum_n |\langle n|\psi_{in}\rangle|^2 e^{-\frac{i}{\hbar}E_n t}. \tag{50}$$

We write this sum as an integral over the energy, weighted by the spectral function,

$$A(t) = \int dE \rho(E) e^{-\frac{i}{\hbar}Et}, \tag{51}$$

where

$$\rho(E) = \sum_n |\langle n|\psi_{in}\rangle|^2 \delta(E - E_n). \tag{52}$$

The persistence amplitude $A(t)$ and the spectral weight $\rho(E)$ are related by Fourier transformation and satisfy an "uncertainty relation", their width are inversely proportional. There is no universal decay law, however a partial resummation of the perturbation series in QED leads to the natural

line width of atomic spectra, a Lorentzian spectral weight

$$\rho(E) = \frac{\Delta E}{\pi[(E-E_0)^2 + \Delta E^2]}, \tag{53}$$

and yields exponential decay,

$$A(t) = e^{-i\frac{E_0}{\hbar}t} e^{-\frac{\Delta E}{\hbar}|t|}. \tag{54}$$

Long time regime: The decay is slower than exponential for long time. This is due to the boundedness of the Hamiltonian from below, $\rho(E) = 0$ for $E < E_0$. In fact, such a shrunk of the support of $\rho(E) = 0$ generates a spread of its Fourier transform, $A(t)$.

E. Quantum Zeno-effect

Zeno (b. Elea, 488BC) argued that Achilles can not pass a tortoise since whenever he reaches the location of tortoise the animal has already moved further. There is a quantum version of the Zeno effect, an closed unstable system never decays if continuously observed.

The quantum Zeno effect is at short time, in the parabolic decay regime. Let us suppose that we observe the system n times, distributed uniformly in time t, at times $j\Delta t$, $\Delta t = t/n$, $j = 1, \ldots, n$. The Schrödinger equation is local in time hence the eventual decay of the system, observed periodically, is generated independently at each observation. Therefore the probability of not having decay at time t is

$$P_0(t) = P_0^n(\Delta t), \tag{55}$$

what we can write as

$$\begin{aligned} P_0(t) &= \left[1 - \left(\frac{t}{nt_Z}\right)^2 + \mathcal{O}\left(n^{-3}\right)\right]^n \\ &= e^{n\ln[1-(\frac{t}{nt_Z})^2 + \mathcal{O}\left(n^{-3}\right)]} \to 1 \end{aligned} \tag{56}$$

where Eq. (44) was used in the first equation and the limit $n \to \infty$ was carried at the end. The continuously monitored radioactive atom does not decay, the undecayed state is completely regenerated by the collapse of the wave function, following the frequent observations: The wave function has no time to spread the latter being an $\mathcal{O}\left(\Delta t^2\right)$ effect.

F. Time-energy uncertainty principle

The algebraic derivation of the uncertainty principle starts with the commutation relation $[A, B] = iC$, A, B and C being observables. We first shift the observables as $A_0 = A - \langle A \rangle$

where the expectation value is $\langle A\rangle = \mathrm{Tr}\rho A$ and ρ denotes the density matrix, cf. Appendix A. The uncertainty of the observable A is defined as $\Delta A^2 = \langle A_0^2\rangle = \langle A^2\rangle - \langle A\rangle^2$. Then the inequality $\langle OO^\dagger\rangle = \mathrm{Tr}\rho OO^\dagger \geq 0$ is used for $O = A_0 + ixB_0$ for real x,

$$\langle OO^\dagger\rangle = \langle A_0^2\rangle - ix\langle [A_0, B_0]\rangle + x^2\langle B_0^2\rangle \geq 0. \tag{57}$$

The inequality holds at the minimum, $x = x_{min} = -\frac{\langle C\rangle}{2\langle B_0^2\rangle}$, where $[A_0, B_0] = iC$ hence

$$\Delta A\Delta B \geq \frac{1}{2}|\langle C\rangle|. \tag{58}$$

There is another, qualitative argument for the Heisenberg uncertainty principle, $\Delta x\Delta p \geq \frac{\hbar}{2}$, based on the Fourier transformation. It goes by comparing the absolute magnitude of wave function of a Gaussian wave packet,

$$\psi(x) = \int \frac{dk}{2\pi} e^{ikx - \frac{k^2}{2\sigma^2}} = \frac{\sqrt{2\pi}}{\sigma} e^{-\frac{\sigma^2 x^2}{2}} \tag{59}$$

in coordinate and momentum space and defining the width, the uncertainty of the Gaussian $e^{-\frac{x^2}{2\Delta x^2}}$ by Δx.

The latter, more intuitive argument can be generalized for time and energy, as well, $\Delta t\Delta E \geq \frac{\hbar}{2}$ without algebraic derivation because the time remains a c-number in quantum mechanics. But there is nevertheless an intuitive argument to support such kind of uncertainty principle. Let us start with the inequality

$$\Delta A\Delta H \geq \frac{1}{2}|\langle [A, H]\rangle|, \tag{60}$$

for a time independent observable A and the Hamiltonian H, written as

$$\Delta A\Delta H \geq \frac{\hbar}{2}\left|\frac{d}{dt}\langle A\rangle\right|, \tag{61}$$

due to

$$\frac{d}{dt}\langle\psi(t)|A|\psi(t)\rangle = i\hbar\langle\psi(t)|[A, H]|\psi(t)\rangle. \tag{62}$$

Therefore we can interpret

$$\tau_A = \frac{\Delta A}{|\frac{d}{dt}\langle A\rangle|} \tag{63}$$

as the characteristic time scale of the expectation value of A, representing the inequality (60) as

$$\tau_A\Delta H \geq \frac{\hbar}{2}. \tag{64}$$

Such a reciprocal uncertainty can be understood qualitatively in the following manner. The measurement of the energy of a stationary state consists of the determination of the period length of an oscillatory phase and it is obvious that the knowledge of the period length of function is more precise if the function is known over a longer interval.

The transition probability (37) provides another support of the time-energy uncertainty relation. The point is that as we move away from the resonance the transition probability is vanishing first at

$$|\omega \pm \omega_{k,n}| = \frac{2\pi}{t}. \tag{65}$$

In other words, the estimate of the energy levels of the system by analyzing the transition probability at time t comes with an error ΔE, satisfying

$$\Delta E t \approx 2\pi\hbar. \tag{66}$$

G. Fermi's golden rule

It happens frequently that the system makes transition between a state in the continuous part of the spectrum and a discrete state, eg. absorption of energy from the radiation field, followed by the ionization an atom or molecule. It is assumed that the final states in the continuum differ macroscopically and are decohered. As a result the interference term among them is negligible and the transition probability can be written as an integral over the continuous spectrum,

$$P_{\text{cont.}\leftarrow\text{discr.}} = \int dE g(E) \frac{|gH_{\text{cont.,discr.}}|^2}{\hbar^2} \frac{4\sin^2 \frac{1}{2}(\omega_{\text{cont.,discr.}} \pm \omega)t}{(\omega_{\text{cont.,discr.}} \pm \omega)^2}, \tag{67}$$

over the where $g(E)$ is the spectral density function, giving the number of state in an energy interval $[E, E+\Delta E]$, as $dN = dEg(E)$. The change of integration variable, $\beta = \frac{1}{2}(\omega_{\text{cont.,discr.}} \pm \omega)t$, $d\beta = dE\frac{t}{2\hbar}$ leads to the integral

$$P_{\text{cont.}\leftarrow\text{discr.}} = \frac{2t}{\hbar} \int d\beta g(E) |gH_{\text{cont.,discr.}}|^2 \frac{\sin^2\beta}{\beta^2}. \tag{68}$$

This integral can be approximated by assuming that the time t is large enough to keep the density of state, $g(E)$, approximately constant when the energy E is changed by the order of magnitude $\Delta E = \hbar/t$. The result is Fermi's golden rule.

$$P_{\text{cont.}\leftarrow\text{discr.}} \approx t\frac{2\pi}{\hbar} g(E) |gH_{\text{cont.,discr.}}|^2, \tag{69}$$

since

$$\int_{-\infty}^{\infty} d\beta \frac{\sin^2\beta}{\beta^2} = \pi. \tag{70}$$

II. ROTATIONS

The implementation of the rich details of a three-dimensional dynamics requires the introduction of new, more sophisticated tools compared to one-dimensional systems. Some of the new issues are related to rotations hence we now turn to a detailed, technical discussion of the we way rotations are realized in the Hilbert space of states.

We start with translation, being more simple and already containing several aspects of the problem. The lesson, learned there, will help to embark the more complex issues of rotations.

A. Translations

1. Translation are carried out in classical physics at the level of the coordinates as

$$\boldsymbol{r} \to T(\boldsymbol{a})\boldsymbol{r} = \boldsymbol{r} + \boldsymbol{a}. \tag{71}$$

2. Functions defined in space, like (probability)distribution functions transforms as

$$f(\boldsymbol{r}) \to f'(\boldsymbol{r}') = f(\boldsymbol{r}' - \boldsymbol{a}). \tag{72}$$

3. Translation are represented in the Hilbert space by operators, acting on the wave function,

$$\psi(\boldsymbol{r}) \to U(T(\boldsymbol{a}))\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} - \boldsymbol{a}). \tag{73}$$

4. Note that for each translation $T(\boldsymbol{a})$ we find now an operator, $U(T(\boldsymbol{a}))$. The mapping $T(\boldsymbol{a}) \to U(T(\boldsymbol{a}))$ is called representation of translation if it preserves the algebraic structure, namely

$$U(T(\boldsymbol{a}))U(T(\boldsymbol{b}))\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} - \boldsymbol{a} - \boldsymbol{b}) = U(T(\boldsymbol{a} + \boldsymbol{b}))\psi(\boldsymbol{r}) \tag{74}$$

5. Translations preserve the scalar product,

$$\int d\boldsymbol{x}\psi^*(\boldsymbol{x} - \boldsymbol{a})\phi(\boldsymbol{x} - \boldsymbol{a}) = \int d\boldsymbol{x}\psi^*(\boldsymbol{x})\phi(\boldsymbol{x}) \tag{75}$$

   thus the operator $U(T)$ is unitary, $U(T)U^\dagger(T) = \mathbb{1}$, we speak of a unitary representation of translation.

6. Infinitesimal translations are of the form

$$\begin{aligned} \boldsymbol{r} &\to \boldsymbol{r} + \delta\boldsymbol{r} \\ \psi(\boldsymbol{r}) &\to \psi(\boldsymbol{r}) - \delta\boldsymbol{r}\boldsymbol{\nabla}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}) - \frac{i}{\hbar}\delta\boldsymbol{r}\vec{G}\psi(\boldsymbol{r}) \end{aligned} \tag{76}$$

   and $\vec{G} = \frac{\hbar}{i}\boldsymbol{\nabla} = \boldsymbol{p}$ is called the generator of translations.

7. Finite translations are represented by $U(\boldsymbol{a}) = e^{-\frac{i}{\hbar}\boldsymbol{ap}}$ on analytical functions according to Taylor expansion,

$$\psi(\boldsymbol{r}) \;\rightarrow\; \psi(\boldsymbol{r}-\boldsymbol{a}) = \sum_{n=0}^{\infty} \frac{(-\boldsymbol{a}\boldsymbol{\nabla})^n}{n!}\psi(\boldsymbol{r}) = e^{-\boldsymbol{a}\boldsymbol{\nabla}}\psi(\boldsymbol{r}) = e^{-\frac{i}{\hbar}\boldsymbol{ap}}\psi(\boldsymbol{r}). \tag{77}$$

B. Rotations

1. Rotations act on the coordinates as

$$\boldsymbol{r} \rightarrow R_{\boldsymbol{n}}(\alpha)\boldsymbol{r} \tag{78}$$

is given by a 3x3 orthogonal matrix where $\boldsymbol{n}$ stands for the axis of the rotation and α denotes the angle of the rotation, $R_{\boldsymbol{n}}^{-1}(\alpha) = R_{\boldsymbol{n}}(-\alpha) = R_{\boldsymbol{n}}^{\mathrm{tr}}(\alpha)$, e.g.

$$R_{\boldsymbol{z}}(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{79}$$

It is easy to find a relation among rotation matrices with different rotation axes, say $R_{\boldsymbol{u}}(\alpha)$ and $R_{\boldsymbol{v}}(\alpha)$. If the rotation A which connects the two axes, $\boldsymbol{v} = A\boldsymbol{u}$, then the the equation

$$R_{\boldsymbol{v}}(\alpha) = AR_{\boldsymbol{u}}(\alpha)A^{-1} \tag{80}$$

follows. In fact, the right hand side, being the product or rotational matrices is itself a rotation. As such, it has one eigenvector with eigenvalue 1, the axis or rotation. The relation $AR_{\boldsymbol{u}}(\alpha)A^{-1}\boldsymbol{v} = AR_{\boldsymbol{u}}(\alpha)\boldsymbol{u} = A\boldsymbol{u} = \boldsymbol{v}$ establishes that this axis is $\boldsymbol{v}$. The argument α is the same on both sides because the matrices A and A^{-1} perform a basis transformation which does not change the angle of rotation. Since the z axis is usually chosen as quantization axis eq. (80) is frequently used as $R_{\boldsymbol{n}}(\alpha) = AR_z(\alpha)A^{-1}$ with $\boldsymbol{n} = A\boldsymbol{z}$.

2. Functions defined in the space transform as

$$f(\boldsymbol{r}) \rightarrow U(R)f(\boldsymbol{r}) = f(R^{-1}\boldsymbol{r}). \tag{81}$$

3. The rotation changes the quantum state as

$$\psi(\boldsymbol{r}) \rightarrow U(R)\psi(\boldsymbol{r}) = \psi(R^{-1}\boldsymbol{r}). \tag{82}$$

4. The algebraic structure of the rotation group is preserved,

$$\begin{aligned} U(R)U(R')\psi(\boldsymbol{r}) &= U(R)\psi(R'^{-1}\boldsymbol{r}) \\ &= \psi(R'^{-1}R^{-1}\boldsymbol{r}) \\ &= \psi((RR')^{-1}\boldsymbol{r}) \\ &= U(RR')\psi(\boldsymbol{r}), \end{aligned} \tag{83}$$

therefore the operator $U(R)$ represent the rotation group in the space of states, $U(R)U(R') = U(RR')$.

5. The scalar product is conserved,

$$\int d\boldsymbol{x}\psi^*(R\boldsymbol{x})\phi(R\boldsymbol{x}) = \int d\boldsymbol{x}\psi^*(\boldsymbol{x})\phi(\boldsymbol{x}), \tag{84}$$

rendering the representation unitary, $U(R)U^\dagger(R) = \mathbb{1}$.

6. Infinitesimal rotations act as

$$\begin{aligned} \boldsymbol{r} &\rightarrow \boldsymbol{r} + \epsilon\boldsymbol{n}\times\boldsymbol{r} \\ \psi(\boldsymbol{r}) &\rightarrow \psi(\boldsymbol{r}) - (\epsilon\boldsymbol{n}\times\boldsymbol{r})\boldsymbol{\nabla}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}) - \epsilon\boldsymbol{n}(\boldsymbol{r}\times\boldsymbol{\nabla})\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}) - \frac{i}{\hbar}\epsilon\boldsymbol{n}\boldsymbol{L}\psi(\boldsymbol{r}), \end{aligned} \tag{85}$$

and the angular momentum $\boldsymbol{L}$ is the generator of rotations.

7. Finite rotations can be constructed by considering the one dimensional subgroup of the rotational group, rotations around a fixed axis, $\{R_{\boldsymbol{n}}(\alpha)\}$. The generator is $\boldsymbol{n}\cdot L$ therefore

$$U(R_{\boldsymbol{n}}(\alpha)) = e^{-\frac{i}{\hbar}\alpha\boldsymbol{n}\boldsymbol{L}}. \tag{86}$$

8. The angular momentum is a vector operator, it can be transformed under rotations as a vector and as an operator and the two transformations agree. To see this we consider the 3×3 rotation matrix A, transforming the coordinate system basis vectors $\boldsymbol{n}_j = A^{-1}\boldsymbol{e}_j$ and write

$$\begin{aligned} U(R_{\boldsymbol{n}_j}(\alpha)) &= U(A^{-1}R_{\boldsymbol{e}_j}(\alpha)A) \\ &= U(A^{-1})U(R_{\boldsymbol{e}_j}(\alpha))U(A) \\ &= U(A^{-1})e^{-\frac{i}{\hbar}\alpha\boldsymbol{e}_j\boldsymbol{L}}U(A) \\ &= \sum_{n=0}^{\infty}\frac{(-\frac{i}{\hbar}\alpha)^n}{n!}U(A^{-1})(\boldsymbol{e}_j\boldsymbol{L})^nU(A) \\ &= \sum_{n=0}^{\infty}\frac{(-\frac{i}{\hbar}\alpha)^n}{n!}[U(A^{-1})\boldsymbol{e}_j\boldsymbol{L}U(A)]^n \\ &= e^{-\frac{i}{\hbar}\alpha U(A^{-1})\boldsymbol{e}_j\boldsymbol{L}U(A)}. \end{aligned} \tag{87}$$

Another way to write this operator is

$$\begin{aligned} U(R_{\boldsymbol{n}_j}(\alpha)) &= e^{-\frac{i}{\hbar}\alpha \boldsymbol{n}_j \boldsymbol{L}} \\ &= e^{-\frac{i}{\hbar}\alpha \boldsymbol{e}_j A \boldsymbol{L}} \end{aligned} \tag{88}$$

since $\boldsymbol{n}_j = A^{-1}\boldsymbol{e}_j = \boldsymbol{e}_j A$. The comparison of the two expressions yields the equation

$$A\boldsymbol{L} = U^{\dagger}(A)\boldsymbol{L}U(A), \tag{89}$$

whose left and right side reflects the vector and operator transformation rules under rotations.

C. Euler angles

Rotations are parametrized in Eq. (78) by their axis, $\boldsymbol{n}$ and the angle of rotation, α. Another parametrization is given in terms of Euler angles:

$$R_{\boldsymbol{n}}(\alpha) = R_{\boldsymbol{z}''}(\alpha)R_{\boldsymbol{y}'}(\theta)R_{\boldsymbol{z}}(\phi) \tag{90}$$

where the rotation axis,

$$\boldsymbol{n} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \tag{91}$$

is given in polar coordinates,

$$\boldsymbol{y}' = R_{\boldsymbol{z}}(\phi)\boldsymbol{y} \tag{92}$$

is the unit vector of the y direction after the rotation $R_{\boldsymbol{z}}(\phi)$ and

$$\boldsymbol{z}'' = R_{\boldsymbol{y}'}(\theta)R_{\boldsymbol{z}}(\phi)\boldsymbol{z} = R_{\boldsymbol{y}'}(\theta)\boldsymbol{z} \tag{93}$$

is the unit vector, pointing in the z axis after the rotation $R_{\boldsymbol{y}'}(\theta)R_{\boldsymbol{z}}(\phi)$. One can find another, more useful way of expressing this rotation by means of fixed axes,

$$\begin{aligned} R_{\boldsymbol{z}''}(\alpha)R_{\boldsymbol{y}'}(\theta)R_{\boldsymbol{z}}(\phi) &= \underbrace{R_{\boldsymbol{y}'}(\theta)R_{\boldsymbol{z}}(\alpha)R^{-1}_{\boldsymbol{y}'}(\theta)}_{R_{\boldsymbol{z}''}(\alpha)} R_{\boldsymbol{y}'}(\theta)R_{\boldsymbol{z}}(\phi) \\ &= \underbrace{R_{\boldsymbol{z}}(\phi)R_{\boldsymbol{y}}(\theta)R^{-1}_{\boldsymbol{z}}(\phi)}_{R_{\boldsymbol{y}'}(\theta)} R_{\boldsymbol{z}}(\alpha)R_{\boldsymbol{z}}(\phi) \\ &= R_{\boldsymbol{z}}(\phi)R_{\boldsymbol{y}}(\theta)R_{\boldsymbol{z}}(\alpha). \end{aligned} \tag{94}$$

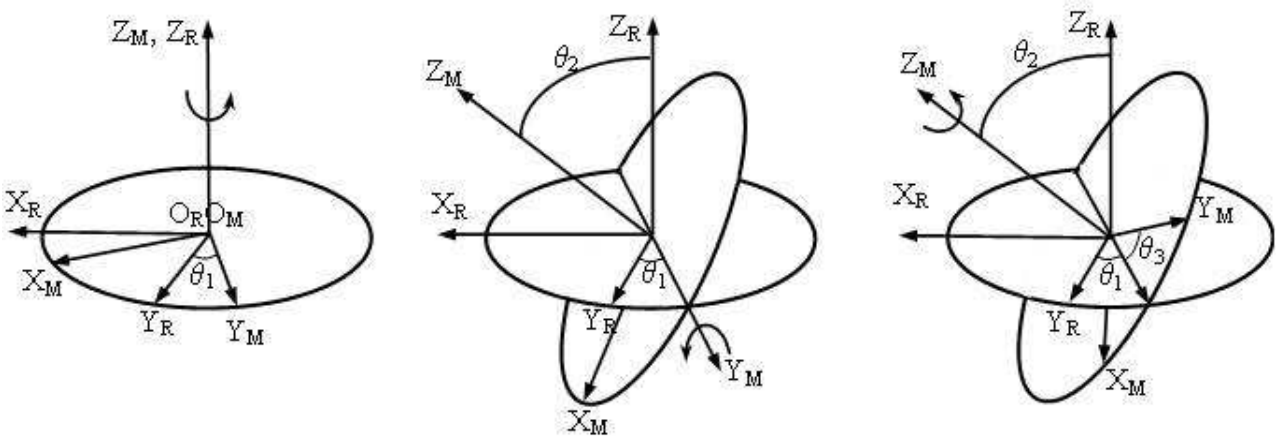


FIG. 3: The successive rotations of $R_{\boldsymbol{z}''}(\Theta_3)R_{\boldsymbol{y}'}(\Theta_2)R_{\boldsymbol{z}}(\Theta_1)$. (https://sites.google.com/site/surilvshah/eajs)

D. Summary of the angular momentum algebra

The orbital angular momentum,

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} \tag{95}$$

satisfies the commutation relations

$$[L_a, L_b] = i\hbar \sum_c \epsilon_{abc} L_c. \tag{96}$$

The operators $\{L_z, \boldsymbol{L}^2\}$ represent a maximal set of commuting operators and their eigenvalues can be used to label the basis vectors,

$$L_z|\ell, m\rangle = \hbar m|\ell, m\rangle, \quad \boldsymbol{L}^2|\ell, m\rangle = \hbar^2 \ell(\ell+1)|\ell, m\rangle, \tag{97}$$

where $\ell = 0, 1, \cdots$ and $m \in \{-\ell, -\ell+1, \cdots, \ell-1, \ell\}$, cf. Fig. 4. One introduces the ladder operators $L_\pm = L_x \pm iL_y$ with commutation relation

$$[L_z, L_\pm] = \pm\hbar L_\pm, \quad [L_+, L_-] = 2\hbar L_z \tag{98}$$

which can be used to prove the relation

$$L_\pm|\ell, m\rangle = \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}|\ell, m\pm 1\rangle. \tag{99}$$

The quantum number ℓ is not changed by the angular momentum operators, hence they are block diagonal in ℓ, $\langle \ell, m|L_a|\ell', m'\rangle = \delta_{\ell,\ell'} F_a(\ell, m, m')$. There might naturally by other quantum numbers labeling the basis vectors. What is important is that rotations can change the quantum number m only. The other, non-rotational quantum numbers will be suppressed in the rest of this chapter.

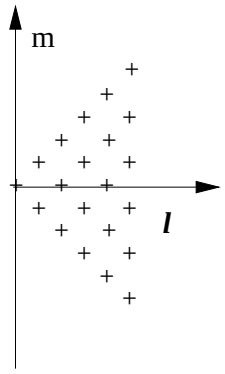


FIG. 4: The spectrum of $\boldsymbol{L}^2$ and L_z.

E. Rotational multiplets

Let us take a state $|\ell, m\rangle$ and apply a rotation,

$$\begin{aligned} e^{-\frac{i}{\hbar}\alpha \boldsymbol{n}\boldsymbol{L}}|\ell,m\rangle &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!}(\boldsymbol{n}\boldsymbol{L})^n|\ell,m\rangle \\ &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!}\left(n_z L_z + \frac{1}{2}n_+ L_- + \frac{1}{2}n_- L_+\right)^n |\ell,m\rangle \end{aligned} \tag{100}$$

where $n_\pm = n_x \pm i n_y$. According to eqs. (97)-(99) we can write

$$e^{-\frac{i}{\hbar}\alpha \boldsymbol{n}\boldsymbol{L}}|\ell,m\rangle = \sum_{-\ell\leq m'}^{\ell} c_{m'}(\alpha,\boldsymbol{n})|\ell,m'\rangle \tag{101}$$

and all coefficients are non-vanishing if $n_\pm \neq 0$. The linear space, $\mathcal{H}_\ell$, span by the vectors (100) is called rotational multiplet and possesses the following properties:

1. The set of vectors $|\ell, m\rangle$, $-\ell \leq m \leq \ell$ is a basis in $\mathcal{H}_\ell$.

2. $\mathcal{H}_\ell$ is closed with respect to rotations, $e^{-\frac{i}{\hbar}\alpha \boldsymbol{n}\boldsymbol{L}}\mathcal{H}_\ell \subset \mathcal{H}_\ell$.

3. $\mathcal{H}_\ell$ is irreducible with respect to rotations.

A linear $\mathcal{H}$ space is called reducible with respect to rotations if it can be split into the direct sum of two subspaces, $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ where each component is closed, $e^{-\frac{i}{\hbar}\alpha \boldsymbol{n}\boldsymbol{L}}\mathcal{H}_j \subset \mathcal{H}_j$, $j = 1, 2$, and non-trivial, $1 \leq dim\mathcal{H}_j$. The irreducibility of a rotational multiplet follows from the action of $L_\pm$, given by eq. (99), by noting that the rotation (100) necessarily generates all basis vectors $|\ell, m'\rangle$, of the multiplet for $n_\pm \neq 0$. A space is irreducible when it is not reducible. Property 3. states that the rotational multiplet $\mathcal{H}_\ell$ is the smallest subspace which is contains the state $|\ell, m_0\rangle$ with a given m_0 and is closed with respect to rotations.

F. Wigner's D matrix

The block diagonality in $\boldsymbol{L}$ is important because it makes the multiplets closed with respect to rotations and allows the description of rotations within each multiplet $\mathcal{H}_\ell$ separately. The action of rotations within a multiplet is described by Wigner's D matrix.

To find the D matrices we start with a resolution of one,

$$\sum_{\ell',m'} |\ell',m'\rangle\langle\ell',m'| = \mathbb{1}, \tag{102}$$

in the space of states, representing rotations. The basis vectors might be labeled by other quantum numbers, as well, which are not related to rotations and one should in principle sum over them, too. Since such a rotational invariant quantum number does not change the argument, followed below, its presence is neglected, i.e. it is assumed that each rotational multiplet occurs only once in the linear space of states. The resolution of the identity, (102), yields the expression

$$\begin{aligned} U(R)|\ell,m\rangle &= \sum_{\ell',m'} |\ell',m\rangle\langle\ell',m'|U(R)|\ell,m\rangle \\ &= \sum_{m'} |\ell,m'\rangle \mathcal{D}^{(\ell)}_{m',m}(R), \end{aligned} \tag{103}$$

for the action of a rotation on a basis vector in terms of the D matrix

$$\mathcal{D}^{(\ell)}_{m',m}(R) = \langle\ell,m'|U(R)|\ell,m\rangle. \tag{104}$$

The representation by Euler angles leads to a factorized form,

$$\begin{aligned} \mathcal{D}^{(\ell)}_{m',m}(R(\alpha,\beta,\gamma)) &= \mathcal{D}^{(\ell)}_{m',m}(R_{\boldsymbol{z}}(\alpha)R_{\boldsymbol{y}}(\beta))R_{\boldsymbol{z}}(\gamma)) \\ &= \sum_{m_1,m_2} \mathcal{D}^{(\ell)}_{m',m_1}(R_{\boldsymbol{z}}(\alpha))\mathcal{D}^{(\ell)}_{m_1,m_2}(R_{\boldsymbol{y}}(\beta))\mathcal{D}^{(\ell)}_{m_2,m}(R_{\boldsymbol{z}}(\gamma)) \\ &= e^{-i\alpha m' - i\gamma m} d^{(\ell)}_{m',m}(\beta) \end{aligned} \tag{105}$$

where the equation

$$\langle\ell,m'|e^{-i\frac{\alpha}{\hbar}L_z}|\ell,m\rangle = \mathcal{D}^{(\ell)}_{m',m}(R_{\boldsymbol{z}}(\alpha)) = \delta_{m',m}e^{-i\alpha m} \tag{106}$$

was used in the last equation and

$$d^{(\ell)}_{m',m}(\beta) = \langle\ell,m'|e^{-i\frac{\beta}{\hbar}L_y}|\ell,m\rangle \tag{107}$$

is called reduced d-matrix.

Let us consider the case of spin half where the generators, the Pauli matrices are defined by

$$\langle\frac{1}{2},m'|\boldsymbol{L}|\frac{1}{2},m\rangle=\frac{\hbar}{2}\boldsymbol{\sigma}=\frac{\hbar}{2}\left\{\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right\}. \tag{108}$$

There are two important relations, satisfied by them,

$$\sigma_a\sigma_b=\delta_{a,b}+i\sum_c\epsilon_{abc}\sigma_c \tag{109}$$

and

$$\sigma_y\boldsymbol{\sigma}\sigma_y=-\boldsymbol{\sigma}^*, \tag{110}$$

they are sufficient to handle the algebra of Pauli matrices. A simple way to write (109) is to contract the indices with two vectors, $(\boldsymbol{u}\boldsymbol{\sigma})\cdot(\boldsymbol{v}\boldsymbol{\sigma})=\mathbb{1}\boldsymbol{u}\boldsymbol{v}+i(\boldsymbol{u}\times\boldsymbol{v})\boldsymbol{\sigma}$.

Finite rotation can be described by the Pauli matrices in a specially simple manner due to the generalized Euler relation

$$\begin{aligned}e^{i\alpha\boldsymbol{n}\boldsymbol{\sigma}}&=\mathbb{1}+i\alpha\boldsymbol{n}\boldsymbol{\sigma}+\frac{(i\alpha)^2}{2!}(\boldsymbol{n}\boldsymbol{\sigma})^2+\frac{(i\alpha)^3}{3!}(\boldsymbol{n}\boldsymbol{\sigma})^3+\frac{(i\alpha)^4}{4!}(\boldsymbol{n}\boldsymbol{\sigma})^4+\cdots\\&=\mathbb{1}+i\alpha\boldsymbol{n}\boldsymbol{\sigma}+\mathbb{1}\frac{(i\alpha)^2}{2!}\boldsymbol{n}^2+\frac{(i\alpha)^3}{3!}\boldsymbol{n}^2\boldsymbol{n}\boldsymbol{\sigma}+\mathbb{1}\frac{(i\alpha)^4}{4!}\boldsymbol{n}^4+\cdots\\&=\mathbb{1}\frac{1}{2}\left(e^{i\alpha}+e^{-i\alpha}\right)+\frac{\boldsymbol{n}\boldsymbol{\sigma}}{2}\left(e^{i\alpha}-e^{-i\alpha}\right)\\&=\mathbb{1}\cos\alpha+i\boldsymbol{n}\boldsymbol{\sigma}\sin\alpha.\end{aligned} \tag{111}$$

This gives the following simple expression for the reduced d matrix:

$$\begin{aligned}d^{(\frac{1}{2})}_{m',m}(\beta)&=\langle\frac{1}{2},m'|e^{-i\frac{\beta\sigma_y}{2}}|\frac{1}{2},m\rangle=\left(\mathbb{1}\cos\frac{\beta}{2}-i\sigma_y\sin\frac{\beta}{2}\right)_{m',m},\\d^{(\frac{1}{2})}(\beta)&=\begin{pmatrix}\cos\frac{\beta}{2}&-\sin\frac{\beta}{2}\\\sin\frac{\beta}{2}&\cos\frac{\beta}{2}\end{pmatrix}.\end{aligned} \tag{112}$$

G. Invariant integration over rotations

The use of the polar coordinate system in the description of a particle in a spherical potential offers a simple separation of the degrees of freedom, related to rotations and radial motion: the polar angles follow free rotations and the radius is subject to the radial dynamical laws. In case of an N-particle system, $N\geq 2$, one can separate three collective coordinates, say the Euler angles of the rotation, connecting the laboratory and the body fixed coordinate systems, the inertial tensor being diagonal in the latter. These angles follow free rotations and the remaining $3(N-1)$

degrees of freedom describe translational motion. Our strategy to solve a dynamical problem is to extract as much information as possible from the free rotational aspects of the dynamics, allowing to concentrate our strength to the solution of the more difficult radial or translational dynamics. The coordinate space to describe the rotations is $SO(3)$ where we use the Euler angles as coordinates. However the construction of translation invariant states is highly non-trivial in curve linear coordinate system, c.f. appendix B. In order to assure that the wave function of a rotational invariant state is constant, a minimal requirement for a reasonable description of the rotational dynamics, we have to use an appropriate, invariant Haar measure in the group space.

Let us start with a single particle where the radial component of the wave function, $\chi(\theta, \phi) = \chi(\boldsymbol{n}(\theta, \phi))$, is defined on the unit sphere whose point are given by the unit vector

$$\boldsymbol{n}(\theta, \phi) = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{113}$$

The wave function $\chi(\theta, \phi) = \langle\theta, \phi|\psi\rangle$ is defined by the help of the orthogonal coordinate eigenstates with normalization

$$\langle\theta', \phi'|\theta, \phi\rangle = \frac{\delta(\theta - \theta')\delta(\phi - \phi')}{s_2(\theta, \phi)}, \tag{114}$$

where $s_2(\theta, \phi) = \sin\theta = d\Sigma/d\theta d\phi$ is the surface density of the unit sphere. In fact, the key equation, the resolution of one,

$$\mathbb{1} = \int d\Sigma|\theta, \phi\rangle\langle\theta, \phi| = \int d\theta d\phi s_2(\theta, \phi)|\theta, \phi\rangle\langle\theta, \phi|, \tag{115}$$

is assured by (114),

$$\langle\theta', \phi'|\mathbb{1}|\theta, \phi\rangle = \frac{\delta(\theta - \theta')\delta(\phi - \phi')}{s_2(\theta, \phi)}. \tag{116}$$

The wave function of the spherical symmetric state,

$$|0\rangle = \frac{1}{\sqrt{4\pi}} \int d\cos\theta d\phi|\theta, \phi\rangle, \tag{117}$$

constructed by the rotational invariant integral measure, $d\Sigma = d\cos\theta d\phi$, is $\chi(\theta, \phi) = \langle\theta, \phi|0\rangle = 1/\sqrt{4\pi}$.

The rotational dynamics takes place in the $SO(3)$ group space for several particles. (One may start with the same group space for a single particle, as well, but on has to keep in mind that we talk about spinless particle and the non-trivial rotations of the point particle located on the z axis

are reduced to $R_z(\phi)R_y(\theta)R_z(\chi) \to R_z(\phi)R_y(\theta)$.) We use the Euler angles as coordinates and seek the normalization in the scalar product

$$\langle \phi', \theta', \chi' | \phi, \theta, \chi \rangle = \frac{\delta(\phi - \phi')\delta(\theta - \theta')\delta(\chi - \chi')}{s_3(\phi, \theta, \chi)}, \tag{118}$$

where $s_3(\phi, \theta, \chi) = \sin\theta = dV/d\phi d\theta d\chi$ is the volume density of $SO(3)$, defined in a rotational invariant manner, by imposing

$$\int_V d\phi d\theta d\chi s_3(\phi, \theta, \chi) = \int_{RV} d\phi d\theta d\chi s_3(\phi, \theta, \chi), \tag{119}$$

where the integration on the left (right) hand side is over an arbitrary volume V (V rotated by an arbitrary $R \in SO(3)$). This condition can be written for an arbitrary function over $SO(3)$ as

$$\int dR f(R) = \int d(R'R) f(R) = \int dR f(R'^{-1}R), \tag{120}$$

with $dR = d\phi d\theta d\chi s_3(\phi, \theta, \chi)$. The integral measures satisfying (120) are called invariant Haar measures and can differ in a normalization constant only.

To find out the normalization $s_3(\phi, \theta, \chi)$ consider the state

$$|0\rangle = \int dR U(R)|\boldsymbol{z}\rangle = \int dR |R\boldsymbol{z}\rangle. \tag{121}$$

which is rotational invariant,

$$U(R')|\boldsymbol{u}\rangle = \int dR U(R')U(R)|\boldsymbol{u}\rangle = \int dR U(R'R)|\boldsymbol{u}\rangle = \int dR |R'R\boldsymbol{u}\rangle = |\boldsymbol{u}\rangle. \tag{122}$$

For the choice $\boldsymbol{u} = \boldsymbol{z}$ (121) simplifies to

$$\begin{aligned} |0\rangle &= \int d\phi d\theta d\chi s_3(\phi, \theta, \chi) |R(\phi, \theta, 0)\boldsymbol{z}\rangle \\ &= \int d\phi d\theta d\chi s_3(\phi, \theta, \chi) |\boldsymbol{n}(\phi, \theta)\rangle \end{aligned} \tag{123}$$

since $R_z(\chi)\boldsymbol{z} = \boldsymbol{z}$ and $R(\phi, \theta, \chi)\boldsymbol{z} = \boldsymbol{n}(\phi, \theta)$. This state is rotational invariant for $\int d\chi s_3(\phi, \theta, \chi) = s_2(\phi, \theta) = \sin\theta$. Since the invariant measure must be the same for R and R^{-1}, $R^{-1}(\phi, \theta, \chi) = R^{\mathrm{tr}}(\phi, \theta, \chi) = R(-\chi, -\theta, -\phi)$ we can take $s_3(\phi, \theta, \chi) = \sin\theta$, a choice which is unique up to a constant multiplicative factor, giving rise to $dR = d\phi d\cos\theta d\chi$. The total surface and volume, using these integral measures are

$$\begin{aligned} \int_{S_2} d\Sigma &= \int_{-1}^{1} dc \int_{-\pi}^{\pi} d\phi = 4\pi, \\ \int_{SO(3)} dR &= \int_{-1}^{1} dc \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\chi = 8\pi^2. \end{aligned} \tag{124}$$

H. Spherical harmonics

Rotations leave r fixed and change θ and ϕ only in polar coordinate system. Hence the wave function of a basis vector $|\ell, m\rangle$,

$$Y_m^\ell(\boldsymbol{n}) = \langle \boldsymbol{n}|\ell, m\rangle, \tag{125}$$

called spherical harmonics, can be considered as a function of θ and ϕ only. We shall show that spherical harmonics are solely determined by the structure of the rotation group.

Spherical harmonics can be defined by the the matrix elements of Eqs. (97),

$$\begin{aligned} L_z Y_m^\ell(\boldsymbol{n}) &= \langle \boldsymbol{n}|L_z|\ell, m\rangle = \hbar m \langle \boldsymbol{n}|\ell, m\rangle = \hbar m Y_m^\ell(\boldsymbol{n}), \\ L_\pm Y_m^\ell(\boldsymbol{n}) &= \langle \boldsymbol{n}|L_\pm|\ell, m\rangle \\ &= \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}\langle \boldsymbol{n}||\ell, m\pm 1\rangle \\ &= \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}Y_{m\pm 1}^\ell(\boldsymbol{n}). \end{aligned} \tag{126}$$

Spherical harmonics, being the eigenvectors of hermitian operators form a basis on the unit sphere. Conversely, a set of functions on the unit sphere satisfying eqs. (126) are the spherical harmonics up to a constant. The absolute magnitude of this constant is fixed by the normalization

$$1 = \int d^2 n |Y_m^\ell(\boldsymbol{n})|^2, \tag{127}$$

where the integration is over the unit sphere, $\boldsymbol{n}^2 = 1$.

The relation between the Euler angles and the polar angles is given by the equation

$$\boldsymbol{n} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} = R(\phi, \theta, \chi)\boldsymbol{z} \tag{128}$$

with $\boldsymbol{z} = (0, 0, 1)$ and χ left arbitrary. The similar rotation in the space of states,

$$|\boldsymbol{n}\rangle = U(R(\phi, \theta, \chi))|\boldsymbol{z}\rangle, \tag{129}$$

can be rewritten by inserting the resolution of unity (102) as

$$|\boldsymbol{n}\rangle = \sum_{\ell, m} U(R(\phi, \theta, \chi))|\ell, m\rangle \otimes \langle \ell, m|\boldsymbol{z}\rangle. \tag{130}$$

the projection of this equation on a basis vector $\langle \ell, m'|$ gives

$$\langle \ell, m'|\boldsymbol{n}\rangle = Y_{m'}^{\ell *}(\boldsymbol{n}) = \sum_m \mathcal{D}_{m', m}^{(\ell)}(R(\phi, \theta, \chi))\langle \ell, m|\boldsymbol{z}\rangle. \tag{131}$$

To find the last factor we consider the matrix element

$$\begin{aligned}\langle \ell, m|U(R_{\boldsymbol{z}}(\phi))|\boldsymbol{z}\rangle &= \sum_{\ell',m'}\langle \ell, m|U(R_{\boldsymbol{z}}(\phi))|\ell', m'\rangle\langle \ell', m'|\boldsymbol{z}\rangle \\ &= \sum_{m'}\mathcal{D}^{(\ell)}_{m,m'}(R_{\boldsymbol{z}}(\phi))\langle \ell, m'|\boldsymbol{z}\rangle \\ &= e^{-im\phi}\langle \ell, m|\boldsymbol{z}\rangle. \end{aligned} \tag{132}$$

The vector $\boldsymbol{z}$ is left invariant by rotations around the z axis thus the ϕ-dependence must be absent, giving

$$\langle \ell, m|\boldsymbol{z}\rangle = \delta_{m,0}c_\ell. \tag{133}$$

As of the normalization, we write

$$1 = \langle \ell, 0|\ell, 0\rangle, \tag{134}$$

as an integral over the solid angle,

$$1 = \int_{S_2} d\boldsymbol{n}\langle \ell, 0|\boldsymbol{n}\rangle\langle \boldsymbol{n}|\ell, 0\rangle \tag{135}$$

or in terms of rotations

$$1 = \frac{1}{2\pi}\int_{SO(3)} dR\langle \ell, 0|U(R)|\boldsymbol{z}\rangle\langle \boldsymbol{z}|U^\dagger(R)|\ell, 0\rangle \tag{136}$$

since the integration weight over S_2 and $SO(3)$ are identical, $s_2(\phi,\theta,\chi) = s_3(\phi,\theta,\chi) = \sin\theta$ and the integrand is χ-independent. We now insert the resolution of unity (102) beside the bra and ket $\boldsymbol{z}$,

$$1 = \frac{1}{2\pi}\sum_{\ell,\ell',m,m'}\int_{SO(3)} dR\langle \ell, 0|U(R)|\ell', m'\rangle\langle \ell', m'|\boldsymbol{z}\rangle\langle \boldsymbol{z}|\ell, m\rangle\langle \ell, m|U^\dagger(R)|\ell, 0\rangle. \tag{137}$$

and use the projection (133) to find

$$1 = \frac{\langle \ell, 0|\boldsymbol{z}\rangle|^2}{2\pi}\underbrace{\int_{SO(3)} dR|\mathcal{D}^{(\ell)}_{0,0}(R)|^2}_{\frac{8\pi^2}{2\ell+1}} \tag{138}$$

and, assuming that c_ℓ is real and positive,

$$c_\ell = \sqrt{\frac{2\ell+1}{4\pi}}. \tag{139}$$

By inserting this into Eq. (131) we find

$$Y^\ell_m(\boldsymbol{n}) = \langle \boldsymbol{n}|\ell, m\rangle = \sqrt{\frac{2\ell+1}{4\pi}}\mathcal{D}^{(\ell)*}_{m,0}(R(\phi,\theta,\chi)) = \sqrt{\frac{2\ell+1}{4\pi}}e^{im\phi}d^{(\ell)*}_{m,0}(\theta). \tag{140}$$

Example: Let us construct the spherical harmonics for $\ell = 1$. These three functions are defined on the unit sphere and transform into each other during rotations in an irreducible manner. The three components of the vector $\boldsymbol{r} = (x, y, z)$ obviously satisfy these requirements and all what is left to find is their linear combinations which correspond to the base $|1, m\rangle$. We start with the observation that the rotations around the z-axes leave the vector $\boldsymbol{z}$ invariant and $L_z z = 0$ according to Eqs. (85). The comparison of this result with the first equation of (126) shows that $Y_0^1(\boldsymbol{n}) = cz/r$, $c = \sqrt{3/4\pi}$ being a normalization factor. To find the remaining functions we use the second equation of (126),

$$Y_{\pm 1}^1(\boldsymbol{n}) = \frac{1}{\sqrt{2}\hbar} L_\pm Y_0^1(\boldsymbol{n}), \tag{141}$$

written as

$$Y_{\pm 1}^1(\boldsymbol{n}) = \frac{c}{\sqrt{2}\hbar r}[yp_z - zp_y \pm i(zp_x - xp_z)]z, \tag{142}$$

yielding

$$\begin{aligned} Y_1^1(\boldsymbol{n}) &= -\sqrt{\frac{3}{8\pi}}\frac{x+iy}{r} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi} \\ Y_0^1(\boldsymbol{n}) &= \sqrt{\frac{3}{4\pi}}\frac{z}{r} = \sqrt{\frac{3}{4\pi}}\cos\theta \\ Y_{-1}^1(\boldsymbol{n}) &= \sqrt{\frac{3}{8\pi}}\frac{x-iy}{r} = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi}. \end{aligned} \tag{143}$$

III. ADDITION OF ANGULAR MOMENTUM

When a system of several particles is considered the quantities, characterizing the individual particles may or may not add up. For instance, the energy is additive for non-interacting particles only, the momentum and angular momentum remain additive in the presence of interactions, as well, in non-relativistic dynamics. But a non-linear function of additive quantities, such as $\boldsymbol{L}^2$ is not additive anymore, rendering the construction of rotational multiplets a non-trivial problem for several particles. We shall consider first additive quantum numbers, such as the momentum $\boldsymbol{p}$ or angular momentum $\boldsymbol{L}$ for two non-interacting particles, followed by the non-additive $\boldsymbol{L}^2$.

A. Additive observables and quantum numbers

Let us consider a system of two non-interactive particles in a state, described by the wave function $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$. We show first that the generators of translations and rotations, the momentum

and angular momentum are additive operators for a system of several particles. After that we address the issue of a non-additive observable, namely the length square of angular momentum.

1. Momentum

Momentum, the generator of translations, can be read off by performing an infinitesimal translation $\boldsymbol{r} \to \boldsymbol{r} + \boldsymbol{\epsilon}$. The equation

$$\delta\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = -\frac{i}{\hbar}\boldsymbol{\epsilon}\boldsymbol{P}\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

defines the total momentum, cf. Eq. (76). The expression

$$\begin{aligned} \delta\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) &= \psi(\boldsymbol{r}_1 - \boldsymbol{\epsilon}, \boldsymbol{r}_2 - \boldsymbol{\epsilon}) - \psi(\boldsymbol{r}_1, \boldsymbol{r}_2) \\ &= -\frac{i}{\hbar}\boldsymbol{\epsilon}(\boldsymbol{p}_1 + \boldsymbol{p}_2)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2), \end{aligned} \tag{144}$$

of the change of the wave function under infinitesimal translation yields the form

$$\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2 \tag{145}$$

of the total momentum. The additivity of the momentum operator implies the additivity of the eigenvalues of $\boldsymbol{p}$ in an obvious manner.

2. Angular momentum

An infinitesimal rotation around the z axis, corresponding to the coordinate transformation

$$\boldsymbol{r} = \begin{pmatrix} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{pmatrix} \to \begin{pmatrix} r\sin\theta\cos(\phi+\epsilon) \\ r\sin\theta\sin(\phi+\epsilon) \\ r\cos\theta \end{pmatrix} \tag{146}$$

induces the change

$$\begin{aligned} \delta\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) &= -\frac{i}{\hbar}\epsilon L_z\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) \\ &= -\epsilon(\partial_{\phi_1} + \partial_{\phi_2})\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) \\ &= -\frac{i}{\hbar}\epsilon(L_{1z} + L_{2z})\psi(\boldsymbol{r}_1, \boldsymbol{r}_2). \end{aligned} \tag{147}$$

It is an obvious generalization of this result that the rotation $R_{\boldsymbol{n}}(\epsilon)$ is generated by $\boldsymbol{n}(\boldsymbol{L}_1+\boldsymbol{L}_2)$. Hence the angular momentum is additive, $\boldsymbol{L}=\boldsymbol{L}_1+\boldsymbol{L}_2$ and satisfies the commutation relations

$$\begin{aligned}[L_a,L_b] &= [L_{1a}+L_{2a},L_{1b}+L_{2b}]\\ &= i\hbar\sum_c \epsilon_{a,b,c}(L_{1c}+L_{2c})\\ &= i\hbar\sum_c \epsilon_{a,b,c}L_c. \end{aligned} \tag{148}$$

Note that the additivity of the components of the angular momentum is not sufficient to determine the quantum number ℓ of the total angular momentum because $\boldsymbol{L}^2=\boldsymbol{L}_1^2+\boldsymbol{L}_2^2+2\boldsymbol{L}_1\boldsymbol{L}_1$ is not additive. This is similar in classical mechanics, as well, where a non-linear function of an additive quantity is naturally non-additive. The determination of the spectrum of such a non-linear combination is non-trivial in the quantum case. For instance, two vectors of classical physics, $\boldsymbol{L}_1$ and $\boldsymbol{L}_2$ produce the sum, $\boldsymbol{L}=\boldsymbol{L}_1+\boldsymbol{L}_2$, in such a manner that

$$\left(\sqrt{\boldsymbol{L}_1^2}-\sqrt{\boldsymbol{L}_2^2}\right)^2 \le \boldsymbol{L}^2 \le \left(\sqrt{\boldsymbol{L}_1^2}+\sqrt{\boldsymbol{L}_2^2}\right)^2. \tag{149}$$

Is there a similar inequality in the quantum case? Furthermore, the construction of any vector, satisfying his inequality is obvious in classical physics. How can we find different states, allowed by the corresponding inequality in the quantum case?

B. System of two particles

Let us consider now two particles in the states $|\phi_1\rangle$ and $|\phi_2\rangle$, respectively, with angular momentum quantum numbers ℓ_1 and ℓ_2, $|\phi_1\rangle\in\mathcal{H}_{\ell_1}$, $|\phi_2\rangle\in\mathcal{H}_{\ell_2}$. Rotations, applied on the system of two particles, $e^{-\frac{i}{\hbar}\alpha\boldsymbol{n}\boldsymbol{L}}|\phi_1\rangle\otimes|\phi_2\rangle$ generate a representatino of rotations in the space $\mathcal{H}=\mathcal{H}_{\ell_1}\otimes\mathcal{H}_{\ell_2}$. The spectrum of $\boldsymbol{L}^2=(\boldsymbol{L}_1+\boldsymbol{L}_2)^2$, $\{\ell_1,\ell_2,\ldots,\ell_n\}$, will be determined by breaking up $\mathcal{H}$ into the direct sum of rotational multiplets $\mathcal{H}=\mathcal{H}_{\ell_1}\oplus\mathcal{H}_{\ell_2}\oplus\cdots\oplus\mathcal{H}_{\ell_n}$. One can prove that the unitary representations can always be broken up into the sum of irreducible representations.

There are two different bases one may use in $\mathcal{H}$. The decoupled basis is defined by the vectors

$$|\ell_1,\ell_2,m_1,m_2\rangle=|\ell_1,m_1\rangle\otimes|\ell_2,m_2\rangle,\quad -\ell_j\le m_j\le\ell_j. \tag{150}$$

Since the quantum numbers m_1 and m_2 are independent we have $dim\mathcal{H}=(2\ell_1+1)(2\ell_2+1)$. The vectors of the coupled basis, $|L,M\rangle$, are labeled by the quantum numbers of the total angular

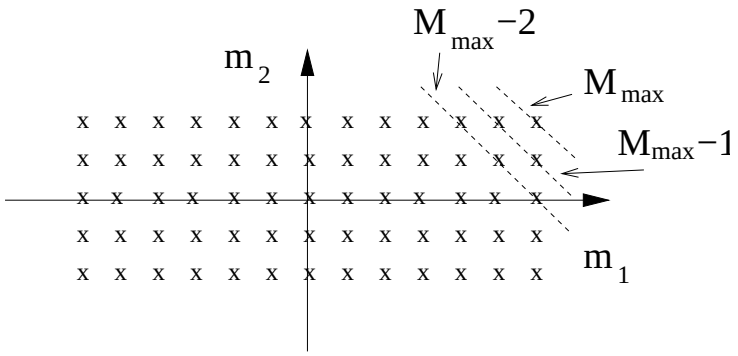


FIG. 5: Decoupled basis: The spectrum of $(L_1)_z$ and $(L_2)_z$ for $\ell_1 = 6$, $\ell_2 = 2$.

momentum $\boldsymbol{L}$,

$$\begin{aligned} \boldsymbol{L}^2|L,M\rangle &= \hbar^2 L(L+1)|L,M\rangle, \\ L_z|L,M\rangle &= \hbar M|L,M\rangle, \end{aligned} \tag{151}$$

and can be constructed as follows.

We start with the decoupled basis vector $|\ell_1,\ell_2,\ell_1,\ell_2\rangle$. Since the components of the angular momentum is additive we have $M = \ell_1 + \ell_2$. Actually this vector has the maximal value of $M = M_{max} = \ell_1 + \ell_2$ in $\mathcal{H}$. Since $\mathcal{H}$ is closed with respect to rotations this vector must be in a multiplet as a coupled basis vector, $|M_{max}, M_{max}\rangle \in \mathcal{H}_{M_{max}}$ and $\mathcal{H} = \mathcal{H}_{M_{max}} \oplus \mathcal{H}'$, where both members of the direct sum are closed with respect to rotations. Since there is no other vector with the same value of M we know that $\mathcal{H}$ contains only one such a multiplet. Thought not obvious at the very beginning, this multiplet might have occurred several times in $\mathcal{H}$. The continuation of the argument is simpler to follow in Figs. 5 and 6 where the basis vectors are represented by crosses.

Let us now apply the ladder operator $L_- = L_{1-} + L_{2-}$ to the decoupled basis vector we have just found and define another element of the multiplet $\mathcal{H}_{M_{max}}$ by the equation

$$|M_{max}, M_{max}-1\rangle = \frac{1}{\hbar\sqrt{2M_{max}}} L_-|M_{max}, M_{max}\rangle. \tag{152}$$

The subspace with $M = M_{max} - 1$ is two dimensional and the unit vector $|\psi\rangle$, orthogonal to $|M_{max}, M_{max}-1\rangle$ can be chosen as a further coupled basis vector within $\mathcal{H}'$. Since $\mathcal{H}'$ is closed with respect to rotations this basis vector must be in a multiplet. There is no further orthogonal states with the same M quantum number therefore $|\psi\rangle = |M_{max}-1, M_{max}-1\rangle \in \mathcal{H}_{M_{max}-1} \subset \mathcal{H}'$ which comes with multiplicity one in $\mathcal{H}'$. We have so far identified two multiplets and found $\mathcal{H} = \mathcal{H}_{M_{max}} \oplus \mathcal{H}_{M_{max}-1} \oplus \mathcal{H}''$, where $\mathcal{H}''$ is closed with respect to rotations.

The repeated application of this procedure, starting always with a decoupled basis vector with one unit lower M quantum number leads to the identification of multiplets $\mathcal{H}_L$ with $L_{min} =$

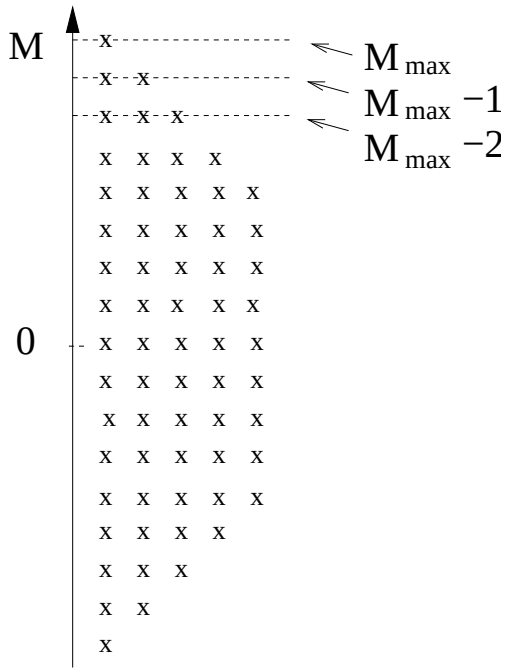


FIG. 6: Coupled basis: The spectrum of L_z for $\ell_1 = 6$, $\ell_2 = 2$.

$|\ell_1 - \ell_2| \leq L \leq L_{max} = \ell_1 + \ell_2$ which occur once only,

$$\mathcal{H} = \mathcal{H}_{|\ell_1-\ell_2|} \oplus \cdots \oplus \mathcal{H}_{\ell_1+\ell_2}, \tag{153}$$

a result summarized symbolically as

$$\ell_1 \otimes \ell_2 = |\ell_1 - \ell_2| \oplus |\ell_1 - \ell_2| + 1 \oplus \cdots \oplus \ell_1 + \ell_2 - 1 \oplus \ell_1 + \ell_2. \tag{154}$$

The "sum rule",

$$\dim\mathcal{H} = (2\ell_1 + 1)(2\ell_2 + 1) = \sum_{|\ell_1-\ell_2|\leq\ell\leq\ell_1+\ell_2} (2\ell + 1), \tag{155}$$

confirms the observation that each multiplet appears once only. The single occurrence of each multiplet in the sum of two angular momentum gives rise to the resolution of the identity

$$\mathbb{1} = \sum_{m_1,m_2} |\ell_1, \ell_2, m_1, m_2\rangle\langle\ell_1, \ell_2, m_1, m_2| = \sum_{L,M} |L, M\rangle\langle L, M| \tag{156}$$

in $\mathcal{H}$.

The simplicity of having each multiplet occurring once in the sum is expected on semi-classical grounds, as well. When two angular momentum vectors are added in quantum mechanics then the different ways of rearranging the total angular momentum quantum number, L, represent the different relative orientations of the angular momentum vectors. The matrix elements of the

right hand side of eq. (96) can be proven to become negligible within a multiplet with angular momentum $\ell \to \infty$ and the classical behavior is recovered in that limit. What happens in classical mechanics? When two angular momentum vectors are added then for each relative orientation of the vectors, parametrized by the angle between the two vectors, there is a well defined length for the sum. This is not the case anymore if three or more vectors are added.

The matrix elements of the unitary transformation, connecting the coupled and the decoupled basis,

$$(\ell_1, \ell_2, m_1, m_2|L, M) = \langle \ell_1, \ell_2, m_1, m_2|L, M\rangle, \tag{157}$$

are called Clebsch-Gordan coefficients and give rise to the expression

$$|L, M\rangle = \sum_{m_1, m_2} |\ell_1, \ell_2, m_1, m_2\rangle (\ell_1, \ell_2, m_1, m_2|L, M) \tag{158}$$

of the coupled base where the resolution of the identity (156) was used. The additivity of L_z yields the property

$$(\ell_1, \ell_2, m_1, m_2|L, M) = \delta_{m_1+m_2, M} (\ell_1, \ell_2, m_1, M - m_1|L, M). \tag{159}$$

One can choose the phase of the basis vectors $|\ell, m\rangle$ in such a manner that Clebsch-Gordan coefficients become real. The procedure, followed above can be extended for the half integer case.

Examples:

1. $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$: Let us now work out the Clebsch-Gordan coefficients for the simplest example, the addition of two spin half, $\ell_1 = \ell_2 = \frac{1}{2}$. The equation

$$|1, \pm 1\rangle = |\pm \frac{1}{2}, \pm \frac{1}{2}\rangle \tag{160}$$

gives $(\frac{1}{2}, \frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2}|1, \pm 1) = 1$. The remaining, third basis vector of the $L = 1$ multiplet is found by the help of the ladder operator,

$$\begin{aligned} |1, 0\rangle &= \frac{1}{\sqrt{2}\hbar} L_- |1, 1\rangle \\ &= \frac{1}{2\sqrt{2}} [\sigma_{1x} + \sigma_{2x} - i(\sigma_{1y} + \sigma_{2y})] |\frac{1}{2}, \frac{1}{2}\rangle \\ &= \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_1 + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_2 \right] |\frac{1}{2}, \frac{1}{2}\rangle \\ &= \frac{1}{\sqrt{2}} \left(|\frac{1}{2}, -\frac{1}{2}\rangle + |-\frac{1}{2}, \frac{1}{2}\rangle \right), \end{aligned} \tag{161}$$

yielding $(\frac{1}{2},\frac{1}{2},\pm\frac{1}{2},\mp\frac{1}{2}|1,0)=\frac{1}{\sqrt{2}}$. Note that all basis vectors of the multiplet are symmetric with respect to the exchange of the two particles. Finally, the fourth basis vector, orthogonal to the already found three is an antisymmetric combination gives

$$|0,0\rangle=\frac{1}{\sqrt{2}}\left(|\frac{1}{2},-\frac{1}{2}\rangle-|-\frac{1}{2},\frac{1}{2}\rangle\right) \tag{162}$$

and $(\frac{1}{2},\frac{1}{2},\pm\frac{1}{2},\mp\frac{1}{2}|1,0)=\pm\frac{1}{\sqrt{2}}$.

2. $d^{(1)}$: The addition of two spin half can be used to find the reduced d-matrix for spin one. We start with the decoupled basis

$$d^{(1)}_{(m_1',m_2'),(m_1,m_2)}(\beta)=\langle m_1',m_2'|e^{-i\frac{\beta}{2}(\sigma_{1y}+\sigma_{2y})}|m_1,m_2\rangle=d^{(\frac{1}{2})}_{m_1',m_2}(\beta)d^{(\frac{1}{2})}_{m_1',m_2}(\beta) \tag{163}$$

and construct

$$d^{(1)}_{m',m}(\beta)=\langle 1,m'|e^{-i\frac{\beta}{\hbar}L_y}|1,m\rangle, \tag{164}$$

by the help of the Eqs. (160)-(162) for the coupled basis,

$$d^{(1)}_{m'm}=\begin{pmatrix} d_{++}d_{++} & \frac{1}{\sqrt{2}}(d_{++}d_{+-}+d_{+-}d_{++}) & d_{+-}d_{+-} \\ \frac{1}{\sqrt{2}}(d_{++}d_{-+}+d_{-+}d_{++}) & \frac{1}{2}(d_{++}d_{--}+d_{+-}d_{-+}+d_{-+}d_{+-}+d_{--}d_{++}) & \frac{1}{\sqrt{2}}(d_{+-}d_{--}+d_{--}d_{+-}) \\ d_{-+}d_{-+} & \frac{1}{\sqrt{2}}(d_{++}d_{+-}+d_{+-}d_{++}) & d_{--}d_{--} \end{pmatrix} \tag{165}$$

where $d_{mm'}=d^{(\frac{1}{2})}_{m,m'}(\beta)$. The explicit expression (112) gives finally

$$d^{(1)}_{m',m}(\beta)=\begin{pmatrix} \cos^2\frac{\beta}{2} & -\frac{1}{\sqrt{2}}\sin\beta & \sin^2\frac{\beta}{2} \\ \frac{1}{\sqrt{2}}\sin\beta & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta \\ \sin^2\frac{\beta}{2} & -\frac{1}{\sqrt{2}}\sin\beta & \cos^2\frac{\beta}{2} \end{pmatrix}. \tag{166}$$

3. $1^{\otimes n}$: What happens when we assemble n particles of spin one? The decoupled basis vectors,

$$|m_1,\ldots,m_n\rangle=|1,m_1\rangle\otimes\cdots\otimes|1,m_n\rangle, \tag{167}$$

have the wave function,

$$\langle\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n|m_1,\ldots,m_n\rangle=\langle\boldsymbol{r}_1|1,m_1\rangle\cdots\langle\boldsymbol{r}_n|1,m_n\rangle, \tag{168}$$

and we choose the single particle wave functions

$$\langle\boldsymbol{r}|1,m\rangle=rY^1_m(\frac{\boldsymbol{r}}{r}), \tag{169}$$

where the spherical harmonics are given by eq. (143). This choice makes the wave functions homogeneous polynomials of the coordinates of order n. One finds angular momentum

multiplets with $0 \leq \ell \leq n$ with different multiplicities, we shall consider the simplest case, $\ell = n$, only. The multiplet $\mathcal{H}_\ell$ ($\ell = n$ from now on) enters with multiplicity one as in the case of Chapter III B because there is a single state with $M = \ell$, namely $|1, \ldots, 1\rangle$. The remaining 2ℓ states of $\mathcal{H}_\ell$ can be obtained by applying $L_- = L_{1-} + \cdots + L_{\ell-}$ on $|1, \ldots, 1\rangle$,

$$|\ell, m\rangle = \frac{1}{N_m} L_-^{\ell-m} |1, \ldots, 1\rangle, \tag{170}$$

with

$$N_m = \prod_{m'=m+1}^{\ell} \hbar\sqrt{\ell(\ell+1) - m'(m'-1)}, \tag{171}$$

up to a phase factor.

The structure of the wave functions of the states in $\mathcal{H}_\ell$ leads to a useful expression for the spherical harmonics. To find it we consider the single particle with wave functions

$$\psi_{m_1,\ldots,m_\ell}(\boldsymbol{r}) = \langle \boldsymbol{r}|1, m_1\rangle \cdots \langle \boldsymbol{r}|1, m_\ell\rangle. \tag{172}$$

This wave function is obtained by collapsing the different coordinates of (168) to a common value, $\boldsymbol{r}_1 = \cdots = \boldsymbol{r}_\ell = \boldsymbol{r}$, hence the transformation properties under rotations which influence each coordinate in a similar manner, in particular the angular momentum, remain the same. Therefore, the wave functions

$$\psi_{\ell,m}(\boldsymbol{r}) = \frac{1}{N_m} L_-^{\ell-m} \psi_{1,\ldots,1}(\boldsymbol{r}), \quad -\ell \leq m \leq \ell \tag{173}$$

form a basis for the multiplet $\mathcal{H}_\ell$ within the state of space of this single particle. The angular momentum operator, $\boldsymbol{L}$ removes a coordinate and multiplies by another and preserve the form of the wave functions, namely being a homogeneous polynomial of the coordinates of order ℓ. The wave function $\psi_{\ell,m}(\boldsymbol{r})$ is the sum of terms

$$\frac{\ell!}{p!q!r!2^r} 2^{q/2+r} (x+iy)^p (\sqrt{2}z)^q (x-iy)^r, \quad p+q+r = \ell, \quad p-r = m \tag{174}$$

up to a common normalization factor. In fact, the combinatorial prefactor denotes the number of possibilities of partitioning ℓ indistinguishable objects into three subsets of size p, q and r. The factors $(\sqrt{2})^q$ and $(\sqrt{2})^{2r}$ are generated by the coefficient $\sqrt{\ell(\ell+1) - m(m-1)}$ on the right hand side of eq. (99) as L_- acts $q+2r$ times. The operator L_- has to act twice on the same factor, $\langle \boldsymbol{r}|1, m_j\rangle$, to reach $m_j = -1$ and the order of the two L_- does not matter. But each order is counted $\ell!$. Such a double counting is removed by the factor 2^r in the

denominator. The condition $p-r=m$ follows from the additivity of L_z. The normalization and the phase conventions, leading to real Clebsch-Gordan coefficients correspond to

$$Y_m^{(\ell)}(\theta,\phi) \;=\; \frac{1}{r^\ell}\sqrt{\frac{2\ell+1}{4\pi}(\ell+m)!(\ell-m)!}\sum_{p+q+r=\ell,p-r=m}\frac{1}{p!q!r!}\left(-\frac{x+iy}{2}\right)^p z^q\left(\frac{x-iy}{2}\right)^r \tag{175}$$

IV. SELECTION RULES

The structure of the rotational group alone restricts the matrix elements of certain operators, calculated between states with well defined angular momentum. Such a simplification is of great importance in the study of involved composite systems. Operators displaying this simplification are called tensor operators and the simplicity of the matrix elements stems from the orthogonality relations and the Wigner-Eckart theorem.

A. Tensor operators

Tensor operator set, $\{T_m^{(\ell)}\}$, $-\ell\le m\le\ell$, transforms as operator acting in the Hilbert space and as tensor, basis vectors of an irreducible multiplet in the linear space of operators,

$$\begin{aligned} U^\dagger(R)T_m^{(\ell)}U(R) \;&=\; \sum_{m'}T_{m'}^{(\ell)}\mathcal{D}^\ell_{m',m}(R^{-1}) \\ &=\; \sum_{m'}\mathcal{D}^{\ell *}_{m,m'}(R)T_{m'}^{(\ell)}, \end{aligned} \tag{176}$$

cf. eq. (89). Tensor operators transform under rotations in two different ways. One the one hand, they are operators and the representation of rotations in the Hilbert space transform them. On the other hand, they are tensors and rotations act on their tensor indices. This equation states that these two ways of rotation are equivalent for tensor operators. We can turn this equation into an invariance property,

$$\sum_{m'}U^\dagger(R)T_{m'}^{(\ell)}U(R)\mathcal{D}^\ell_{m',m}(R)=T_m^{(\ell)}. \tag{177}$$

Example: Let us consider the spherical harmonics, transforming under rotations as

$$\begin{aligned} Y_m^\ell(R\boldsymbol{n}) \;&=\; U(R^{-1})Y_m^\ell(\boldsymbol{n}) \\ &=\; \langle\boldsymbol{n}|U(R^{-1})|\ell,m\rangle=\sum_{m'}Y_{m'}^\ell(\boldsymbol{n})D^{(\ell)}_{m',m}(R^{-1}), \end{aligned} \tag{178}$$

where a resolution of the identity is inserted after the bra $\langle\boldsymbol{n}|$ in the second line. Such a transformation rule suggests that the operator, $Y_m^\ell(\hat{\boldsymbol{A}})$, obtained by the help of a vector operator,

$R\hat{\boldsymbol{A}} = U^\dagger(R)\hat{\boldsymbol{A}}U(R)$, is a tensor operator. In fact,

$$\begin{aligned} Y^\ell_m(R\boldsymbol{A}) &= \sum_{m'} Y^\ell_{m'}(\hat{\boldsymbol{A}}) D^{(\ell)}_{m',m}(R^{-1}) \\ &= Y^\ell_m(U^\dagger(R)\hat{\boldsymbol{A}}U(R)) \\ &= U^\dagger(R) Y^\ell_m(\hat{\boldsymbol{A}}) U(R) \end{aligned} \tag{179}$$

B. Orthogonality relations

The orthogonality theorem, stating that the set of matrix elements of all irreducible representations of a group form a complete orthogonal basis for functions on the group, plays a central role in the theory of representation of groups. Rather than presenting a general proof we follow a short-cut, needed to use this theorem for rotations.

We have seen that the spherical harmonics, defined by

$$\sqrt{\frac{2\ell+1}{4\pi}} d^{(\ell)*}_{m,m'}(\theta) e^{im\phi} \tag{180}$$

with $m' = 0$, represent a basis on the unit sphere with the integral measure $d\phi d(\cos\theta)$. One can generalize this result for $m' \neq 0$ by showing that those functions are linearly independent and satisfy the same eigenvalue conditions with the operators $\boldsymbol{L}^2$ and L_z. Therefore the D matrix elements,

$$\begin{aligned} \mathcal{D}^{(\ell)}_{m',m}(R(\phi,\theta,\chi) &= \langle \ell, m' | U(R_{\boldsymbol{z}}(\phi) U(R_{\boldsymbol{y}}(\theta) U(R_{\boldsymbol{z}}(\chi) | \ell, m \rangle \\ &= e^{-im'\phi - im\chi} d^{(\ell)}_{m',m}(\theta), \end{aligned} \tag{181}$$

give a basis for the rotation group $SO(3) = \{R(\phi,\theta,\chi)\}$ with the integral measure $dR = d\phi d(\cos\theta) d\chi$ because the factor $e^{-im\chi}$ provides a basis for the dependence on χ.

Hence the equation, expressing the orthogonality of different basis vectors,

$$\int dR \mathcal{D}^{(\ell_1)*}_{m_1',m_1}(R) \mathcal{D}^{(\ell_2)}_{m_2',m_2}(R) = \frac{8\pi^2}{2\ell_1+1} \delta_{\ell_1,\ell_2} \delta_{m_1',m_2'} \delta_{m_1,m_2}, \tag{182}$$

follows where the normalization is obtained from (138). The completeness implies the representations

$$f(\phi,\theta,\chi) = \sum_{\ell,m,m'} f_{\ell,m,m'} \mathcal{D}^{(\ell)}_{m,m'}(R(\phi,\theta,\chi)) \tag{183}$$

where

$$f_{\ell,m,m'} = \frac{2\ell_1+1}{8\pi^2} \int_{-\pi}^{\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_{-\pi}^{\pi} d\chi \mathcal{D}^{(\ell)*}_{m,m'}((\phi,\theta,\chi)) f(\phi,\theta,\chi) \tag{184}$$

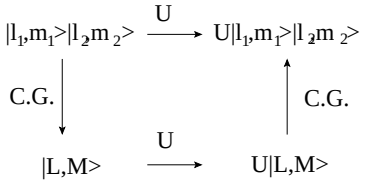


FIG. 7: Two ways of performing rotations on a decoupled basis element.

for square integrable functions over $SO(3)$.

We now work out an inportant consequence of the orthogonality relation for the addition of angular momentum. The basis transformation from the decoupled to the coupled basis is not only unitary but orthogonal because the Clebsch-Gordan coefficient are real. Therefore the transformation

$$|L,M\rangle = \sum_{m_1,m_2} |\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle (\ell_1,\ell_2,m_1,m_2|L,M) \tag{185}$$

can be inverted with the result

$$|\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle = \sum_{L,M} |L,M\rangle (\ell_1,\ell_2,m_1,m_2|L,M). \tag{186}$$

We can write rotations on the decoupled basis on two different manners by following the two different paths of Fig. 7. By applying the rotation on each factor of the direct product basis vector we have

$$U(R)|\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle = \sum_{m_1',m_2'} |\ell_1,m_1'\rangle \otimes |\ell_2,m_2'\rangle \mathcal{D}^{(\ell_1)}_{m_1',m_1}(R)\mathcal{D}^{(\ell_2)}_{m_2',m_2}(R). \tag{187}$$

The use of Eq. (186) gives

$$U(R)|\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle = \sum_{L,M,M'} |L,M'\rangle \mathcal{D}^{(L)}_{M',M}(R)(\ell_1,\ell_2,m_1,m_2|L,M) \tag{188}$$

where the right hand side can be rewritten by the help of the decoupled basis vectors as

$$\begin{aligned} U(R)|\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle \;=\; & \sum_{L,M,M',m_1',m_2'} |\ell_1,m_1'\rangle \otimes |\ell_2,m_2'\rangle (\ell_1,\ell_2,m_1',m_2'|L,M') \\ & \mathcal{D}^{(L)}_{M',M}(R)(\ell_1,\ell_2,m_1,m_2|L,M). \end{aligned} \tag{189}$$

Comparing this result with (187) we find

$$\begin{aligned} \mathcal{D}^{(\ell_1)}_{m_1',m_1}(R)\mathcal{D}^{(\ell_2)}_{m_2',m_2}(R) \;&=\; \sum_{L,M,M'} (\ell_1,\ell_2,m_1',m_2'|L,M')\mathcal{D}^{(L)}_{M',M}(R)(\ell_1,\ell_2,m_1,m_2|L,M) \\ &=\; \sum_{L,M,M'} \langle \ell_1,\ell_2,m_1',m_2'|L,M'\rangle \mathcal{D}^{(L)}_{M',M}(R)\langle L,M|\ell_1,\ell_2,m_1,m_2\rangle. \end{aligned} \tag{190}$$

The usual bracket formalism is used in the second equation because it indicates in an obvious manner that we have here the same rotation in the coupled and the decoupled bases.

We finally multiply this equation by $\mathcal{D}^{(L)*}_{M',M}(R)$ and carry out the integration over the rotational group to find

$$\int dR \mathcal{D}^{(L)*}_{M',M}(R)\mathcal{D}^{(\ell_1)}_{m'_1,m_1}(R)\mathcal{D}^{(\ell_2)}_{m'_2,m_2}(R) = \frac{8\pi^2}{2L+1}(\ell_1,\ell_2,m'_1,m'_2|L,M')(\ell_1,\ell_2,m_1,m_2|L,M), \quad (191)$$

where Eq. (182) has been used to simplify the right hand side. This equation, called orthogonality relation for Clebsch-Gordan coefficients, expresses the addition of angular momenta, corresponding to the two indices of the D matrix, the projection of $|\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle$ and $\langle \ell_1,m'_1|\otimes\rangle \ell_2,m'_2|$ on $\langle L,M|$ and $|L,M'\rangle$, respectively. We see no complex conjugation on the Clebsch-Gordan coefficient, corresponding to the left indices because $(\ell_1,\ell_2,m'_1,m'_2|L,M')$ is real.

C. Wigner-Eckart theorem

To obtain a useful parametrization of the matrix elements of tensor operators we split the quantum numbers, labeling our basis vectors into rotational and non-rotational classes. The former includes ℓ and m and the remaining quantum numbers belong to the latter, denoted by n. Therefore a generic matrix element of a tensor operator is

$$\mathcal{M} = \langle n_1,\ell_1,m_1|T^{(\ell)}_m|n_2,\ell_2,m_2\rangle. \quad (192)$$

We use the identity (177) to write $\mathcal{M}$ as

$$\begin{aligned}\mathcal{M} &= \sum_{m'}\langle n_1,\ell_1,m_1|U^\dagger(R)T^{(\ell)}_{m'}U(R)|n_2,\ell_2,m_2\rangle\mathcal{D}^{\ell}_{m',m}(R)\\ &= \sum_{m'_1m'_2m'}\langle n_1,\ell_1,m_1|U^\dagger(R)\underbrace{|n_1,\ell_1,m'_1\rangle\langle n_1,\ell_1,m'_1|}_{\mathbb{1}}T^{(\ell)}_{m'}\underbrace{|n_2,\ell_2,m'_2\rangle\langle n_2,\ell_2,m'_2|}_{\mathbb{1}}U(R)|n_2,\ell_2,m_2\rangle\\ &\quad\times\mathcal{D}^{\ell}_{m',m}(R). \end{aligned} \quad (193)$$

An integration over rotations eliminates the R-dependence,

$$\mathcal{M}\int dR = \sum_{m'_1,m'_2,m'}\langle n_1,\ell_1,m'_1|T^{(\ell)}_{m'}|n_2,\ell_2,m'_2\rangle\int dR\mathcal{D}^{(\ell_1)*}_{m'_1,m_1}(R)\mathcal{D}^{(\ell)}_{m',m}(R)\mathcal{D}^{(\ell_2)}_{m'_2,m_2}(R), \quad (194)$$

and the orthogonality relation (191) results

$$\mathcal{M}\int dR = \frac{8\pi^2}{2\ell_1+1}(\ell,\ell_2,m,m_2|\ell_1,m_1)\sum_{m'_1,m'_2,m'}(\ell,\ell_2,m',m'_2|\ell_1,m'_1)\langle n_1,\ell_1,m'_1|T^{(\ell)}_{m'}|n_2,\ell_2,m'_2\rangle. \quad (195)$$

The Wigner-Eckart theorem,

$$\mathcal{M} = (\ell, \ell_2, m, m_2|\ell_1, m_1) \ll n_1, \ell_1|T^{(\ell)}|n_2, \ell_2 \gg, \tag{196}$$

expresses the matrix elements of a tensor operator in a factorized form. One factor, the Clebsch-Gordan coefficient, reflects the structure of the rotation group because it depends on rotational quantum numbers only, and represents the kinematic feature of the matrix element in question. The other factor, the so called reduced matrix element,

$$\ll n_1, \ell_1|T^{(\ell)}|n_2, \ell_2 \gg = \frac{1}{2\ell_1 + 1} \sum_{m_1', m_2', m'} (\ell, \ell_2, m', m_2'|\ell_1, m_1')\langle n_1, \ell_1, m_1'|T^{(\ell)}_{m'}|n_2, \ell_2, m_2'\rangle, \tag{197}$$

contains the dynamical aspects of the matrix element as indicated by the dependence on the non-rotational quantum numbers n_1 and n_2.

If the Clebsch-Gordan coefficient in (196) is vanishing then whole matrix element is canceled. When this happens in the calculation of transitional amplitude then such a cancellation is called selection rule, a kinematic consideration restricts the possible outcome.

Examples:

1. Tensor operator with $\ell = 0$: The triviality of the Clebsch-Gordan coefficients

$$(\ell_2, 0, m_2, 0|\ell_1, m_1) = \delta_{\ell_1,\ell_2}\delta_{m_1,m_2} \tag{198}$$

gives the factorization

$$\langle n_1, \ell_1, m_1|T^{(0)}_m|n_2, \ell_2, m_2\rangle = \delta_{\ell_1,\ell_2}\delta_{m_1,m_2} \ll n_1, \ell_1|T^{(0)}|n_2, \ell_2 \gg . \tag{199}$$

Such a factorization actually appears in the calculation of the matrix elements of spherical symmetric functions in problems with rotational invariant potential, such as the Hydrogen atom,

$$\langle n_1, \ell_1, m_1|r^p|n_2, \ell_2, m_2\rangle = \underbrace{\int d\phi \int d(\cos\theta) Y^{\ell_1 *}_{m_1}(\theta, \phi) Y^{\ell_2}_{m_2}(\theta, \phi)}_{(\ell_2, 0, m_2, 0|\ell_1, m_1)} \underbrace{\int dr r^{2+p} \eta^*_{n_1,\ell_1}(r)\eta_{n_2,\ell_2}(r)}_{\ll n_1, \ell_1|r^p|n_2, \ell_2 \gg} . \tag{200}$$

2. Tensor operator with $\ell = 1$: The results (**??**)-(**??**) can be generalized to the angular momentum operator which give $\ell = 1$ tensor operators, namely,

$$T^{(1)}_0 = L_z, \quad T^{(1)}_{\pm 1} = \mp\frac{1}{\sqrt{2}} L_\pm, \tag{201}$$

and the Wigner-Eckart theorem gives

$$\langle n_1, \ell_1, m_1 | L_m | n_2, \ell_2, m_2 \rangle = (1, \ell_2, m, m_2 | \ell_1, m_1) \ll n_1, \ell_1 | L | n_2, \ell_2 \gg . \tag{202}$$

This relation can be used to obtain the reduced matrix elements in a simple manner, by considering the case

$$\langle n_1, \ell_1, \ell_1 | L_0 | n_2, \ell_2, \ell_2 \rangle = (1, \ell_2, 0, \ell_2 | \ell_1, \ell_1) \ll n_1, \ell_1 | L | n_2, \ell_2 \gg . \tag{203}$$

In fact, we have

$$\langle n_1, \ell_1, m | L_0 | n_2, \ell_2, m \rangle = \hbar m \delta_{n_1, n_2} \delta_{\ell_1, \ell_2} \tag{204}$$

and the Clebsh-Gordan coefficient,

$$(1, \ell_1, 0, \ell_1 | \ell_1, \ell_1) = \sqrt{\frac{\ell_1}{\ell_1 + 1}} \tag{205}$$

can be used to find the reduced matrix element

$$\ll n_1, \ell_1 | L | n_2, \ell_2 \gg = \delta_{n_1, n_2} \delta_{\ell_1, \ell_2} \hbar \sqrt{\ell(\ell + 1)}. \tag{206}$$

V. SYMMETRIES IN QUANTUM MECHANICS

Yet another chapter dealing with symmetries is needed to address realistic problems in atomic physics, namely to clarify the impact of symmetries on the dynamics and to include discrete symmetry transformation, in particular space and time inversions. We start with a more careful definition of the symmetry and mention its important consequences on the dynamics, followed by an extension of the class of symmetry transformations. The Chapter is closed by discussing space and time inversion symmetries.

A. Representation of symmetries

Symmetry transformation of a classical system is easier to define in the phase space where the equation of motion is of a first order differential equation in time. The state of motion of the system is described by a point in the phase space, $c = (x, p)$ and a transformation, $c \to s(c)$, acting on the canonical variables is a symmetry if it maps a trajectory $c(t)$ of the system into another one. This condition can be expressed in a simple manner if the initial condition $c(t_i) = c_i$, imposed at $t = t_i$

kept explicitly in the corresponding solution of the equation of motion, $c(t;c_i)$, ie. $c(t_i;c_i)=c_i$. Now, the transformation $c\to s(c)$ is a symmetry if

$$c(t;s(c_i))=s(c(t;c_i)). \tag{207}$$

The system is evolved in quantum mechanics in a linear space by a first order equation of motion, $i\hbar\partial_t|\psi\rangle=H|\psi\rangle$, as

$$|\psi(t)\rangle=e^{-\frac{i}{\hbar}(t-t_i)H}|\psi(t_i)\rangle \tag{208}$$

and the symmetry transformations s are acting within the linear space of state, $|\psi\rangle\to S|\psi\rangle$ is a symmetry if

1. Solution of the equation of motion is mapped into solution,

$$S|\psi(t)\rangle=e^{-\frac{i}{\hbar}(t-t_i)H}S|\psi(t_i)\rangle, \tag{209}$$

which is equivalent with the condition

$$[S,H]=0. \tag{210}$$

2. Observable quantities are preserved by S. It will be mentioned below that the preservation of the transition probability $P(|\psi\rangle\leftarrow|\psi\rangle)=|\langle\phi|\psi\rangle|^2$ requires that S be unitary or anti-unitary operator. This feature, the preservation of the absolute magnitude of the scalar product, is specially important. It gives a justification of the construction of the coupled basis, followed in Chapter III B, because it assures that basis vectors are mapped into basis vectors. This point allows us to generalize the procedure for any symmetry and stating that the multiplets of a symmetry, the linear subspaces which are closed with respect to the symmetry operations, can always be broken up into the direct sum of irreducible multiplets.

The following properties of the way, symmetries are realized in quantum mechanics play an important role in applications.

- The set of symmetry transformations forms a **group**. One has to check four features to prove this statement. (i) The identity, $S=\mathbb{1}$ is always a symmetry, (ii) When two symmetry transformations are applied one after the other then the result is again a symmetry. (iii) The property $(S_1S_2)S_3=S_1(S_2S_3)$ is obvious. (iv) Both unitary and anti-unitary operators possess an inverse.

- A symmetry transformation indicates a **degeneracy** of the Hamiltonian. In fact, let us consider an eigenstate $H|\psi\rangle = E|\psi\rangle$. This state is degenerate with its image with respect to the symmetry transformation since

$$HS|\psi\rangle = SH|\psi\rangle = ES|\psi\rangle. \tag{211}$$

  An important example is the case of rotational invariant Hamiltonian, $[\boldsymbol{L}, H] = 0$ where the symmetry with respect to the rotations, $S = e^{-\frac{i}{\hbar}\alpha \boldsymbol{n}\boldsymbol{L}}$, makes the rotational multiplets degenerate.

- Each subspace of an energy eigenvalue, either degenerate or not, is **closed** with respect to symmetry operation. The reasoning is given by eqs. (211), too. Hence we have a representation of the symmetry group for each eigenvalues of the Hamiltonian.

- A unitary symmetry generates a **conservation law**. In fact, let us start the motion from an initial state which is an eigenstate of the symmetry transformation, $S|\psi(t_i)\rangle = \lambda|\psi(t_i)\rangle$, then the state remains an eigenstate, corresponding to the same eigenvalue since

$$S|\psi(t)\rangle = Se^{-\frac{i}{\hbar}(t-t_i)H}|\psi(t_i)\rangle = e^{-\frac{i}{\hbar}(t-t_i)H}S|\psi(t_i)\rangle = \lambda|\psi(t)\rangle. \tag{212}$$

  Note an important difference between the classical and quantum case. On the one hand, Noether theorem assures that continuous symmetries generate conserved quantities without giving any role to discrete symmetries, on the other hand, both continuous and discrete symmetries lead to conservation laws in quantum mechanics.

B. Unitary and anti-unitary symmetries

It is an important condition against symmetry transformation that observables should be preserved. This condition brings in a surprising element because the correspondence between physical states and vectors in the space of states is not unique. The one-dimensional linear subspace $z|\psi\rangle$, span by the vector $|\psi\rangle$ belongs to the same physical state. Even if we use normalized vectors $e^{i\alpha}|\psi\rangle$ representing the same state, the physics states are realized by a ray-representation in quantum mechanics. This circumstance is important in discussing symmetries because the image of a symmetry transformation is well defined up to a phase, namely a symmetry transformation $|\psi\rangle \to S|\psi\rangle$ can always be generalized to $S|\psi\rangle \to |\tilde{\psi}\rangle = e^{i\alpha_\psi}S|\psi\rangle$ where α_ψ is a suitable defined phase. Thus the requirement $\langle\psi|\phi\rangle = \langle\tilde{\psi}|\tilde{\phi}\rangle$ can be relaxed to $\langle\psi|\phi\rangle = |\langle\tilde{\psi}|\tilde{\phi}\rangle|$.

To accommodate such a weaker condition we generalize the idea of operators in the following manner. An operator S is called linear or anti-linear if

$$S(a|\phi\rangle + b|\psi\rangle) = aS|\phi\rangle + bS|\psi\rangle, \tag{213}$$

or

$$S(a|\phi\rangle + b|\psi\rangle) = a^*S|\phi\rangle + b^*S|\psi\rangle, \tag{214}$$

respectively. The linear operator U is unitary if it is linear and

$$|\psi\rangle \to U|\psi\rangle = |\tilde{\psi}\rangle, \quad \langle\psi|\phi\rangle = \langle\tilde{\psi}|\tilde{\phi}\rangle. \tag{215}$$

An anti-unitary operator A is an anti-linear operator and it satisfies

$$|\psi\rangle \to A|\psi\rangle = |\tilde{\psi}\rangle, \quad \langle\psi|\phi\rangle = \langle\tilde{\psi}|\tilde{\phi}\rangle^*. \tag{216}$$

An important theorem, due to E. Wigner, assures that one can always choose the phases $\{\alpha_n\}$ in such a manner that a symmetry transformation is always either unitary or anti-unitary.

Dirac's bracket formalism is prepared to deal with linear operators and produces inconsistencies when anti-linear operators appear. We mention here three unusual properties of the simplest anti-linear operator, the complex conjugation, K, $Kc|\psi\rangle = c^*K|\psi\rangle$.

1. There are restrictions in the bracket formalism when anti-linear operators are allowed.

   (a) K is basis dependent. This comes about because we may use real wave functions for the description of any basis, for instance $\psi_j = \delta_{j,j_0}$ or $\psi_{x_0}(x) = \delta(x - x_0)$, in a linear space with discrete or continuous spectrum, respectively. In other words,

   $$K\sum_n c_n|\psi_n\rangle = \sum_n c_n^*|\psi_n\rangle, \tag{217}$$

   K does nothing with the basis vectors in which it is defined.

   Let us now use another basis set, $\{|\phi_j\rangle\}$, related to the previous one as $|\psi_n\rangle = \sum_j u_{nj}|\phi_j\rangle$, where we find

   $$K\sum_{jn} c_n u_{nj}|\phi_j\rangle = \sum_{jn} c_n^* u_{nj}^*|\phi_j\rangle. \tag{218}$$

   The complex conjugation does not stop after c_n in this basis and gives a result which agrees with (217) for real u_{nj} only.

(b) K acts always to right, never to left and $K^\dagger$ is ill defined. This problem comes from the inconsistency of the bracket formalism when it deals with anti-linear operators,

$$\langle\psi|K_{\rightarrow}a|\phi\rangle = a^*\langle\psi|K|\phi\rangle \neq \langle\psi|_{\leftarrow}Ka|\phi\rangle = a\langle\psi|K|\phi\rangle, \tag{219}$$

where the arrow shows the direction K is acting. As a result the hermitian conjugate, $\langle\psi|K|\phi\rangle = \langle\phi|K^\dagger|\psi\rangle^*$, can not be introduced neither.

2. Symmetries, realized by anti-linear operators do not lead to conserved quantities. In fact, let us suppose that an anti-linear operator A corresponds to a symmetry, $[A, H] = 0$ and the initial condition is an eigenvector if the symmetry transformation, $A|\psi(t_i)\rangle = \lambda|\psi(t_i)\rangle$. The solution of the Schrödinger equation is not an eigenvector since

$$A|\psi(t)\rangle = Ae^{-\frac{i}{\hbar}(t-t_i)H}|\psi(t_i)\rangle = e^{\frac{i}{\hbar}(t-t_i)H}A|\psi(t_i)\rangle \neq \lambda|\psi(t)\rangle. \tag{220}$$

There is a useful representation of anti-unitary operators, they can be written as $A = UK$, the product of a unitary operator U,$U^\dagger U = \mathbb{1}$ and complex conjugation. The product $A = UK$ is obviously anti-linear, what is left to check is anti-unitarity. For this end consider the states $|\phi\rangle = \sum_n a_n|n\rangle$, $|\psi\rangle = \sum_n b_n|n\rangle$, written in a basis with real wave functions, $K|n\rangle = |n\rangle$. The scalar product $\langle\phi|\psi\rangle$ transforms

$$\begin{aligned}
\langle\tilde{\phi}|\tilde{\psi}\rangle &= (UK\sum_m a_m|m\rangle)^\dagger UK\sum_n b_n|n\rangle \\
&= (\sum_m a_m^* U|m\rangle)^\dagger \sum_n b_n^* U|n\rangle \\
&= \sum_{mn} a_m b_n^* \langle m|U^\dagger U|n\rangle \\
&= (\sum_{mn} a_m^* b_n \langle n|m\rangle)^* \\
&= \langle\phi|\psi\rangle^*
\end{aligned} \tag{221}$$

indeed as required by (216). The representation $A = UK$ can be used to construct basis independent anti-unitary operator. All we have to do is to use a unitary operator U which is basis dependent in such a manner that it compensates the basis dependence of K.

C. Space inversion

The space inversion is the simplest to define in coordinate basis, $P|\boldsymbol{x}\rangle = e^{i\alpha}|-\boldsymbol{x}\rangle$. It is a unitary transformation because the scalar product is preserved, $\langle\boldsymbol{x}|\boldsymbol{y}\rangle = \langle-\boldsymbol{x}|-\boldsymbol{y}\rangle$. It is a useful

convention to choose the phases of the basis states $\{|\boldsymbol{x}\rangle\}$ in such a manner that $\delta = 0$, giving $P^2 = \mathbb{1}$, $P = P^{-1} = P^\dagger$.

It is easy to find out the transformation of the canonical variables under space inversion. The relation

$$\langle\phi|P^\dagger \boldsymbol{x} P|\psi\rangle = -\langle\phi|\boldsymbol{x}|\psi\rangle \tag{222}$$

gives the operator equation

$$P^\dagger \boldsymbol{x} P = -\boldsymbol{x}. \tag{223}$$

The transformation rule for the momentum can be found by requiring the invariance of the canonical commutation relation under space inversion,

$$P^\dagger \left[x_j, p_k\right] P = -[x_j, P^\dagger p_k P] = i\hbar\delta_{j,k}, \tag{224}$$

giving

$$P^\dagger \boldsymbol{p} P = -\boldsymbol{p}. \tag{225}$$

As a result we find another useful transformation rule,

$$P^\dagger \boldsymbol{L} P = \boldsymbol{L}. \tag{226}$$

The wave function transform as

$$P\psi(\boldsymbol{x}) = \langle\boldsymbol{x}|P|\psi\rangle = \langle\boldsymbol{x}|P^\dagger|\psi\rangle = \langle -\boldsymbol{x}|\psi\rangle = \psi(-\boldsymbol{x}), \tag{227}$$

and we find the same result in momentum space,

$$P\psi(\boldsymbol{p}) = \psi(-\boldsymbol{p}), \tag{228}$$

too.

The eigenstate of space inversion posses well defined parity, $P|\psi\rangle = \pi_\psi|\psi\rangle$, $\pi_\psi^2 = 1$, $\pi_\psi = \pm 1$. The wave function of states with parity 1 or -1 is even or odd, respectively. One can introduce space inversion parity for operators, as well, $P^\dagger O P = \pi_O O$. It is important to know the parity of the electromagnetic field. To find these parities one may start by noting that the parity of the four-current, $j^\mu = (c\rho, \boldsymbol{j})$ is $\pi_\rho = -\pi_{\boldsymbol{j}} = 1$ and the interaction Lagrangian, $ej^\mu A_\mu$ with $A_\mu = (\phi, -\boldsymbol{A})$, is space inversion invariant, giving $\pi_\phi = -\pi_{\boldsymbol{A}} = -\pi_{\boldsymbol{E}} = \pi_{\boldsymbol{B}} = 1$.

The spherical harmonics, given by eq. (175) transform as

$$PY_m^{(\ell)}(\boldsymbol{n}) = Y_m^{(\ell)}(-\boldsymbol{n}) = (-1)^\ell Y_m^{(\ell)}(\boldsymbol{n}), \tag{229}$$

and we have in general

$$P|\ell, m\rangle = (-1)^\ell |\ell, m\rangle. \tag{230}$$

Note that in a system of two particles the parity, $\pi_{|\ell,m\rangle} = (-1)^{\ell_1+\ell_2}$ may or may not be identical with $(-1)^L$.

We mention a simple theorem, stating that the non-degenerate eigenstate of a space inversion invariant Hamiltonian $H|\psi\rangle = E|\psi\rangle$ possesses well defined parity. The proof uses the projection operator, $P_\pm = \frac{1}{2}(\mathbb{1} \pm P)$, onto the subspace of parity $\pi = \pm 1$. The inversion symmetry, $[P, H] = 0$, gives $HP_\pm|\psi\rangle = EP_\pm|\psi\rangle$ and the theorem follows by remarking only that one of the subspace can contain a non-degenerate eigenvector. As an application, one may mention the case of a double well potential, $U(x) = -ax^2 + bx^2$, with $a, b > 0$. The theorem states that despite the potential barrier between the minimas each stationary state in this potential have even or odd wave function.

Permanent electric dipole moments present a non-trivial use of space inversion symmetry. The electric dipole of a multi-particle system is

$$\boldsymbol{d} = \sum_n e_n \boldsymbol{r}_n, \tag{231}$$

where e_n and $\boldsymbol{r}_n$ denote the charge and the coordinate of the n-th particle. The dipole moment is permanent if it is non-vanishing in the absence of external electric field. The dipole operator has -1 parity its expectation value changes sign under space inversion,

$$\langle\psi|\boldsymbol{d}|\psi\rangle = \langle\psi|P^\dagger P\boldsymbol{d}P^\dagger P|\psi\rangle = -\langle\psi|P^\dagger \boldsymbol{d}P|\psi\rangle. \tag{232}$$

If the state $|\psi\rangle$ is a non-degenerate eigenstate of the space inversion invariant Hamiltonian then it has a well defined parity, π_ψ, furthermore we have

$$\langle\psi|\boldsymbol{d}|\psi\rangle = -\langle\psi|P^\dagger \boldsymbol{d}P|\psi\rangle = -\pi_\psi^2\langle\psi|\boldsymbol{d}|\psi\rangle = -\langle\psi|\boldsymbol{d}|\psi\rangle, \tag{233}$$

making the permanent electric dipole vanishing. If the state $|\psi\rangle$ is degenerate then permanent electric dipole is possible, as observed in the $n = 2$, fourfold degenerate state of the hydrogen atom.

D. Time inversion

To every solution of a dynamical system corresponds another one, obtained by sending the time in opposite direction. Time reversal of classical mechanics consists of the the transformation $x(t) \to x(-t)$ or $(x,p) \to (x,-p)$ of the trajectories or canonical variables, respectively. Though time inversion deals with the time evolution of the system nevertheless it can be stated in terms of the transformation of the canonical variable at a given time because the equation of motion is of first order in the phase space.

The time reversal, $T|\psi(t)\rangle = |\psi(t)^T\rangle$, is anti-linear in quantum mechanics because the Schrödinger equation, $i\hbar\partial_t|\psi\rangle = H|\psi\rangle$, reads for the time reversed system as

$$i\hbar\partial_t T|\psi\rangle = -HT|\psi\rangle = -TH|\psi\rangle = -Ti\hbar\partial_t|\psi\rangle, \tag{234}$$

where it is assumed that the Hamiltonian is time independent, $[T,H]=0$.

The determination of the transformation rule of observables under time reversal is facilitated by the relation

$$\langle\phi|O|\psi\rangle = \langle\psi^T|TO^\dagger T^{-1}|\phi^T\rangle, \tag{235}$$

holding for any linear operator O. The proof of this equation is simplified by introducing the state $|\chi\rangle = O^\dagger|\phi\rangle$,

$$\begin{aligned}
\langle\phi|O|\psi\rangle &= \langle\chi|\psi\rangle \\
&= \langle\psi^T|\chi^T\rangle \\
&= \langle\psi^T|TO^\dagger|\phi\rangle \\
&= \langle\psi^T|TO^\dagger T^{-1}T|\phi\rangle \\
&= \langle\psi^T|TO^\dagger T^{-1}|\phi^T\rangle.
\end{aligned} \tag{236}$$

The coordinate is time independent.

$$T^{-1}\boldsymbol{x}T = \boldsymbol{x}, \tag{237}$$

hence we have $\langle\phi^T|\boldsymbol{x}|\psi^T\rangle = \langle\phi|\boldsymbol{x}|\psi\rangle$, and

$$\hat{\boldsymbol{x}}T|\boldsymbol{y}\rangle = T\hat{\boldsymbol{x}}|\boldsymbol{y}\rangle = \boldsymbol{y}T|\boldsymbol{y}\rangle, \tag{238}$$

leading to

$$T|\boldsymbol{x}\rangle = e^{i\gamma(\boldsymbol{x})}|\boldsymbol{x}\rangle. \tag{239}$$

We shall use time inversion which is based on the coordinate representation, meaning $\gamma(\boldsymbol{x}) = 0$. The transformation rule for the momentum is inferred from the invariance of the canonical commutation relation under time reversal. The commutation relation, applied to an arbitrary state,

$$[x_j, p_k]\,|\psi\rangle = i\hbar\delta_{j,k}|\psi\rangle, \tag{240}$$

implies

$$T\,[x_j, p_k]\,T^{-1}T|\psi\rangle = \left[x_j, Tp_kT^{-1}\right]T|\psi\rangle = -i\hbar\delta_{j,k}T|\psi\rangle \tag{241}$$

which gives

$$T^{-1}\boldsymbol{p}T = -\boldsymbol{p}. \tag{242}$$

The transformed momentum eigenstate satisfies the equations

$$\hat{\boldsymbol{p}}T|\boldsymbol{p}'\rangle = -T\hat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = -\boldsymbol{p}'T|\boldsymbol{p}'\rangle, \tag{243}$$

resulting in

$$T|\boldsymbol{p}\rangle = e^{i\kappa(\boldsymbol{p})}|-\boldsymbol{p}\rangle. \tag{244}$$

The transformation rules (237) and (242) give the transformation rule

$$T^{-1}\boldsymbol{L}T = -\boldsymbol{L} \tag{245}$$

for angular momentum.

The wave function transform as

$$\begin{aligned} T\psi(\boldsymbol{x}) &= \langle\boldsymbol{x}|T|\psi\rangle \\ &= \int d^3y\langle\boldsymbol{x}|T|\boldsymbol{y}\rangle\langle\boldsymbol{y}|\psi\rangle \\ &= \int d^3y\langle\boldsymbol{x}|\boldsymbol{y}\rangle\langle\boldsymbol{y}|\psi\rangle^* \\ &= \psi(\boldsymbol{x})^* \end{aligned} \tag{246}$$

in the coordinate representation. The application of this rule to $\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle\boldsymbol{x}|\boldsymbol{p}\rangle = e^{\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}}$ yields the transformation

$$T\psi_{\boldsymbol{p}}(\boldsymbol{x}) = Te^{\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}} = e^{-\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}} = \psi_{-\boldsymbol{p}}(\boldsymbol{x}), \tag{247}$$

which in turn gives

$$T|\boldsymbol{p}\rangle = T\int d^3x|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle = \int d^3x|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle^* = \int d^3x|\boldsymbol{x}\rangle\langle\boldsymbol{x}|-\boldsymbol{p}\rangle = |-\boldsymbol{p}\rangle, \tag{248}$$

and $\kappa(\boldsymbol{p}) = 0$ in (244). The momentum space wave function transforms as

$$\begin{aligned} T\psi(\boldsymbol{p}) &= \langle \boldsymbol{p}|T|\psi\rangle \\ &= \int \frac{d^3p'}{(2\pi\hbar)^3}\langle \boldsymbol{p}|T|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'|\psi\rangle \\ &= \int \frac{d^3p'}{(2\pi\hbar)^3}\langle \boldsymbol{p}|-\boldsymbol{p}'\rangle\psi(\boldsymbol{p}')^* \\ &= \psi(-\boldsymbol{p})^* \end{aligned} \tag{249}$$

The transformation rule of the spherical harmonics, (175),

$$TY_m^{(\ell)}(\boldsymbol{n}) = (-1)^m Y_{-m}^{(\ell)}(\boldsymbol{n}), \tag{250}$$

gives

$$T|\ell, m\rangle = (-1)^m|\ell, -m\rangle. \tag{251}$$

One can introduce time reversal parity for states, $T|\psi\rangle = \tau_\psi|\psi\rangle$, and operators, $T^{-1}OT = \tau_O O$. Since applying time reversal twice one regains the original time direction and the same physical state we have

$$T^2|\psi\rangle = e^{2i\gamma}|\psi\rangle, \tag{252}$$

and $\tau_\psi = e^{i\gamma}$. As noted above, this parity is not conserved. As of the electromagnetic field is concerned, $\tau_\rho = -\tau_{\boldsymbol{j}} = 1$ leads to $\tau_\phi = -\tau_{\boldsymbol{A}} = \tau_{\boldsymbol{E}} = -\tau_{\boldsymbol{B}} = 1$.

It is easy to find the theorem, analogues to the case of space inversion. The non-degenerate eigenstate, $H|\psi\rangle = E|\psi\rangle$, of the time reversal invariant Hamiltonian, $[T, H] = 0$ has a space independent phase. To prove this we start with the equations

$$HT|\psi\rangle = TH|\psi\rangle = ET|\psi\rangle, \tag{253}$$

yielding $T|\psi\rangle = e^{i\delta}|\psi\rangle$. Comparing this result with the transformation rule (246) we find for the wave function parametrized as $\psi(\boldsymbol{x}) = \rho(\boldsymbol{x})e^{i\chi(\boldsymbol{x})}$

$$\chi(\boldsymbol{x}) = -\frac{\delta}{2}. \tag{254}$$

An important lesson is to be learned from the application of time inversion on the spin operator $\boldsymbol{S} = \hbar\boldsymbol{\sigma}/2$. According to eq. (245) we find

$$T^{-1}\boldsymbol{\sigma}T = -\boldsymbol{\sigma} \tag{255}$$

which gives for $T = UK$

$$U^\dagger \sigma_{\underset{z}{x}} U = -\sigma_{\underset{z}{x}}, \quad U^\dagger \sigma_y U = \sigma_y. \tag{256}$$

This equation can be satisfied by the choice $U = e^{i\theta}\sigma_y$ when eq. (110) is used. The usual convention is

$$U = -i\sigma_y = e^{-i\frac{\pi}{2}\sigma_y} = e^{-\frac{i}{\hbar}\pi S_y} = U(R_y(\pi)) \tag{257}$$

which gives

$$T^2 = U(R_y(2\pi)). \tag{258}$$

This is a highly non-trivial and important result, relating time reversal and rotations. The application of T^2 on a state $|J, \Sigma\rangle$ with well defined angular total momentum,

$$T^2|J,\Sigma\rangle = U(R_y(2\pi))|J,\Sigma\rangle = (-1)^{2J}|J,\Sigma\rangle = \pm|J,\Sigma\rangle, \tag{259}$$

shows that the application of two time reversal and rotation by 2π produces a multiplicative factor, 1 or -1 within the subspace of integer or half-integer angular momentum.

We are now in the position to show an important theorem for half integer spin states with time reversal invariant dynamics, $[T, H] = 0$. Let us take an eigenstate of the Hamiltonian, $|\psi\rangle$. The state $T|\psi\rangle$ has the same eigenvalue and let us now ask the question if these two vectors correspond to the same physical state. Let us suppose for the moment that the answer is affirmative and they correspond to the same state, $T|\psi\rangle = e^{i\alpha}|\psi\rangle$. Another time reversal gives

$$T^2|\psi\rangle = Te^{i\alpha}|\psi\rangle = e^{-i\alpha}T|\psi\rangle = e^{-i\alpha}e^{+i\alpha}|\psi\rangle = |\psi\rangle, \tag{260}$$

a condition which is compatible with integer angular momentum only. For particles with half integer angular momentum the states $|\psi\rangle$ and $T|\psi\rangle$ are different and degenerate. Such a Kramers degeneracy is usually a trivial spin up, spin down reduplication of the electron states. But the theorem becomes highly non-trivial for inhomogeneous electric field. For instance, odd or even umber of electrons had fundamentally different spectrum in an arbitrary external electric field which is time reversal even and the degeneracy for odd number of electron persists for arbitrary electric field but can be broken by a magnetic field.

Three space coordinates and the time are joined to form a four dimensional manifold in relativity and suggest some kind of similarity between space and time. But this similarity is rather limited, the time usually plays a distinguished role in physics. It has different signature as the space

coordinates in the Minkowski geometry, it is oriented as witnessed by irreversibility, it remains a c-number, passive parameter in quantum mechanics where the coordinates are traded into operators. Here we see another point where time creates exceptions, it makes us looking for an extension of Dirac's bracket formalism.

VI. RELATIVISTIC CORRECTIONS TO THE HYDROGEN ATOM

A. Scale dependence of physical laws

The relativistic corrections to the dynamics of the hydrogen atom represent a nice manifestation of an interesting feature of the physical laws, namely that *any observation depends on the scale involved*.

Scales refer in physics to dimensional quantities. What is the meaning of dimensions? What is the difference between say $\sqrt{2}$ and the diameter $20cm$ of a ball? The former is an element of the set of real numbers. The latter expresses a ratio between the size of the ball and the unit of length, a convention. Hence dimensional quantities always express a ratio of properties of physical objects and chosen units.

A measuring process always contains dimensional parameters, for instance the mass or size of the apparatus and the time of the measurement. When these parameters are modified then the measurement involves different physical quantities, different set of elementary constituents, briefly it covers different physics. Therefore the result of the observation changes, c.f. Fig. 8 where the emergent phenomenas are indicated as the function of the spatial resolution of the observations. The understanding and the reproduction of such a scale dependence is the goal of the renormalization group method, developed approximately fifty years ago in high energy and statistical physics. Our concepts are based on our experiences, conveyed to us by our senses and are formed in our childhood when our brains plasticity is still high. We play with macroscopic toys in that time and our concept cover few orders of magnitudes around our natural scale, around say a meter. This is the reason we need the formal concepts of mathematics to navigate among the results, produced by our "extended senses", the microscopes and telescopes. Both the quantitative numerical values and the qualitative laws depend on the scale of the observations. This is why our intuition, based on macroscopic physics, is completely lost when the resolution of the observation reaches a scale somewhere between a cell and molecule, where the quantum world opens up.

It is fair to say that there are no constants physical values and what are called "constants" in

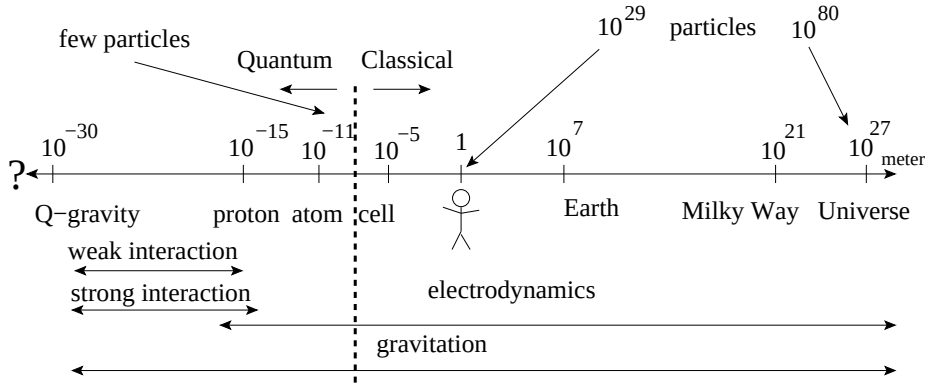


FIG. 8: Few relevant length scales and the fundamental interactions as the function of length.

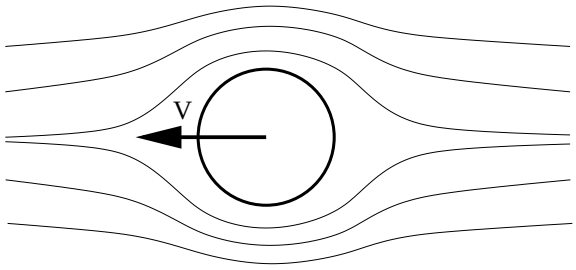


FIG. 9: A ball, moving in a fluid. The realistic fluid is viscous and its flow patter is turbulent, leading to more fluid moving with the ball.

physics and engineering are actually (slowly) changing functions of observation scales with possible long plateau. The Bureau of Standard exists just to monitor and maintain the special environment, needed to keep certain physical quantities fixed. Consider for instance the mass of a ball which is well defined for an isolated body but the situation changes as soon as the environment is taken into account. In fact, a ball, shown in Fig. 9 moving with velocity v with respect to a fluid, has an ill defined mass since certain fluid molecules are dragged along the motion and there is no clear separation between the molecules, belonging to the ball and the fluid. A possible strategy to define the mass is to measure the energy, assumed to be the sum of the ball and the fluid energy, $E_{tot}(v) = E_{ball}(v) + E_{fl}$, and write $E_{ball} = \frac{m(v)}{2}v^2$, yielding $m(v) = \frac{d^2 E_{tot}(v)}{dv^2}$. This quantity is "running", i.e. depends on the scale parameter, v, of the experimental setup. A similar analysis reveals the scale-dependence of other physical "constants".

A more realistic example is a system of electrons, described for the sake of simplicity by QED, a theory containing two parameters, the electron mass, m and charge, e. The dependence of these parameters can be represented by a curve, the renormalized trajectory, in the parameter space of the theory as depicted in Fig. 10.

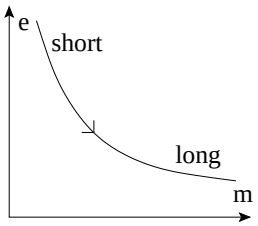


FIG. 10: The electron mass and the charge as the function of the resolution in the space-time in QED.

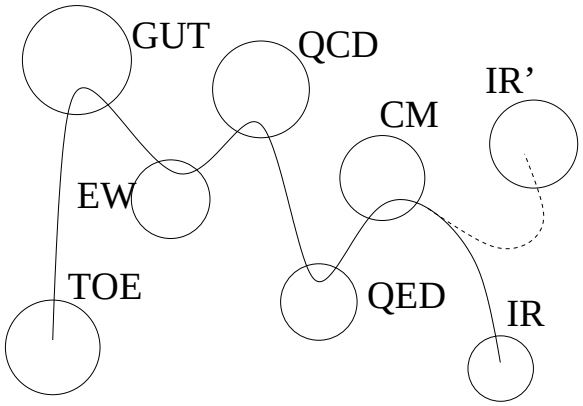


FIG. 11: The renormalized trajectory of the Theory of Everything.

It is instructive to try to imagine the Theory Of Everything whose parameters cover all "constants", used in physics. Its renormalized trajectory is a curve in this high dimensional space. There are special theories, called renormalizable theories, which in the limit of very fine resolution produce scale independent observables. These are indicated by circles in Fig. 11 and the renormalized trajectory, the observed values of the "physical constants", visit them as the resolution changes. The renormalized trajectory provides us a "guided tour of physics" and defines the effective theories which are valid in certain limited scale windows. The search of the Theory Of Everything, perhaps the most attractive problem in physics, remains a remote possibility for us, being able to cover phenomenas in finite scale windows. But even if it were found, the possible chaotic feature of the renormalized trajectory would render the its knowledge irrelevant at our scales.

B. Hierarchy of scales in QED

The strength of the electromagnetic interaction can be characterized by the dimensionless coupling constant

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137} \tag{261}$$

which can be used to order the relativistic effects in the hydrogen atom as well since

$$\frac{v^2}{c^2} \approx \frac{\hbar^2}{m^2 a_0^2 c^2} = \frac{e^4}{\hbar^2 c^2} = \alpha^2. \tag{262}$$

The smallness of this coupling strength leads the the emergence of a hierarchy of the length scales in quantum electrodynamics. In fact, starting with the scale of atomic physics, a_0, the perturbation expansion expressions contain the length scales $r_n = a_0 \alpha^n$ with $n = 1, 2, ...$

1. $n = 0$: The first scale, the longest length scale is the Bohr radius, $a_0 \approx 0.053nm$ which is the order of magnitude of the size of a hydrogen atom. The spectrum, seen at such a space resolution is the $\mathcal{O}\left(c^0\right)$ non-relativistic energy levels.

2. $n = 1$: The second length scales is the Compton wavelength,

$$\lambda_C = \frac{\hbar}{mc} \approx 3.86 \cdot 10^{-11} cm = 386 fm. \tag{263}$$

being independent of the electric charge, e, it belongs to the dynamics of the electron without taking into account its coupling to the electromagnetic field. The Compton wavelength belongs to the spatial extension of a maximally localized particle. In fact, the characteristic length of the wave function of a particle, localized in a region of size ℓ, is ℓ and the electron has the kinetic energy

$$E = c\sqrt{m^2c^2 + \boldsymbol{p}^2} \approx c\sqrt{m^2c^2 + \frac{\hbar^2}{\ell^2}}, \tag{264}$$

in this state. This energy is sufficient to create an particle-anti particle pair and delocalize it if $\ell \lessapprox \lambda_C$. When we attempt to localize a charged particle within a region of extension smaller than the Compton wavelength then the generated anti-particles escape and render the usual, first quantized formalism of quantum mechanics where the number of particle is fixed, inappropriate. The emergent anti-particle radiation can be described by using the second quantized formalism of quantum field theory.

3. $n = 2$: The third scale is the classical electron radius, r_c, the order of magnitude of the electron-proton separation where the Coulomb energy is sufficient to create electron-positron pairs. It is defined by

$$\frac{e^2}{r_c} = mc^2, \tag{265}$$

giving

$$r_c = \frac{e^2}{mc^2} \approx 2.8fm. \tag{266}$$

This scale does not contain $\hbar$ therefore it belongs to the realm of classical physics. To understand the physical relevance of this scale consider an imaginary world without quantum mechanics. The electrodynamics of point charges has a single intrinsic length scale, r_c. The careful solution of the theory reveals that the electromagnetic interactions, known to us are dominant at length scales longer than r_c only and singularities and acausalities show up at distances shorter than r_c. The physical process which becomes stronger as we approach the scale r_c from longer distance is the interaction of the charge with the electromagnetic field, generated by itself, the Abraham-Lorentz force. Naturally, being deeply in the quantum domain the corresponding classical phenomenon is embedded into quantum processes in our world.

4. $n = 3$: One finds yet another scale, an accidental degeneracy of the spectrum of the hydrogen atom in the total angular momentum after having taken into account the leading order relativistic corrections is spited by the Lamb shift and this interaction takes place at scale

$$\ell_L = \frac{e^4}{mc^3\hbar} \approx 0.02fm \tag{267}$$

Further, higher order, shorter length scales are more difficult to identify because they belong to involved, multi-particle effects.

C. Unperturbed, non-relativistic dynamics

The non-relativistic discussions is based on the separation of the center of mass motion, by writing the Hamiltonian as $H_{nr} = H_{cm} + H_r$, with

$$\begin{aligned} H_{cm} &= \frac{\boldsymbol{P}^2}{2M}, \\ H_r &= \frac{\boldsymbol{p}^2}{2m} - \frac{e^2}{r}, \end{aligned} \tag{268}$$

where $\boldsymbol{P} = \boldsymbol{p}_e + \boldsymbol{p}_p$ is the total momentum, $M = m_e + m_p$ stands for the total mass, $\boldsymbol{p} = \boldsymbol{p}_e - \boldsymbol{p}_p$ and $\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_p$ denote the relative momentum and coordinate, respectively and

$$\frac{1}{m} = \frac{1}{m_e} + \frac{1}{m_p} \approx \frac{1}{m_e}. \tag{269}$$

The eigenstates of H_r can be written in the factorized form

$$\psi_{n,\ell,m,s_e,s_p}(r,\theta,\phi,\sigma,\Sigma) = \eta_{n,\ell}(r) Y_m^\ell(\theta,\phi)\chi_{s_e}(\sigma)\chi_{s_p}(\Sigma), \tag{270}$$

where the radial dynamics determines $\eta_{n,\ell}(r)$, the rotational symmetric potential leads to the directional dependence, given by the spherical harmonics $Y_m^\ell(\theta,\phi)$ and $\chi_{s_e}(\sigma)$ and $\chi_{s_p}(\Sigma)$ denote the electron and proton spin wave functions, respectively. The energy eigenvalue of such a state is

$$E_{n,\ell,m,s} = -\frac{R}{n^2}, \tag{271}$$

with $\ell = 0,\ldots,n-1$ and $-\ell \leq m \leq \ell$, where $R = \frac{\hbar^2}{2ma_0^2} \approx 13.6eV$ denotes the Rydberg constant and a_0 stands for the Bohr radius, $a_0 = \frac{\hbar^2}{me^2} \approx 0.53A$. The $(2S_p+1)(2S_e+1)n^2 = 4n^2$-fold degeneracy of the energy levels is the result of an accidental degeneracy, the independence of the energy of the angular momentum and the spin independence of the Coulomb interaction.

The spectrum and the stationary states of the hydrogen atom, mentioned above, are appropriate when used with the resolution in space-time, comparable with the Bohr radius. The shorter distance scale structure of the wave function is modified by the relativistic corrections to the kinetic energy, by the creation of virtual electron-positron pairs and byt the induction of magnetic field.

The relativistic transformation rules are different for the coordinates and the spin vectors, leading to a non-trivial coupling of the spins and $\boldsymbol{r}$. The coupling of the electron spin and orbital angular momentum destroys the symmetry with respect to the independent rotations of the electron coordinate $\boldsymbol{r}$ and spin $\boldsymbol{s}$, leaving the simultaneous rotation of the total angular momentum, $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{s}$ as a symmetry generator. These effect can easily be sorted out experimentally because the sensitivity of the spectrum on the perturbation in the subspaces where the unperturbed Hamiltonian is degenerate.

D. Fine structure

The operators, reflecting the relativistic effects of the electron should be symmetric with respect to three-rotations and space inversion. This requirement restricts them to $\boldsymbol{r}^2$, $\boldsymbol{p}^2$, $\boldsymbol{rp}$ and $\boldsymbol{L}^2$ as far as the orbital motion is concerned. The electron spin appear in the rotational invariant form in the combinations $\boldsymbol{Sr}$, $\boldsymbol{Sp}$ and $\boldsymbol{S}\cdot\boldsymbol{L}$ the last being the only one which is invariant under space inversion, too.

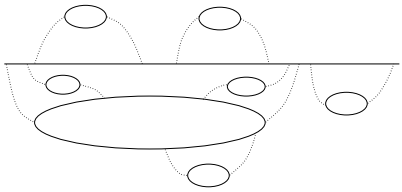


FIG. 12: Elementary processes in QED, contributing to the spread of the charge distribution by vacuum polarization.

1. Relativistic corrections to the kinetic energy

1. Origin: The relativistic corrections to the kinetic energy,

$$E = c\sqrt{m^2c^2 + \boldsymbol{p}^2} = mc^2 + \frac{\boldsymbol{p}^2}{2m} - \frac{\boldsymbol{p}^4}{8m^3c^2} + \mathcal{O}\left(\left(\frac{v}{c}\right)^6\right) \tag{272}$$

   modify the stationary states of a free particle.

2. Form: The energy spectrum of a free particle is

$$H_0 = \frac{\boldsymbol{p}^2}{2m} - \frac{\boldsymbol{p}^4}{8m^3c^2} = \frac{\boldsymbol{p}^2}{2m} + H_m. \tag{273}$$

3. Magnitude: The order of magnitude of the shift of the spectrum is

$$\frac{|H_m|}{\frac{\boldsymbol{p}^2}{2m}} \approx \frac{v^2}{c^2} = \alpha^2 \tag{274}$$

2. Darwin term

1. Origin: A point charge is surrounded by a cloud of virtual electron-positron pairs, reflecting the vacuum polarization of the Dirac-see, in close analogy with the polarization of a classical dielectric material. Such a spread of the elementary charge distribution can be followed in QED, a typical Feynman graph being shown in Fig. 12.

2. Form: Let us suppose that a point charge distribution, $\rho(\boldsymbol{r}) = \delta(\boldsymbol{r})$ is smeared to $\rho(\boldsymbol{r})$, $\int d\boldsymbol{r}\rho(\boldsymbol{r}) = 1$, by elementary processes in QED. This amounts to a dressing of the Coulomb

potential, $U_C(r) \to U(r) = U_C(r) + U_D(\boldsymbol{r})$, where $U_C(r) = \frac{e^2}{r}$ and

$$\begin{aligned} U(\boldsymbol{r}) &= \int d\boldsymbol{r}'\rho(\boldsymbol{r}')U_C(\boldsymbol{r}+\boldsymbol{r}') \\ &= \int d\boldsymbol{r}'\rho(\boldsymbol{r}')\left[U_C(\boldsymbol{r}) + \boldsymbol{r}'\boldsymbol{\nabla}U_C(\boldsymbol{r}) + \frac{1}{2}r'_j r'_k \partial_j\partial_k U_C(\boldsymbol{r}) + \cdots\right] \\ &= U_C(\boldsymbol{r}) + \frac{1}{6}\boldsymbol{\nabla}^2 U_C(\boldsymbol{r}) \underbrace{\int d\boldsymbol{r}'\boldsymbol{r}'^2\rho(\boldsymbol{r}')}_{\frac{3}{4}\lambda_C^2} \\ &= U_C(\boldsymbol{r}) + U_D(\boldsymbol{r}). \end{aligned} \tag{275}$$

The explicit form of the Darwin term is $H_D = -U_D$, where

$$U_D(\boldsymbol{r}) = \frac{1}{8}\lambda_C^2\boldsymbol{\nabla}^2 U_C(\boldsymbol{r}) = -\frac{1}{2}\pi e^2\lambda_C^2\delta(\boldsymbol{r}) = -\frac{\pi\hbar^2 e^2}{2m^2c^2}\delta(\boldsymbol{r}). \tag{276}$$

3. Magnitude: The estimate

$$\langle U_D\rangle = \frac{\pi\hbar^2e^2}{2m^2c^2}\underbrace{|\psi(0)|^2}_{\approx\frac{1}{a_0^3}} \approx \frac{e^2\hbar^2}{m^2c^2}\frac{m^3e^6}{\hbar^6} = mc^2\frac{e^8}{\hbar^4c^4} = mc^2\alpha^4, \tag{277}$$

together with

$$\langle H_0\rangle \approx R = \frac{\hbar^2}{2ma_0^2} = \frac{\hbar^2}{2m}\frac{m^2e^4}{\hbar^4} = \frac{me^4}{2\hbar^2} = \frac{1}{2}mc^2\alpha^2 \tag{278}$$

yields

$$\frac{|\langle H_D\rangle|}{\langle H_0\rangle} \approx \alpha^2. \tag{279}$$

3. Spin-orbit coupling

1. Origin: The spin and the angular momentum represent a magnetic moment and a magnetic field, respectively in this case.

   Let us start by recalling the interaction energy,

$$H_i = -\boldsymbol{m}\boldsymbol{B}, \tag{280}$$

   between a magnetic moment $\boldsymbol{m}$ and the classical magnetic field $\boldsymbol{B}$. To find the magnetic moment, induced by the motion of charge in quantum mechanics we consider the classical Lagrangian of the charge, in the presence of an external electromagnetic field. The interaction

is described by the term $-\frac{e}{c}j^\mu A_\mu$, including the current $j^\mu = (nc, n\dot{\boldsymbol{x}})$ where n denotes the density and the vector potential $A^\mu = (\phi, \boldsymbol{A})$ hence the total Lagrangian is

$$L = \frac{m}{2}\dot{\boldsymbol{x}}^2 - e\phi(t,\boldsymbol{x}) + \frac{e}{c}\dot{\boldsymbol{x}}\boldsymbol{A}(t,\boldsymbol{x}). \tag{281}$$

The momentum,

$$\begin{aligned} \boldsymbol{p} &= \frac{\partial L(\dot{\boldsymbol{x}},\boldsymbol{x})}{\partial\dot{\boldsymbol{x}}} \\ &= m\dot{\boldsymbol{x}} + \frac{e}{c}\boldsymbol{A}(t,\boldsymbol{x}), \end{aligned} \tag{282}$$

is used to find the Hamiltonian,

$$\begin{aligned} H &= \boldsymbol{p}\dot{\boldsymbol{x}} - L \\ &= \frac{(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})^2}{2m} + e\phi, \end{aligned} \tag{283}$$

with $\boldsymbol{p} = \frac{\hbar}{i}\boldsymbol{\nabla}$.

While the interaction of a classical charge with the electromagnetic field can be described by the gauge invariant electric and magnetic fields, $\boldsymbol{E}$ and $\boldsymbol{B}$, respectively the possibility of interference requires a more detailed scheme in quantum mechanics. In fact, a charge follows a closed orbit, a circle in homogeneous magnetic field and it enters into an interference with itself. The need of keeping track of the phase factor, governing such an interference, requires the coupling to the magnetic field, appearing in the Lagrangian (281).

Let us assume a homogeneous magnetic field for the sake of simplicity, $\phi = 0$, $\boldsymbol{A} = -\frac{1}{2}\boldsymbol{r}\times\boldsymbol{B}$ and the Hamiltonian,

$$\begin{aligned} H &= \frac{\boldsymbol{p}^2}{2m} - \frac{e}{2mc}(\boldsymbol{pA}+\boldsymbol{Ap}) + \frac{e^2}{2mc^2}\boldsymbol{A}^2 \\ &= \frac{\boldsymbol{p}^2}{2m} - \frac{e}{mc}\boldsymbol{Ap} + i\frac{e\hbar}{2mc}\boldsymbol{\nabla A} + \frac{e^2}{2mc^2}\boldsymbol{A}^2 \\ &= \frac{\boldsymbol{p}^2}{2m} + \frac{e}{2mc}(\boldsymbol{r}\times\boldsymbol{B})\boldsymbol{p} + \frac{e^2}{2mc^2}\boldsymbol{A}^2 \\ &= \frac{\boldsymbol{p}^2}{2m} - \frac{e}{2mc}\boldsymbol{LB} + \frac{e^2}{2mc^2}\boldsymbol{A}^2 \end{aligned} \tag{284}$$

shows that the magnetic moment, due to the angular momentum is $\boldsymbol{m} = \frac{e}{2mc}\boldsymbol{L}$.

One expects a similar relation between the spin and the magnetic moment, as well. But the relativistic extension of the Schrödinger equation, the Dirac equation introduces a further factor 2 in these expressions. One can understand this by the help of a simpler equation, proposed by Pauli in 1927, the replacement, $\boldsymbol{P} = \boldsymbol{p} - \frac{e}{c}\boldsymbol{A} \to \boldsymbol{\sigma P}$ in the kinetic energy

$$H = \frac{\boldsymbol{P}^2}{2m} \to \frac{(\boldsymbol{\sigma P})^2}{2m} \tag{285}$$

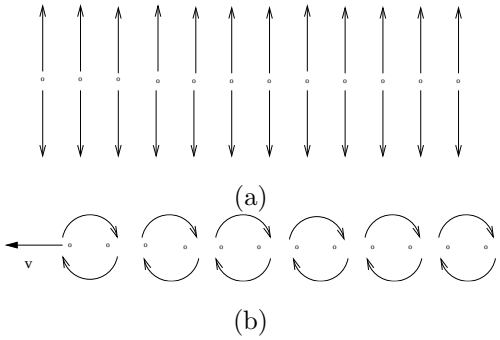


FIG. 13: (a): The electric field of a stationary current in the co-moving coordinate system with the charges. (b): The induced magnetic field in the laboratory frame.

A year later Dirac came forward with his relativistic equation of motion which reproduces Pauli's equation and introduces further $\mathcal{O}\left(p^4/m^3c^2\right)$ corrections. The Hamiltonian (285) can be written as

$$H = \frac{\{\sigma^j, \sigma^k\}\{P^j, P^k\} + [\sigma^j, \sigma^k][P^j, P^k]}{8m}. \tag{286}$$

The property (109) of the Pauli matrices yields $\{\sigma^j, \sigma^k\} = 2\delta^{jk}$, $[\sigma^j, \sigma^k] = 2i\epsilon^{jk\ell}\sigma^\ell$ which together with the relation $[\nabla^j + f^j, \nabla^k + f^k] = \nabla^j f^k - \nabla^k f^j$ give

$$\begin{aligned} \frac{(\boldsymbol{\sigma P})^2}{2m} &= \frac{\boldsymbol{P}^2}{2m} - \frac{\hbar e}{2mc}\epsilon^{jk\ell}\nabla^j A^k \sigma^\ell \\ &= \frac{\boldsymbol{P}^2}{2m} - \boldsymbol{mB} \end{aligned} \tag{287}$$

where the spin magnetic moment is $\boldsymbol{m} = \frac{\hbar e}{2mc}\boldsymbol{\sigma}$ is customary written in terms of the Bohr magneton, $\frac{e\hbar}{2mc}$ and the spin gyromagnetic factor $g = 2$ as $\boldsymbol{m} = g\mu_B \frac{\boldsymbol{S}}{\hbar}$. The important consequence of this result is that the magnetic moment arising from the motion of the electron and its spin is

$$\boldsymbol{m} = \mu_B \frac{\boldsymbol{L} + g\boldsymbol{S}}{\hbar} = \mu_B \frac{\boldsymbol{J} + (g-1)\boldsymbol{S}}{\hbar} \neq \mu_B \frac{\boldsymbol{J}}{\hbar} \tag{288}$$

where $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$.

But what is the magnetic field in the hydrogen atom? The naive answer to this question, stating that the magnetic field due to the proton at rest is vanishing holds in the reference frame attached to the proton. It is more appropriate to ask this question in the reference frame where the electron is at rest at a given time. The point is that the Lorentz boost, connecting these two reference frames mixes the temporal end spatial components of the vector potential A_μ which induces a mixing of the electric and magnetic fields. In particular,

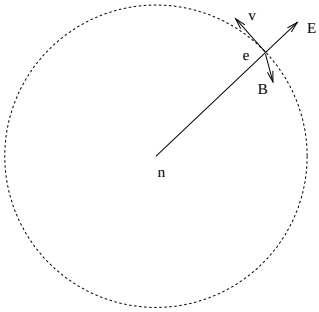


FIG. 14: Origin of the spin-orbit force.

an electric field $\boldsymbol{E}$ produces a magnetic field

$$\boldsymbol{B} = -\frac{1}{c}\boldsymbol{v} \times \boldsymbol{E} \tag{289}$$

when seen from a reference frame, moving with velocity $\boldsymbol{v}$ with respect to the electric field, cf. Fig. 13. Therefore the Coulomb field of the proton induces a magnetic field when seen from the instantaneous reference frame where the electron is at rest.

2. Form: The interaction Hamiltonian (280), corresponding to the Coulomb field

$$\boldsymbol{E}(\boldsymbol{r}) = -\boldsymbol{e}_r \partial_r \frac{e}{r} = \frac{e}{r^2}\boldsymbol{e}_r \tag{290}$$

turns out

$$\begin{aligned} H_{so} &= -\boldsymbol{m}_s \boldsymbol{B} = 2\mu_B \frac{\boldsymbol{s}}{\hbar}\frac{\boldsymbol{v} \times \boldsymbol{E}}{c} \\ &= -\frac{\hbar e^2}{m^2} \cdot \frac{1}{\hbar c^2}\boldsymbol{s}(\boldsymbol{p} \times \boldsymbol{r})\frac{1}{r}\partial_r \frac{1}{r} \\ &= \frac{e^2}{m^2 c^2}\boldsymbol{s}\boldsymbol{L}\frac{1}{r}\partial_r \frac{1}{r}. \end{aligned} \tag{291}$$

3. Magnitude:

$$\frac{\langle H_{so}\rangle}{\langle U_C\rangle} \approx \frac{\frac{e^2\hbar^2}{m^2c^2a_0^3}}{\frac{e^2}{a_0}} = \frac{e^4}{\hbar^2 c^2} = \alpha^2 \tag{292}$$

E. Hyperfine structure

The proton moves in the electromagnetic field, generated by the electron. The former has been taken into account in the fine structure, discussed above which gives rise an effect which is suppressed by $m_e/m_p \sim 0.51MeV/938MeV \sim 1/2000$, called hyperfine structure.

1. Origin: The spin and the orbital momentum of the electron generates a magnetic field which interacts with the proton spin.

2. Form: The interaction energy (280) is

$$H_{hf} = -\frac{1}{c^2}\left\{\frac{e}{m_e R^3}\boldsymbol{L}\boldsymbol{m}_p + \frac{1}{R^3}[3(\boldsymbol{m}_e\boldsymbol{n})(\boldsymbol{m}_p\boldsymbol{n}) - \boldsymbol{m}_e\boldsymbol{m}_p] + \frac{8\pi}{3}\boldsymbol{m}_e\boldsymbol{m}_p\delta^{(3)}(R)\right\} \tag{293}$$

   where the electron and proton magnetic moments are

$$\begin{aligned}\boldsymbol{m}_e &= 2\frac{e\hbar}{2m_e}\frac{\boldsymbol{s}_n}{\hbar},\\ \boldsymbol{m}_p &= g_p\frac{e\hbar}{2m_n}\frac{\boldsymbol{s}_n}{\hbar},\end{aligned} \tag{294}$$

   where the proton magnetic moment, $g_p \approx 5.585$, is far from 2 due to the internal quark structure.

3. Magnitude:

$$\langle H_{hf}\rangle \approx \frac{e^2\hbar^2}{m_e m_p c^2 a_0^3} \approx \langle H_{so}\rangle\frac{m_e}{m_p}. \tag{295}$$

F. Splitting of the fine structure degeneracy

Most of the degeneracy in the spectrum of the non-relativistic hydrogen atom is split by the relativistic corrections, represented by the fine structure Hamiltonian

$$H_f = H_m + H_D + H_{so}. \tag{296}$$

The $\boldsymbol{L}\boldsymbol{s}$ coupling, appearing in the spin-orbit interaction can be diagonalized when the total angular momentum, $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{s}$ is used since

$$\boldsymbol{L}\boldsymbol{s} = \frac{1}{2}(\boldsymbol{J}^2 - \boldsymbol{L}^2 - \boldsymbol{s}^2). \tag{297}$$

Therefore we use the coupled basis

$$|n, J, M, \ell\rangle = \sum_{s_e} |n, \ell, M - s_e, s_e\rangle(\ell, \frac{1}{2}, M - s_e, s_e|J, M). \tag{298}$$

We shall use the traditional spectroscopic notations, the states will be labeled by the quantum numbers $n\ell_J$, and $\ell = 0, 1, 2, 3, \ldots = s, p, d, f, g, \ldots$.

1. $n = 1$

The $1s$ level has a 2×2 degeneracy in the spins. To find the first order correction to the energy, $E_n^{(1)} = \langle n|H_f|n\rangle$, we need the spectrum and the eigenstates of the non-relativistic Hamiltonian, H_0. The diagonal matrix elements $\langle n, \ell, m, s_s|H_f|n, \ell, m, s_s\rangle$ are calculated for the state with wave function

$$\langle r, \theta, \phi, s_s|n, \ell, m, s_s\rangle = R_{n,\ell}(r)Y_m^\ell(\theta, \phi)u(s_e) \tag{299}$$

where

$$R_{1,0}(r) = \frac{2}{a_0^{\frac{3}{2}}} e^{-\frac{r}{a_0}}, \tag{300}$$

and

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}. \tag{301}$$

$\boldsymbol{H_m}$: To find the matrix elements of the relativistic correction to the kinetic energy we write

$$\boldsymbol{p}^4 = 4m^2 \left(H_0 + \frac{e^2}{r}\right)^2 \tag{302}$$

where

$$H_0 = \frac{\boldsymbol{p}^2}{2m} - \frac{e^2}{r} \tag{303}$$

is the non-relativistic Hamiltonian of spectrum $E_n = -\frac{\alpha^2 mc^2}{2n^2}$. We now have the expression

$$H_m = -\frac{(H_0 + \frac{e^2}{r})^2}{2mc^2} \tag{304}$$

for the leading relativistic correction to the kinetic energy. Its expectation values are

$$\langle H_m\rangle = -\frac{1}{2mc^2}\left(E_n^2 + 2E_n\langle\frac{e^2}{r}\rangle + \langle\frac{e^4}{r^2}\rangle\right), \tag{305}$$

The calculation of the matrix elements of r^n is facilitated by the use of the generator functional

$$I(\kappa) = \int_0^\infty dr e^{-\kappa r} = \frac{1}{\kappa}, \tag{306}$$

because we have

$$\langle\frac{1}{r^n}\rangle = \frac{4\pi}{4\pi}\int_0^\infty dr r^{2-n}\frac{4}{a_0^3}e^{-\frac{2r}{a_0}} = \frac{4}{a_0^3}(-1)^{2-n}\frac{d^{2-n}I(\kappa)}{d\kappa^{2-n}}_{|\kappa=\frac{2}{a_0}} \tag{307}$$

for $n = 1, 2$, in particular,

$$\langle \frac{1}{r} \rangle = \frac{1}{a_0}, \qquad \langle \frac{1}{r^2} \rangle = \frac{2}{a_0^2} \tag{308}$$

give

$$\langle H_m \rangle = -\frac{1}{2mc^2} \left(\frac{\alpha^4 m^2 c^4}{4} - \frac{\alpha^2 mc^2 e^2}{a_0} + \frac{2e^4}{a_0^2} \right) = -\frac{5}{8} \alpha^4 mc^2. \tag{309}$$

$\boldsymbol{H_D}$: The calculation of the diagonal matrix is obvious, leading to

$$\langle H_D \rangle = \frac{e^2 \hbar^2 \pi}{2m^2 c^2} |\psi_{n,\ell,m}(0)|^2 = \frac{e^2 \hbar^2}{8m^2 c^2} |R_{1,0}(0)|^2 = \frac{1}{2} \alpha^4 mc^2. \tag{310}$$

$\boldsymbol{H_{so}}$: The matrix element is vanishing in the s-wave sector.

We find the shift $\Delta E = -\frac{1}{8} \alpha^4 mc^2$ in $1s_{\frac{1}{2}}$ and the degeneracy prevails.

2. $n = 2$

The fine structure within the shell $n = 2$ is non-trivial. This shell has the degeneracy

$$\underbrace{2}_{2s_{\frac{1}{2}}} + \underbrace{2}_{2p_{\frac{1}{2}}} + \underbrace{4}_{2p_{\frac{3}{2}}} = 8. \tag{311}$$

The fine structure is simplified by the absence of mixing of the states $2s$ and $2p$,

$$H_f = \begin{pmatrix} H_{2s} & 0 \\ 0 & H_{2p} \end{pmatrix}. \tag{312}$$

The radial wave functions,

$$R_{2,0} = \frac{2}{(2a_0)^{\frac{3}{2}}} \left(1 - \frac{r}{2a_0} \right) e^{-\frac{r}{2a_0}}, \qquad R_{2,1} = \frac{1}{\sqrt{2}(2a_0)^{\frac{3}{2}}} \frac{r}{a_0} e^{-\frac{r}{2a_0}}, \tag{313}$$

give the matrix elements

$$\langle 2s | \frac{1}{r} | 2s \rangle = \frac{1}{4a_0}, \qquad \langle 2s | \frac{1}{r^2} | 2s \rangle = \frac{1}{12a_0^2}, \qquad \langle 2s | \frac{1}{r^3} | 2s \rangle = \frac{1}{24a_0^3}. \tag{314}$$

The diagonal matrix elements within the subspace $2s$,

$$\begin{aligned} \langle H_m \rangle &= -\frac{13}{128} mc^2 \alpha^4 \\ \langle H_D \rangle &= -\frac{1}{16} mc^2 \alpha^4 \\ \langle H_{so} \rangle &= 0 \end{aligned} \tag{315}$$

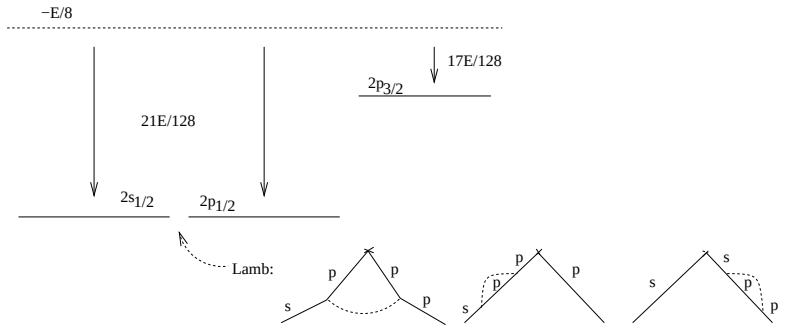


FIG. 15: Splitting of the shell $n = 2$ and the Lamb shift.

leave the degeneracy and produce the energy shift, $\Delta E_{2s_{\frac{1}{2}}} = -\frac{21}{128}\alpha^4 mc^2$. The $2p$ sector is

$$\begin{aligned}
\langle H_m\rangle &= -\frac{55}{384}mc^2\alpha^4 \\
\langle H_D\rangle &= 0 \\
\langle H_{so}\rangle &= \langle 2p, m, s_e|\frac{e^2}{2m^2c^2}\frac{1}{r^3}\boldsymbol{SL}|2p, m', s'_e\rangle = \underbrace{\frac{e^2}{2m^2c^2}\int_0^\infty dr r^2 \frac{1}{r^3}|R_{2,1}(r)|^2}_{\frac{mc^2\alpha^4}{48\hbar^2}}\langle 1, m, s_e|\boldsymbol{SL}|1, m', s'_e\rangle
\end{aligned} \tag{316}$$

where the vanishing of $\langle H_D\rangle$ is due to the asymptotic behavior $R_\ell = \mathcal{O}\left(r^\ell\right)$. The action of the operator $\boldsymbol{SL}$ on an angular momentum eigenstate,

$$\begin{aligned}
\boldsymbol{SL}|\ell, m, s\rangle &= \frac{1}{2}(\vec{J}^2 - \boldsymbol{L}^2 - \boldsymbol{S}^2)|\ell, m, s\rangle \\
&= \frac{\hbar^2}{2}\left[J(J+1) - \ell(\ell+1) - \frac{1}{2}\frac{3}{2}\right]|\ell, m, s\rangle \\
&= \frac{\hbar^2}{2}\left[J(J+1) - \frac{11}{4}\right]|\ell, m, s\rangle \\
&= \begin{cases} -\hbar^2|1, m, s_e\rangle & J = \frac{1}{2} \\ \frac{\hbar^2}{2}|1, m, s_e\rangle & J = \frac{3}{2} \end{cases}
\end{aligned} \tag{317}$$

gives

$$\langle H_{so}\rangle = \begin{cases} -\frac{1}{48}mc^2\alpha^4 & J = \frac{1}{2}, \\ \frac{1}{96}mc^2\alpha^4 & J = \frac{3}{2}. \end{cases} \tag{318}$$

The degeneracy in J is split, $\Delta E_{2p_{\frac{1}{2}}} = -\frac{21}{128}\alpha^4 mc^2$, $\Delta E_{2p_{\frac{3}{2}}} = -\frac{17}{128}\alpha^4 mc^2$ but the subspaces $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ remain degenerate. This degeneracy is split in $\mathcal{O}\left(\alpha^2\right)$ by photon emission and absorption processes.

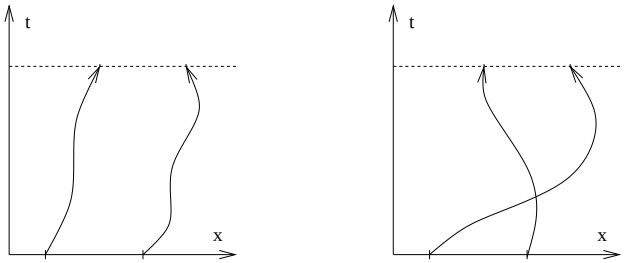


FIG. 16: Two possible propagations which may be impossible to distinguish in quantum mechanics.

VII. IDENTICAL PARTICLES

The quantum effects are proportional to some positive power of $\hbar$ and the small value of Planck constant in macroscopic units makes them unimportant for macroscopic system, except few remarkable exceptions.

A. A macroscopic quantum effect

How do we distinguish particles? We may classify them according to the internal quantum numbers, such as mass, spin, charge, etc. If these agree for two particles then we may look into their behavior in space, into their external quantum numbers, such as energy, momentum, angular momentum, etc.

Let us consider identical particles, particles with identical internal properties in classical physics and label them by the index n. Their state of motion is characterized by the set of initial conditions $\boldsymbol{x}_n(t_i) = \boldsymbol{x}_{ni}$ and $\dot{\boldsymbol{x}}_n(t_i) = \boldsymbol{v}_{ni}$. Suppose that we can determine the space points where a particle can be found at time t and find the set of locations $\{\boldsymbol{x}^{(j)}\}$. Can we establish a correspondence $n \leftrightarrow j$, between the initial particles and the locations where particle is found at a later time? As long as the kinetic energy is finite the particle trajectories have finite derivative and a sufficiently frequent check of the particle positions can be used to establish the unique trajectories and the correspondence $n \leftrightarrow j$, distinguishing the particles from each other.

The state of affairs changes in quantum mechanics where due to the uncertainty principle we can not keep the whole phase space for the characterization of the motion. For instance, whatever frequently do we measure the particle locations we can not construct their velocity, the observation interferes with the particle dynamics as reflected by the uncertainty principle. As soon as the precision to follow the motion in phase space is restricted the possibility of distinguishing the particles is limited, too. If the unique distribution of the index n among the particles is impossible

the distinguishability of the particles might partially be regained by the inspection of their spatial behavior. But as far as states at a given time are concerned we have lost the possibility of tracing down the individuality of particles with identical internal quantum numbers.

If the state $|x_1, x_2\rangle$ is not distinguishable from the one, obtained by the exchange of the two particles, $\pi|x_1, x_2\rangle = |x_2, x_1\rangle$ then

$$|x_2, x_1\rangle = e^{i\theta_e}|x_1, x_2\rangle, \tag{319}$$

the exchange produces a change of phase only. In terms of wave function we have

$$\psi(x_2, x_1) = e^{i\theta_e}\psi(x_1, x_2). \tag{320}$$

The loss of the distinguishability of identical particles reduces the number of possible physical states for N particles by $N!$. Such a reduction is dramatic for macroscopic system and one may wonder if it has already been noticed before the advent of quantum mechanics. One may say that the resolution of the paradox of the non-additivity of entropy in ideal gas, put forward by Gibbs is based on an intuitive realization of the indistinguishability of identical particles.

B. Fermions and bosons

One would naively conclude that the performance of two consecutive exchange oaf the particles is the identity transformation,$\pi^2 = 1$, allowing $e^{i\theta_e} = \pm 1$. But this is not necessarily so, all we can safely say that the physical state $\pi^2|x_1, x_2\rangle$ is identical of $|x_1, x_2\rangle$, $\pi^2|x_1, x_2\rangle = e^{2i\theta_e}|x_1, x_2\rangle$. But on can show that $e^{2i\theta_e} = 1$ in three dimensional space. The argument is based on another phase, hidden in our two-particle state. A rotation of a particle by 2π preserves the physical state and can produce a phase only,

$$U_j(R_{\boldsymbol{n}}(2\pi))|x_1, x_2\rangle = e^{i\theta_r}|x_1, x_2\rangle, \tag{321}$$

where the operator $U_j(R)$ represents rotations of the particle $j = 1, 2$. the spin-statistics theorem assures that the phase, acquired by rotating on of the identical particles by 2π is the same as the one, obtained by exchanging them. The rather deep spin-statistics theorem, proven by the methods of algebraic topology assures the identity of the two phases,

$$\theta_r = \theta_e. \tag{322}$$

Due to the double connected topology of the rotation group $SO(3)$ rotation by 4π is always trivial, $U_j(R_{\boldsymbol{n}}(4\pi)) = \mathbb{1}$, thus $\theta_r = 0$ or π in three dimensions. Particles with $\theta_r = 0$ have integer

angular momentum and are called bosons. States with $\theta_r = \pi$ correspond to half-integer angular momentum and represent fermions. It is advantageous to introduce the exchange statics, $\xi = e^{i\theta_r}$, assuming the value $+1$ and -1 for bosons and fermions, respectively, and write the spin-statistics theorem as

$$U(R_{\boldsymbol{n}}(2\pi)) = \xi. \tag{323}$$

In two dimensions the rotation group, $SO(2)$ is infinitely many connected, θ_r remains arbitrary and we have anyons, particle classes corresponding to arbitrary values of θ_r.

The different behavior of fermions and bosons under rotation by 2π can be observed for tensor operators, too. Namely, tensor operator with integer or half integer angular momentum preserve their form or change their sign under rotation by 2π according to Eq. (176). Classical physics has been known before quantum mechanics and is expressed in terms of vectors and tensors, all belonging to integer angular momentum. In other words, classical physics and observables are invariant under rotation by 2π. Let us now consider a matrix element $\langle\psi_{\xi'}|T^{(\ell)}_m|\phi_\xi\rangle$ of a tensor operator between states with well defined exchange statistics, written as

$$\langle\psi_{\xi'}|T^{(\ell)}_m|\phi_\xi\rangle = \langle\psi_{\xi'}|U^\dagger(R_{\boldsymbol{n}}(2\pi))U(R_{\boldsymbol{n}}(2\pi))T^{(\ell)}_m U^\dagger(R_{\boldsymbol{n}}(2\pi))U(R_{\boldsymbol{n}}(2\pi))|\phi_\xi\rangle. \tag{324}$$

We now apply the tensor operator transformation rule (176) for $R = R_{\boldsymbol{n}}(-2\pi)$),

$$\langle\psi_{\xi'}|T^{(\ell)}_m|\phi_\xi\rangle = \sum_{m'} \mathcal{D}^\ell_{m',m}(R_{\boldsymbol{n}}(-2\pi))\langle\psi_{\xi'}|U^\dagger(R_{\boldsymbol{n}}(2\pi))T^{(\ell)}_{m'}U(R_{\boldsymbol{n}}(2\pi))|\phi_\xi\rangle, \tag{325}$$

and the spin-statistics theorem (323),

$$\langle\psi_{\xi'}|T^{(\ell)}_m|\phi_\xi\rangle = \xi'\xi\sum_{m'} \mathcal{D}^\ell_{m',m}(R_{\boldsymbol{n}}(-2\pi))\langle\psi_{\xi'}|T^{(\ell)}_{m'}|\phi_\xi\rangle. \tag{326}$$

Since rotations by 2π leave tensor operators with integer angular momentum invariant, $\mathcal{D}^\ell_{m',m}(R_{\boldsymbol{n}}(-2\pi)) = \delta_{m,m'}$, the matrix element is vanishing for $\xi' \neq \xi$. This is a superselection rule, namely interactions, described by a Hamiltonian composed of integer angular momentum tensor operators can not mix states with different exchange symmetry. In other words, the Hamiltonian is an $\ell = 0$ tensor operator thus no interaction can generate for a fermion (boson) components with bosonic (fermionic) properties. A two particle wave function can always be written as a sum of even and odd components,

$$\underbrace{\psi(1,2)}_{\mathcal{H}_{12}} = \underbrace{\frac{1}{2}(\psi(1,2)+\psi(2,1))}_{\mathcal{H}_s} \underbrace{+}_{\oplus} \underbrace{\frac{1}{2}(\psi(1,2)-\psi(2,1))}_{\mathcal{H}_a} \tag{327}$$

expressing that the two particle space of states is the direct sum of a fermion and a bosonic parts, $\mathcal{H}_{12} = \mathcal{H}_s \oplus \mathcal{H}_a$, not mixed by interactions.

It is not difficult to generalize the bosonic and fermion states for several particles. Multi-particle state of bosons (fermion) transform under the exchange of any pair of particles,

$$\psi(x_1, \ldots, x_j, x_{j+1}, \ldots, x_n) = \xi\psi(x_1, \ldots, x_{j+1}, x_j, \ldots, x_n). \tag{328}$$

(One can see easily that it is sufficient to impose this property for the exchange of neighbouring particles of the wave function.) We can construct a basis for a system of N identical particles by starting with a complete set of one-particle states $\{|k\rangle\}$ as

$$|k_1, \ldots, k_N\rangle = \mathcal{N}^{-1} \sum_{\pi \in S_N} \xi^{\sigma(\pi)} |k_{\pi(1)}\rangle \otimes \cdots \otimes |k_{\pi(N)}\rangle \tag{329}$$

where $\mathcal{N}$ is a normalization factor and π denotes a permutation of N objects and $\sigma(\pi)$ is the parity of the permutation, defined in the following manner. Any permutation

$$\pi = \binom{1\ ,\ldots,\ N}{\pi(1),\ldots,\pi(N)} \tag{330}$$

can be visualized as a set of N curves, connecting N dots, representing the particles as shown in Fig. 17. The curves correspond to particles and we find a series of crossings, particle exchanges, as the dotted vertical line is moved from the right to the left. Each crossing generates a multiplicative factor ξ in the state (329). The number of crossings is depends on the way the lines are drown and is not uniquely defined, a continuous deformation of the curves may induce more or less crossings. Nevertheless such a deformation of the lines may change the number of crossing in units of 2 since whenever the deformation which preserves the order of the lines at the two ends but makes two lines cross somewhere in the inner part of the figure must induce another crossing where the lines return to the original order. This argument, borrowed from knot theory, a chapter of topology, shows that (i) any permutation can be decomposed into the product of exchanges of neighboring objects and (ii) the number of exchanges ℓ is not unique but its parity, $\sigma(\pi) = \ell(\mathrm{mod}2)$ is well defined. For example, for $N = 3$ we have

$$\begin{aligned} 1 &= \sigma\left(\binom{1,2,3}{1,2,3}\right) = \sigma\left(\binom{1,2,3}{3,1,2}\right) = \sigma\left(\binom{1,2,3}{2,3,1}\right) \\ -1 &= \sigma\left(\binom{1,2,3}{1,3,2}\right) = \sigma\left(\binom{1,2,3}{3,2,1}\right) = \sigma\left(\binom{1,2,3}{2,1,3}\right). \end{aligned} \tag{331}$$

What is left to show is that the state (329) has the desired transformation property under particle exchange. To prove this we start with the identity

$$\sum_{\pi \in S_N} F(\pi) = \sum_{\pi \in S_N} F(\pi\pi'). \tag{332}$$

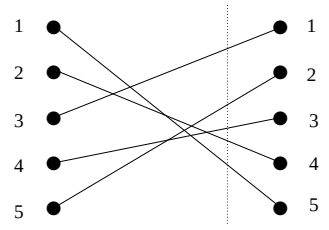


FIG. 17: Graphical representation of the permutation $\binom{1,2,3,4,5}{3,5,4,2,1}$.

It holds because the map $\pi \to \pi\pi'$ of S_N for a given $\pi' \in S_N$ is bijective (onto and one-to-one), hence we have the same quantities on both sides summed up in different order. Addition is commutative hence Eq. (332) follows. This identity allows us write

$$\begin{aligned} |k_{\pi'(1)}, \ldots, k_{\pi'(N)}\rangle &= \mathcal{N}^{-1} \sum_{\pi \in S_N} \xi^{\sigma(\pi)} |k_{\pi\pi'(1)}\rangle \otimes \cdots \otimes |k_{\pi\pi'(N)}\rangle \\ &= \xi^{\sigma(\pi')} |k_1, \ldots, k_N\rangle, \end{aligned} \tag{333}$$

where the equations $\sigma(\pi\pi') = \sigma(\pi) + \sigma(\pi')$, $\xi^{2\sigma(\pi')} = 1$ have been used in arriving at the second line. The wave function of the state (329),

$$\begin{aligned} \psi^{(+)}_{k_1,\ldots,k_n}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) &= \mathcal{N}^{-1} \sum_{\pi \in S_N} \psi_{k_1}(\boldsymbol{x}_{k_{\pi(1)}}) \cdots \psi_{k_N}(\boldsymbol{x}_{k_{\pi(N)}}) \\ \psi^{(-)}_{k_1,\ldots,k_n}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) &= \mathcal{N}^{-1} \sum_{\pi \in S_N} (-1)^{\sigma(\pi)} \psi_{k_1}(\boldsymbol{x}_{k_{\pi(1)}}) \cdots \psi_{k_N}(\boldsymbol{x}_{k_{\pi(N)}}) \\ &= \mathcal{N}^{-1} \det \begin{vmatrix} \psi_{k_1}(\boldsymbol{x}_1) & \psi_{k_1}(\boldsymbol{x}_2) & \cdots & \psi_{k_1}(\boldsymbol{x}_N) \\ \psi_{k_2}(\boldsymbol{x}_1) & \psi_{k_2}(\boldsymbol{x}_2) & \cdots & \psi_{k_2}(\boldsymbol{x}_N) \\ \vdots & \vdots & \cdots & \vdots \\ \psi_{k_N}(\boldsymbol{x}_1) & \psi_{k_N}(\boldsymbol{x}_2) & \cdots & \psi_{k_N}(\boldsymbol{x}_N) \end{vmatrix} \end{aligned} \tag{334}$$

where the subscript indicates the exchange statistics ξ. The fermionic wave function is called Slater determinant. It displays Pauli's exclusion principle, namely two fermions can not occupy the same quantum state. In fact, the determinant is vanishing if two lines are equivalent.

C. Occupation number representation

The (anti)symmetrized states, (329), are unpractical for calculations with more than 4-5 particles due to their complicated structure. The reason of complication is that the construction is based on the product wave function $\psi_{k_1}(\boldsymbol{x}_1), \ldots \psi_{k_N}(\boldsymbol{x}_N)$ which contains too much information, it

treats the identical particles distinguishable and we have to sum over a large number of terms to cancel the unphysical information. The problem can be circumvented by the use of basis states which has physical information only. This is achieved in the occupation number representation where instead of keeping track of the state of each particle we store the occupation number, n_k, of each one-particle state, the number of particles which are in the state $|k\rangle$. A many-particle state can be visualized by a series of boxes, one for each one-particle state. We distribute indistinguishable balls in the boxes, each ball representing a particle and the occupation number is the number of balls in a given box. A basis for the many-particle system is given by the states $|n\rangle$ for each occupation number n_k. Additive quantum numbers, such as the particle number, the momentum or the energy of non-interacting particles, can easily be recovered in this basis,

$$N[n] = \sum_k n_k, \quad \boldsymbol{P} = \sum_k n_k \boldsymbol{p}_k, \quad E[n] = \sum_k n_k E_k \tag{335}$$

where $\boldsymbol{p}_k$ and E_k denote the momentum and the energy of the state $|k\rangle$. Note that the number of particles becomes a dynamical quantity in this representation which opens the way to describe processes with variable number of degrees of freedom. This is the starting point to construct an extension of non-relativistic quantum mechanics, the quantum field theory.

D. Exchange interaction

The (anti)symmetrization of states may introduce correlations among quantum numbers. Let us for instance consider two particles with identical exchange statistics ξ and place them in two different one-particle states with wave functions $\psi_j(\boldsymbol{x}, \sigma)$ where $j = 1, 2$ and σ stands for the spin. When the two particles make up a system then their wave function is

$$\psi_{12}(\boldsymbol{x}_1, \sigma_1, \boldsymbol{x}_2, \sigma_2) = \frac{1}{\sqrt{2}}[\psi_1(\boldsymbol{x}_1, \sigma_1)\psi_2(\boldsymbol{x}_2, \sigma_2) + \xi\psi_2(\boldsymbol{x}_1, \sigma_1)\psi_1(\boldsymbol{x}_2, \sigma_2)]. \tag{336}$$

Let us now suppose that the one-particle wave functions are factorisable,

$$\psi_j(\boldsymbol{x}, \sigma) = \chi_j(\boldsymbol{x})\phi_j(\sigma). \tag{337}$$

This does not lead to factorisable two-particle wave functions but suggests the use of a factorisable basis,

$$\psi_{12}(\boldsymbol{x}_1, \sigma_1, \boldsymbol{x}_2, \sigma_2) = \chi_{12}(\boldsymbol{x}_1, \boldsymbol{x}_2)\phi_{12}(\sigma_1, \sigma_2), \tag{338}$$

where we assume that both components on the right hand side have well defined transformation property under the exchange of the particles,

$$\chi_{12}(\boldsymbol{x}_2, \boldsymbol{x}_1) = \xi_c\chi_{12}(\boldsymbol{x}_1, \boldsymbol{x}_2), \quad \chi_{12}(\boldsymbol{x}_2, \boldsymbol{x}_1) = \xi_s\phi_{12}(\sigma_1, \sigma_2). \tag{339}$$

Since this wave function has a definite exchange statistics there is a correlation between the transformation properties of the components under particle exchange,

$$\xi_c \xi_s = \xi. \tag{340}$$

Such a correlation between the coordinate and the spin dynamics of the basis vectors seems surprising and leads to an unusual phenomenon, called exchange interaction.

The exchange interactions is the easiest to find in a the bound states of two identical fermions interacting with a spherical symmetric potential which is strongly attractive at short distances,

$$H = \frac{\boldsymbol{p}_1^2}{2m} + \frac{\boldsymbol{p}_2^2}{2m} + U(r_{12}). \tag{341}$$

One usually separates the trivial dynamics of the center of mass motion by introducing the variables $\boldsymbol{X} = \frac{1}{2}(\boldsymbol{x}_1 + \boldsymbol{x}_2)$, $\boldsymbol{P} = \frac{1}{2}(\boldsymbol{p}_1 + \boldsymbol{p}_2)$, $\boldsymbol{x} = \boldsymbol{x}_1 - \boldsymbol{x}_2$, and $\boldsymbol{p} = \boldsymbol{p}_1 - \boldsymbol{p}_2$ and write the coordinate-dependent factor of the wave function as

$$\chi(\boldsymbol{x}_1, \boldsymbol{x}_2) = e^{-\frac{i}{\hbar}\boldsymbol{P}\vec{X}} \eta_{n,\ell}(r) Y_m^\ell(\theta, \phi). \tag{342}$$

Note that the exchange of the two particles induces $\boldsymbol{x} \to -\boldsymbol{x}$ hence $\xi_x = (-1)^\ell$. The two spin can be coupled into states $S = 0$ and $S = 1$ and $\xi_x = -1$ or 1 for $S = 0$ or 1, respectively according to the first example of Chapter III B. We find in this manner a correlation between the total electron spin and the orbital angular momentum, ℓ is even or odd for $S = 0$ or 1, respectively. This leads to a spin characteristic energy spectrum, the ground state being the spin singlet. The reason is that the coordinate eigenstate has the asymptotic behavior $\eta_{n,\ell}(r) = \mathcal{O}\left(r^\ell\right)$, letting the potential to lower considerably the interaction energy when the particles are close to each other, as it happens for $\ell = 0$. Such an observation seems surprising in view of the spin independence of the interaction potential.

VIII. POTENTIAL SCATTERING

The microscopic interactions among atoms or elementary particles is easier to explore in scattering experiments, an extension of the idea of microscope to matter waves. We shall consider the simplest realization of this idea, the elastic, energy conserving, scattering of an incoming, coherent beam of spinless particles on a localized, spherical potential, depicted in Fig. 18.

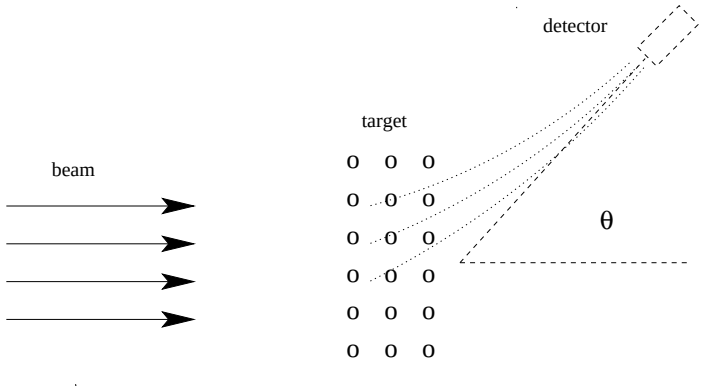


FIG. 18: Schematic view of a scattering experiment

A. Cross section

The result of a collision experiment, the number of particles scattered at a given angle, dN, is proportional to the beam flux, given by the magnitude of the probability current, $|\boldsymbol{j}_i|$,

$$dN = |\boldsymbol{j}_i| d\sigma, \tag{343}$$

and the proportionality constant is called differential cross section. The total cross section,

$$\sigma = \int d\sigma = \int d\Omega \frac{d\sigma}{d\Omega}, \tag{344}$$

is the integral of the differential cross section over the full solid angle. For instance the total cross section of colliding with a rigid sphere of radius a is $\sigma = a^2\pi$ in classical physics. Another expression for number of scattered particles, given in terms of the probability current of the scattered particles, $\boldsymbol{j}_s$,

$$dN = \boldsymbol{j}_s d\boldsymbol{S} \tag{345}$$

where $d\boldsymbol{S}$ stands for the active surface of the detector yields

$$d\sigma = \frac{\boldsymbol{j}_s d\boldsymbol{S}}{|\boldsymbol{j}_i|}. \tag{346}$$

The quantum mechanical calculation of the cross section is based on the assumption that the detector is sufficiently far from the collision region where the potential is non-negligible therefore one seeks a stationary state with wave function

$$\psi = \psi_i + \psi_s, \tag{347}$$

where

$$\lim_{r\to\infty}\psi_i = e^{ikz} \tag{348}$$

represents the incoming, monochromatic beam and

$$\lim_{r\to\infty}\psi_d = f(\theta,\phi)\frac{e^{ikr}}{r} \tag{349}$$

describes the scattered waves in terms of the scattering amplitude $f(\theta,\phi) = f(\theta)$. The incoming and scattered probability currents are

$$\boldsymbol{j}_i = \langle\psi_i|\boldsymbol{j}|\psi_i\rangle = \frac{\hbar}{2mi}\left(\psi_i^*\boldsymbol{\nabla}\psi_i - \boldsymbol{\nabla}\psi_i^*\psi_i\right) = \boldsymbol{e}_z\frac{\hbar k}{m} \tag{350}$$

and

$$\boldsymbol{j}_s = \langle\psi_s|\boldsymbol{j}|\psi_s\rangle = \boldsymbol{e}_r\frac{\hbar k}{mr^2}|f(\theta)|^2, \tag{351}$$

respectively. The number of scattered particles is therefore

$$dN = \frac{\hbar k}{m}d\sigma = r^2\frac{\hbar k}{mr^2}|f(\theta)|^2 d\Omega \tag{352}$$

and the resulting differential cross section, (346), is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2. \tag{353}$$

The total cross section reads as

$$\sigma = 2\pi\int_{-1}^{1} d(\cos\theta)|f(\theta)|^2. \tag{354}$$

B. Optical theorem

The unitarity of the time evolution, the conservation of the probability flux, imposes a constraint on the scattering amplitude and the cross section. The collision is described by a stationary state therefore the total particle flux, traversing of radius R around the center of the scattering potential is vanishing,

$$\int d^3r\,\delta(|\boldsymbol{r}| - R)\boldsymbol{r}\langle\psi|\boldsymbol{j}|\psi\rangle = 0. \tag{355}$$

The form (347) of the state allows us to rewrite this condition as

$$\begin{aligned}
0 &= \int_{|\boldsymbol{r}|=R} d\Omega\boldsymbol{r}\frac{\hbar}{2mi}\left[(\psi_i^*+\psi_s^*)\boldsymbol{\nabla}(\psi_i+\psi_s) - \boldsymbol{\nabla}(\psi_i^*+\psi_s^*)(\psi_i+\psi_s)\right] \\
&= \int_{|\boldsymbol{r}|=R} d\Omega\boldsymbol{r}\left[\boldsymbol{j}_i + \boldsymbol{j}_s + \frac{\hbar}{2mi}\left(\psi_i^*\boldsymbol{\nabla}\psi_s + \psi_s^*\boldsymbol{\nabla}\psi_i - \boldsymbol{\nabla}\psi_i^*\psi_s - \boldsymbol{\nabla}\psi_s^*\psi_i\right)\right] \\
&= \int_{|\boldsymbol{r}|=R} d\Omega\boldsymbol{r}\left[\boldsymbol{j}_i + \boldsymbol{j}_s + \frac{\hbar}{m}Im\left(\psi_i^*\boldsymbol{\nabla}\psi_s + \psi_s^*\boldsymbol{\nabla}\psi_i\right)\right].
\end{aligned} \tag{356}$$

The asymptotic behavior of the wave function is known hence we consider the limit $R \to \infty$ where one finds

$$\begin{aligned} 0 &= \int_{|\boldsymbol{r}|=R} d\Omega \left[\boldsymbol{r}(\boldsymbol{j}_i + \boldsymbol{j}_s) + \frac{\hbar}{m} Im \left(e^{-ikz} \partial_r f(\theta,\phi) \frac{e^{ikr}}{r} + f^*(\theta,\phi) \frac{e^{-ikr}}{r} \partial_r e^{ikz} \right) \right] \\ &= \int_{|\boldsymbol{r}|=R} d\Omega \left[\boldsymbol{r}(\boldsymbol{j}_i + \boldsymbol{j}_s) + \frac{\hbar}{m} Im \left(ikf(\theta,\phi) \frac{e^{ik(r-z)}}{r} + ik\cos\theta f^*(\theta,\phi) \frac{e^{-ik(r-z)}}{r} \right) \right]. \end{aligned} \quad (357)$$

The total flux of the incoming plane wave is vanishing and the last equation can be written as

$$\begin{aligned} \frac{\sigma\hbar k}{mR^2} &= -\frac{\hbar k}{mR} Re \int d\Omega \left[f(\theta,\phi) e^{ik(R-z)} + \cos\theta f^*(\theta,\phi) e^{-ik(R-z)} \right] \\ &= -\frac{\hbar k}{mR} \int d\Omega (1+\cos\theta) \left[Ref(\theta,\phi)\cos k(R-z) - Imf(\theta,\phi)\sin k(R-z) \right]. \end{aligned} \quad (358)$$

The contribution to the integral is vanishing for $\theta \neq 0$ due to the oscillatory integrand and we find

$$\begin{aligned} \sigma &= 4\pi R \lim_{R\to\infty} \lim_{\delta\to 0} \int_{1-\delta c}^{1} dc \left[Imf(0,\phi)\sin kR(1-c) - Ref(0,\phi)\cos kR(1-c) \right] \\ &= 4\pi \lim_{R\to\infty} \lim_{\delta\to 0} \left[Imf(0,\phi) \frac{1-\cos kR\delta c}{kR} - Ref(0,\phi) \frac{\sin kR\delta c}{kR} \right] \\ &= \frac{4\pi}{k} Imf(0,\phi), \end{aligned} \quad (359)$$

a simple proportionality of the total cross section and the imaginary part of the forward transition amplitude.

C. Lippmann-Schwinger equation

There are two frequently followed, different ways to calculate cross sections, one is based exclusively on plane wave states and shows the peculiarity of continuous spectrum. One starts with the Hamiltonian

$$H = H_0 + V, \quad (360)$$

where

$$H_0 = \frac{\boldsymbol{p}^2}{2m}, \quad (361)$$

supposes that it has continuous spectrum and constructs the eigenstates $|\psi\rangle$

$$(H_0 + V)|\psi\rangle = E|\psi\rangle. \quad (362)$$

It is advantageous to introduce the unperturbed eigenstate of the same energy, $H_0|\phi\rangle = E|\phi\rangle$ which represents the incoming beam and write

$$|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle + |\phi\rangle. \tag{363}$$

This equation has to be modified to make the resolvent, $(E - H_0)^{-1}$, well defined within the null-space of $E - H_0$, the subspace corresponding to the eigenvalue E of H_0. The spectrum of H_0 is real therefore the introduction of an infinitesimal imaginary part in the free Hamiltonian, $H_0 \to H_0 \pm i\epsilon$, is sufficient. The resulting Lippmann-Schwinger equation,

$$|\psi^{(\pm)}\rangle = \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle + |\phi\rangle \tag{364}$$

identifies the full scattering state starting from the incoming beam state $|\phi\rangle$. There are two degenerate states for each energy, corresponding to the orientation of the scattered wave in time, $|\psi^{(\pm)}\rangle$ which can describe in- or out-going waves. Time inversion maps one state onto the other and changes the sign of the anti-Hermitian part of the Hamiltonian. By starting with the state

$$\langle \boldsymbol{x}|\phi\rangle = e^{i\boldsymbol{x}\boldsymbol{k}} \tag{365}$$

we find the Lippmann-Schwinger equation

$$\langle \boldsymbol{x}|\psi^{(\pm)}\rangle = \int d^3x' \langle \boldsymbol{x}| \frac{1}{E - H_0 \pm i\epsilon} |\boldsymbol{x'}\rangle V(\boldsymbol{x'}) \langle \boldsymbol{x'}|\psi^{(\pm)}\rangle + \langle \boldsymbol{x}|\phi\rangle. \tag{366}$$

The matrix element in this equation,

$$G_\pm(\boldsymbol{x}, \boldsymbol{x'}) = \frac{\hbar^2}{2m} \langle \boldsymbol{x}| \frac{1}{E - H_0 \pm i\epsilon} |\boldsymbol{x'}\rangle, \tag{367}$$

can be found by going over momentum space representation,

$$\begin{aligned} G_\pm(\boldsymbol{x}, \boldsymbol{x'}) &= \frac{\hbar^2}{2m} \int \frac{d^3k'}{(2\pi)^3} \frac{d^3k''}{(2\pi)^3} \langle \boldsymbol{x}|\boldsymbol{k'}\rangle \langle \boldsymbol{k'}| \frac{1}{E(\boldsymbol{k}) - H_0 \pm i\epsilon} |\boldsymbol{k''}\rangle \langle \boldsymbol{k''}|\boldsymbol{x'}\rangle \\ &= \frac{\hbar^2}{2m} \int \frac{d^3k'}{(2\pi)^3} \frac{d^3k''}{(2\pi)^3} \langle \boldsymbol{x}|\boldsymbol{k'}\rangle \frac{1}{E(\boldsymbol{k}) - \frac{\hbar^2 \boldsymbol{k''}^2}{2m} \pm i\epsilon} \underbrace{\langle \boldsymbol{k'}|\boldsymbol{k''}\rangle}_{(2\pi)^3 \delta(\boldsymbol{k'} - \boldsymbol{k''})} \langle \boldsymbol{k''}|\boldsymbol{x'}\rangle \\ &= \frac{\hbar^2}{2m} \int \frac{d^3k'}{(2\pi)^3} \frac{e^{i\boldsymbol{k'}(\boldsymbol{x} - \boldsymbol{x'})}}{E(\boldsymbol{k}) - \frac{\hbar^2 \boldsymbol{k'}^2}{2m} \pm i\epsilon} \end{aligned} \tag{368}$$

with $E(\boldsymbol{k}) = \frac{\hbar^2 k^2}{2m}$. The Fourier integral can easily be carried out,

$$\begin{aligned} G_\pm(\boldsymbol{x},\boldsymbol{x'}) &= \frac{\hbar^2}{2m(2\pi)^3}\int_0^\infty dqq^2\int_{-\pi}^{\pi}d\phi\int_{-1}^{1}d(\cos\theta)\frac{e^{iq|\boldsymbol{x}-\boldsymbol{x'}|\cos\theta}}{\frac{\hbar^2k^2}{2m}-\frac{\hbar^2q^2}{2m}\pm i\epsilon} \\ &= \frac{1}{(2\pi)^3}\int_0^\infty dqq^2\int_{-\pi}^{\pi}d\phi\int_{-1}^{1}d(\cos\theta)\frac{e^{iq|\boldsymbol{x}-\boldsymbol{x'}|\cos\theta}}{k^2-q^2\pm i\epsilon} \\ &= -\frac{1}{2(2\pi)^2 i|\boldsymbol{x}-\boldsymbol{x'}|}\int_{-\infty}^{\infty}dqq\underbrace{\frac{e^{iq|\boldsymbol{x}-\boldsymbol{x'}|}-e^{-iq|\boldsymbol{x}-\boldsymbol{x'}|}}{q^2-k^2\mp i\epsilon}}_{(q-k\mp i\epsilon')(q+k\pm i\epsilon')} \\ &= -\frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{x'}|}\left[\frac{(\pm k)e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|}}{\pm 2k}+\frac{(\pm k)e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|}}{\pm 2k}\right] \\ &= -\frac{e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|}}{4\pi|\boldsymbol{x}-\boldsymbol{x'}|}, \end{aligned} \tag{369}$$

and it reduces (366) to

$$\langle\boldsymbol{x}|\psi^{(\pm)}\rangle = -\frac{2m}{\hbar^2}\int d^3x'\frac{e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|}}{4\pi|\boldsymbol{x}-\boldsymbol{x'}|}V(\boldsymbol{x'})\langle\boldsymbol{x'}|\psi^{(\pm)}\rangle + \langle\boldsymbol{x}|\phi\rangle. \tag{370}$$

The scattering amplitude is read off from the stationary state at spatial infinity, thus we go into the limit $r = |\boldsymbol{x}| \gg r' = |\boldsymbol{x'}|$, where

$$\begin{aligned} |\boldsymbol{x}-\boldsymbol{x'}| &= \sqrt{r^2-2rr'\cos\theta+r'^2} \\ &= r\sqrt{1-\frac{2r'}{r}\cos\theta+\frac{r'^2}{r^2}} \\ &\approx r-\boldsymbol{n}\boldsymbol{x'} \end{aligned} \tag{371}$$

where $\boldsymbol{n} = \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$ and

$$e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|} \approx e^{\pm ikr\mp i\boldsymbol{k'}\boldsymbol{x'}}, \tag{372}$$

with $\boldsymbol{k'} = k\boldsymbol{n}$, giving

$$\begin{aligned} \lim_{r\to\infty}\langle\boldsymbol{x}|\psi^{(\pm)}\rangle &= -\frac{2m}{\hbar^2}\frac{e^{\pm ikr}}{4\pi r}\int d^3x' e^{\mp i\boldsymbol{k'}\boldsymbol{x'}}V(\boldsymbol{x'})\langle\boldsymbol{x'}|\psi^{(\pm)}\rangle + \langle\boldsymbol{x}|\boldsymbol{k}\rangle \\ &= e^{i\boldsymbol{k}\boldsymbol{x}}+\frac{e^{\pm ikr}}{r}f^{(\pm)}(\boldsymbol{k'},\boldsymbol{k}). \end{aligned} \tag{373}$$

With the time evolution $|\psi^{(\pm)}(t)\rangle = e^{-\frac{i}{\hbar}E(\boldsymbol{k})t}|\psi^{(\pm)}\rangle$ we find spherical out- and in-going scattered waves in $\psi^{(+)}\rangle$ and $\psi^{(-)}\rangle$, respectively. The differential cross section is therefore

$$\frac{d\sigma}{d\Omega} = |f^{(+)}(\boldsymbol{k'},\boldsymbol{k})|^2. \tag{374}$$

The Lippmann-Schwinger equation is easiest to solve by iteration. The first order result, the Born approximation, where the replacement $\langle\boldsymbol{x'}|\psi^{(+)}\rangle \to \langle\boldsymbol{x'}|\phi\rangle = e^{i\boldsymbol{k}\boldsymbol{x'}}$ is made on the right hand

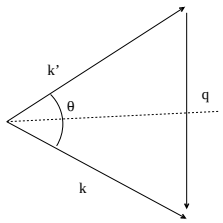


FIG. 19: The vectors q, $\boldsymbol{k}$ and $\boldsymbol{k'}$ for the calculation of $f_B(\theta)$.

side, leads to

$$\begin{aligned} f_B(\boldsymbol{k'},\boldsymbol{k}) &= -\frac{m}{2\pi\hbar^2}\int d^3x' e^{i(\boldsymbol{k}-\boldsymbol{k'})\boldsymbol{x'}}V(\boldsymbol{x'}) \\ &= -\frac{m}{2\pi\hbar^2}\tilde{V}(\boldsymbol{k'}-\boldsymbol{k}). \end{aligned} \tag{375}$$

Let us take for the sake of an example a spherically symmetric scattering potential, $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$ and use $q = |\boldsymbol{k'}-\boldsymbol{k}| = 2k\sin\theta/2$ (cf. Fig. 19),

$$\begin{aligned} f_B(\theta) &= -\frac{m}{\hbar^2}\int_0^\infty dr r^2 V(r)\int d(\cos\theta)e^{iqr\cos\theta} \\ &= -\frac{m}{\hbar^2}\int_0^\infty dr r^2 V(r)\frac{e^{iqr}-e^{-iqr}}{iqr} \\ &= -\frac{2m}{q\hbar^2}\int_0^\infty dr r V(r)\sin qr. \end{aligned} \tag{376}$$

In particular, the screened Coulomb potential, $V(r) = ge^{-\mu r}/r$, gives

$$\begin{aligned} f_B(\theta) &= -\frac{mg}{iq\hbar^2}\int_0^\infty dr[e^{(iq-\mu)r}-e^{-(iq+\mu)r}] \\ &= \frac{mg}{iq\hbar^2}\left(\frac{1}{iq-\mu}+\frac{1}{iq+\mu}\right) \\ &= -\frac{2mg}{\hbar^2}\frac{1}{q^2+\mu^2}. \end{aligned} \tag{377}$$

The identity

$$q^2 = 4k^2\sin^2\frac{\theta}{2} = 2k^2(1-\cos\theta) \tag{378}$$

produces finally

$$\frac{d\sigma}{d\Omega} = \frac{4m^2g^2}{\hbar^4}\frac{1}{[2k^2(1-\cos\theta)+\mu^2]^2}. \tag{379}$$

The choice $\mu = 0$ and $g = ZZ'e^2$ gives

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{4m^2(ZZ'e^2)^2}{\hbar^4}\frac{1}{4k^4(1-\cos\theta)^2} \\ &= \frac{4m^2(ZZ'e^2)^2}{\hbar^4}\frac{1}{16k^4\sin^4\frac{\theta}{2}} \\ &= \frac{(ZZ'e^2)^2}{16E_0^2(\hbar k)}\frac{1}{\sin^4\frac{\theta}{2}} \end{aligned} \tag{380}$$

with $E_0(\hbar k) = \frac{\hbar^2 k^2}{2m}$, the Rutherford cross section for scattering of two nuclei of charge Z_1 and Z_2 by a Coulomb potential.

It is worthwhile noting the following features of the Born approximation:

1. $\frac{d\sigma}{d\Omega}$ is independent of the sign of $V(r)$.

2. The cross section is given by

$$f_B(\theta) = -\frac{m}{2\pi\hbar^2}\int d^3x' V(\boldsymbol{x'}) \tag{381}$$

   at low energy, $kr_{ch} \ll 1$.

3. The Born approximation is valid for weak potential or high energy, $k \to \infty$,

$$\left| \int d^3x' \frac{e^{\pm ikr'}}{4\pi r'} V(\boldsymbol{x'}) e^{i\boldsymbol{k}\boldsymbol{x'}} \right| \ll \frac{\hbar^2}{2m}. \tag{382}$$

D. Partial waves

Another approximation for the cross section which remains valid at low energy is based on phase shift, induced by the scattering potential on the spherical harmonic components of the stationary scattering state.

One start here with the solution $\psi(r,\theta,\phi) = R_\ell^{(0)}(k,r)Y_m^\ell(\theta,\phi)$ of the free Schrödinger equation,

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\partial_r r^2 \partial_r - \frac{\ell(\ell+1)}{r^2}\right] R_\ell^{(0)}(k,r) = E R_\ell^{(0)}(k,r), \tag{383}$$

written as

$$\left[\partial_x^2 + \frac{2}{x}\partial_x + 1 - \frac{\ell(\ell+1)}{x^2}\right] R_\ell^{(0)}(k,r) = 0 \tag{384}$$

by means of the dimensionless radius $x = kr$ and $E = \frac{\hbar^2 k^2}{2m}$. We have two kinds of solutions,

- Bessel functions: $R_\ell^{(0)}(k,r) = j_\ell(kr)$, $j_\ell(0) < \infty$,

$$\begin{aligned} r \to 0: \; j_0(x) &= \frac{\sin x}{x}, \quad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \dots \\ r \to \infty: \; j_\ell(x) &= \frac{1}{x}\sin\left(x - \frac{\ell\pi}{2}\right). \end{aligned} \tag{385}$$

- Neumann functions: $R_\ell^{(0)}(k,r) = n_\ell(kr)$, $n_\ell(0) = \infty$,

$$\begin{aligned} r \to 0: \; n_0(x) &= -\frac{\cos x}{x}, \quad n_1(x) = \frac{\cos x}{x^2} - \frac{\sin x}{x}, \dots \\ r \to \infty: \; n_\ell(x) &= \frac{1}{x}\cos\left(x - \frac{\ell\pi}{2}\right). \end{aligned} \tag{386}$$

The divergence of the Neumann function at the origin excludes them from the description of a free particle state.

In the presence of the scattering potential we write the wave function of the scattered particle as

$$\psi_s(r,\theta,\phi) = \sum_{\ell,m} C_{\ell,m} R_\ell(k,r) Y_m^\ell(\theta,\phi) \tag{387}$$

where

$$\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\partial_r r^2 \partial_r - \frac{\ell(\ell+1)}{r^2}\right) + U(r)\right] R_\ell(k,r) = E R_\ell(k,r). \tag{388}$$

It is advantageous to use the same dimensionless radius x and the potential $V(x) = \frac{2m}{\hbar^2}U(\frac{x}{k})$, giving

$$\left[\partial_x^2 + \frac{2}{x}\partial_x - V(x) + 1 - \frac{\ell(\ell+1)}{x^2}\right] R_\ell(k,r) = 0. \tag{389}$$

The solution of this equation is made unique by the boundary conditions.

1. $r \to 0$: We start with a useful relation obtained by the orthogonality of eigenvectors of the Hamiltonian, $H|\psi\rangle = E|\psi\rangle$, $H|\psi'\rangle = E'|\psi'\rangle$,

$$(E - E')\langle\psi'|\psi\rangle = 0 \tag{390}$$

To find this relation for the scattering states we consider two solutions, $R_\ell(k,r) = u(r)/r$ and $\tilde{R}_\ell(\tilde{k},r) = \tilde{u}(r)/r$ of the Schrödinger equation,

$$\begin{aligned} E u_\ell(r) &= \left(-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + U(r)\right) u_\ell(r), \\ \tilde{E}\tilde{u}_\ell^*(r) &= \left(-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + U(r)\right) \tilde{u}_\ell^*(r). \end{aligned} \tag{391}$$

By multiplying the first and the second equation with $\tilde{u}_\ell^*(r)$ and $u_\ell(r)$, respectively and subtracting the resulting two equations we find

$$\begin{aligned} (E-\tilde{E})\tilde{u}_\ell^*(r)u_\ell(r) &= \tilde{u}_\ell^*(r)\left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + U(r)\right] u_\ell(r) \\ &\quad -u_\ell(r)\left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + \tilde{U}(r)\right] \tilde{u}_\ell^*(r) \\ &= -\frac{\hbar^2}{2m}\partial_r[\tilde{u}_\ell^*(r)\partial_r u_\ell(r) - u_\ell(r)\partial_r\tilde{u}_\ell^*(r)]. \end{aligned} \tag{392}$$

The integration of this equation over r gives

$$0 = (E-\tilde{E})\langle\tilde{u}_\ell|u_\ell\rangle = (E-\tilde{E})\int_0^\infty dr\,\tilde{u}_\ell^*(r)u_\ell(r) = \frac{\hbar^2}{2m}[\tilde{u}_\ell^*(0)\partial_r u_\ell(0) - u_\ell(0)\partial_r\tilde{u}_\ell^*(0)]. \tag{393}$$

Let us now turn our attention to the behavior of the wave functions at small r where the functional forms

$$\begin{aligned} U(r) &= r^p(U_0 + U_1 r + U_2 r^2 + \cdots), \\ u_\ell(k,r) &= rR_\ell(k,r) = r^s(c_0 + c_1 r + c_2 r^2 + \cdots), \end{aligned} \tag{394}$$

are assumed with $c_0 \neq 0$ and write the Schrödinger equation as

$$Er^s(c_0 + \cdots) = \left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + r^p(U_0 + U_1 r + \cdots)\right] r^s(c_0 + \cdots) \tag{395}$$

The equivalence of the terms $\mathcal{O}\left(r^{s-2}\right)$ yields the equation

$$0 = \begin{cases} -\frac{\hbar^2}{2m}[s(s-1) - \ell(\ell+1)] & p \geq -1, \\ -\frac{\hbar^2}{2m}[s(s-1) - \ell(\ell+1)] + U_0 & p = -2. \end{cases} \tag{396}$$

For the more realistic case, $p \geq -1$, we have $s = -\ell$ or $s = \ell+1$. The orthogonality condition, (393), restricts the solution to $s = \ell + 1$, giving $u_\ell(r) = \mathcal{O}\left(r^{\ell+1}\right)$ and $R_\ell(k,r) = \mathcal{O}\left(r^\ell\right)$.

2. $r \to \infty$: It is assumed that the scattering potential is negligible at large distances, $\lim_{r\to\infty} rU(r) = 0$ where the solution approaches a linear superposition of the free Schrödinger equation of the same energy, involving both the Bessel and the Neumann functions,

$$\lim_{r\to\infty} R_\ell(k,r) = j_\ell(kr)\cos\delta_\ell + n_\ell(kr)\sin\delta_\ell = \frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)}{kr} \tag{397}$$

The mixing angle, δ_ℓ is the phase shift of the scattered particle with respect to the free propagation.

1. Scattering amplitude

The scattering amplitude is determined by the wave function as $r \to \infty$ which is found by considering the wave function of the complete state with $m = 0$,

$$\psi(r,\theta,\phi) = \sum_\ell C_\ell R_\ell(k,r) P_\ell(\cos\theta). \tag{398}$$

Since

$$\begin{aligned} e^{ikz} &= \sum_\ell (2\ell+1) i^\ell j_\ell(kr) P_\ell(\cos\theta) \\ &\to \sum_\ell (2\ell+1) i^\ell \frac{\sin\left(kr - \frac{\ell\pi}{2}\right)}{kr} P_\ell(\cos\theta) \end{aligned} \tag{399}$$

in this limit the wave function of the scattered particle is

$$\begin{aligned}\psi - e^{ikz} &\rightarrow f(\theta)\frac{e^{ikr}}{r} \\ &= \frac{1}{kr}\sum_\ell P_\ell(\cos\theta)\left[C_\ell \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right) - (2\ell+1)i^\ell \sin\left(kr - \frac{\ell\pi}{2}\right)\right] \\ &= \frac{1}{2kri}\sum_\ell P_\ell(\cos\theta) \\ &\quad \times \left[e^{i(kr-\frac{\ell\pi}{2})}\left(C_\ell e^{i\delta_\ell} - (2\ell+1)i^\ell\right) - e^{-i(kr-\frac{\ell\pi}{2})}\left(C_\ell e^{-i\delta_\ell} - (2\ell+1)i^\ell\right)\right]. \quad (400)\end{aligned}$$

The second term in the square bracket is vanishing in the absence of ingoing spherical waves thus

$$C_\ell = e^{i\delta_\ell}(2\ell+1)i^\ell \quad (401)$$

and

$$f(\theta) = \sum_\ell (2\ell+1) f_\ell P_\ell(\cos\theta) \quad (402)$$

where the partial scattering amplitudes,

$$f_\ell = \frac{e^{2i\delta_\ell}-1}{2ik} = \frac{e^{i\delta_\ell}\sin\delta_\ell}{k} = \frac{1}{k}\frac{1}{e^{-i\delta_\ell}\frac{1}{\sin\delta_\ell}} = \frac{1}{k\cot\delta_\ell - ik}, \quad (403)$$

are given in terms of the phase shifts. The orthogonality of the spherical harmonics,

$$\int_{-1}^{1} d(\cos\theta) P_\ell(\cos\theta) P_{\ell'}(\cos\theta) = \delta_{\ell,\ell'}\frac{2}{2\ell+1} \quad (404)$$

leads to the total cross section

$$\sigma = 2\pi\int_{-1}^{1} d(\cos\theta)|f(\theta)|^2 = 4\pi\sum_\ell (2\ell+1)|f_\ell|^2 = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell = \sum_\ell \sigma_\ell, \quad (405)$$

shown in Fig. 20. Note that the upper bound of the partial cross section is

$$\sigma_\ell \leq \sigma_{\ell\ \max} = \frac{4\pi(2\ell+1)}{k^2}. \quad (406)$$

The decomposition of the scattered state into spherical harmonics is useful and converges fast, $\sigma_\ell \sim 0$, if the impact parameter b and the characteristic length, r_0, satisfy $b > r_0$. This inequality assumes the form $\ell > r_0 k$ because the impact parameter can be defined by the angular momentum as $L_x = bp = \hbar\ell$.

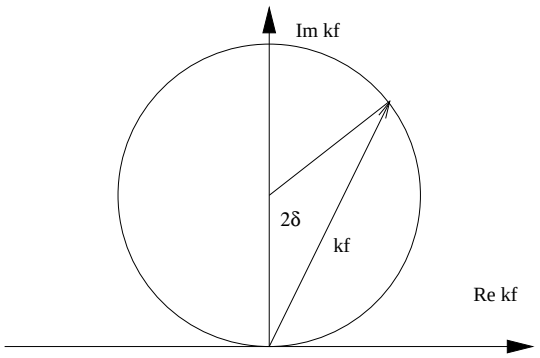


FIG. 20: Argand diagram for $kf_\ell = \frac{i}{2}(e^{2i\delta_\ell} - 1)$.

2. Phase shift

One can obtain a more explicit expression for the phase shift by following the strategy of eqs. (391)-(392) by two wave functions, $R_\ell(r) = u(r)/r$ and $\tilde{R}_\ell(r) = \tilde{u}(r)/r$, of the same energy and satisfying the Schrödinger equation with potentials $U(r)$ and $\tilde{U}(r)$, respectively,

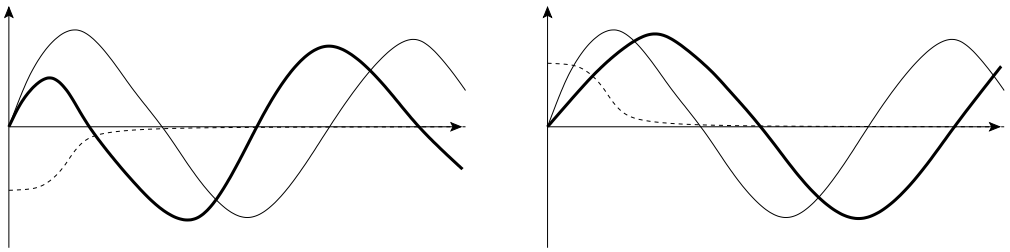
$$\begin{aligned}
Eu_\ell(r) &= \left(-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + U(r)\right) u_\ell(r), \\
E\tilde{u}_\ell(r) &= \left(-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + \tilde{U}(r)\right) \tilde{u}_\ell(r), \\
0 &= \tilde{u}_\ell(r)\left(-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + U(r)\right) u_\ell(r) \\
&\quad -u_\ell(r)\left(-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + \tilde{U}(r)\right) \tilde{u}_\ell(r) \\
&= [U(r) - \tilde{U}(r)]\tilde{u}_\ell(r)u_\ell(r) - \frac{\hbar^2}{2m}\partial_r[\tilde{u}_\ell(r)\partial_r u_\ell(r) - u_\ell(r)\partial_r\tilde{u}_\ell(r)].
\end{aligned} \tag{407}$$

The integration over r now gives

$$\Delta = \int_0^\infty dr[U(r) - \tilde{U}(r)]\tilde{u}_\ell(r)u_\ell(r) = \frac{\hbar^2}{2m}[\tilde{u}_\ell(r)\partial_r u_\ell(r) - u_\ell(r)\partial_r\tilde{u}_\ell(r)]_{|r=\infty} \tag{408}$$

One assumes the asymptotic form

$$\lim_{r\to\infty} u_\ell(k,r) = \frac{1}{k}\left[\sin\left(kr - \frac{\ell\pi}{2}\right) + \cos\left(kr - \frac{\ell\pi}{2}\right)\tan\delta_\ell\right] \tag{409}$$



(a) (b)

FIG. 21: A qualitative plot of the radial wave function, $u_0(r)$, of the free particle (thin solid line), the scattered particle (fat solid line) and the potential, $U(r)$, (dashed line) as functions of r. (a): The potential is attractive, increasing the curvature of $u_0(r)$, "pulling back" the particle and inducing $\delta_0 > 0$. (b): The potential is repulsive, decreasing the curvature of $u_0(r)$, "pushing out" the particle and inducing $\delta_0 < 0$.

and finds

$$\begin{aligned}\Delta &= \frac{\hbar^2}{2mk^2}\Bigg\{\left[\sin\left(kr-\frac{\ell\pi}{2}\right)+\cos\left(kr-\frac{\ell\pi}{2}\right)\tan\tilde{\delta}_\ell\right]\\ &\quad\times\partial_r\left[\sin\left(kr-\frac{\ell\pi}{2}\right)+\cos\left(kr-\frac{\ell\pi}{2}\right)\tan\delta_\ell\right]\\ &\quad-\left[\sin\left(kr-\frac{\ell\pi}{2}\right)+\cos\left(kr-\frac{\ell\pi}{2}\right)\tan\delta_\ell\right]\\ &\quad\times\partial_r\left[\sin\left(kr-\frac{\ell\pi}{2}\right)+\cos\left(kr-\frac{\ell\pi}{2}\right)\tan\tilde{\delta}_\ell\right]\Bigg\}_{|r=\infty}\\ &= \frac{\hbar^2}{2mk}(\tan\tilde{\delta}_\ell-\tan\delta_\ell).\end{aligned} \tag{410}$$

One way to use this result is to establish a differential equation for the phase shift,

$$\frac{d\delta_\ell}{d\lambda} = -\frac{2mk}{\hbar^2}\int_0^\infty dr\frac{dU(r)}{d\lambda}u_\ell^2(kr), \tag{411}$$

indicating that a more attractive potential induces more phase shift, delaying more the wave function as a function of r, compared to the free propagation, cf. Fig. 21. But the phase shifts do not characterize the potential completely, in particular sufficiently strong potentials may reach $\delta_\ell = 0(\mathrm{mod}2\pi)$ and $\sigma_0 = 0$ (Ramser-Townsed effect).

A more explicit expression is found for the phase shift by setting $\tilde{U}(r) = 0$,

$$\tan\delta_\ell = -\frac{2mk}{\hbar^2}\int_0^\infty drr^2U(r)j_\ell(kr)R_\ell(r). \tag{412}$$

One can conveniently characterize the scattering process by means of the scattering matrix, S whose matrix element for ℓ-waves, S_ℓ, is defined in the limit $r\to\infty$ by

$$\psi \to \frac{1}{2kri}\sum_\ell(2\ell+1)i^\ell P_\ell(\cos\theta)\left[S_\ell e^{i(kr-\frac{\ell\pi}{2})}-e^{-i(kr-\frac{\ell\pi}{2})}\right]. \tag{413}$$

The comparison of this equation with the expression

$$\psi \to \frac{1}{kr}\sum_\ell P_\ell(\cos\theta)e^{i\delta_\ell}(2\ell+1)i^\ell \sin\left(kr-\frac{\ell\pi}{2}+\delta_\ell\right) \tag{414}$$

results

$$S_\ell = e^{2i\delta_\ell}. \tag{415}$$

The scattering matrix allows us to write the scattered state as

$$|\psi_s\rangle = S|\psi_i\rangle. \tag{416}$$

3. Low energy scattering

The scattering is simplified considerably in the limit $k \to 0$ mainly because it dominated by s-waves, $\ell = 0$. Assuming that the potential is of finite range we have $u_0''(r) = 0$ and $u(r) \sim r - a$ at large distances, a being a characteristic length scale, the scattering length. We have for the scattered wave, (397),

$$\frac{u_0'(r)}{u_0(r)} = k\cot(kr+\delta_0) \to \frac{1}{r-a} \tag{417}$$

as $k \to 0$ which allows us to write

$$\lim_{k\to 0} k\cot\delta_0 \to -\frac{1}{a} \tag{418}$$

even though the wave function (397) is valid at large r. The total cross section is therefore

$$\sigma = \sigma_0 = \lim_{k\to 0}\frac{4\pi}{k^2|\cot\delta_\ell - i|^2} = 4\pi a^2, \tag{419}$$

by using eqs. (403), (405) and (418).

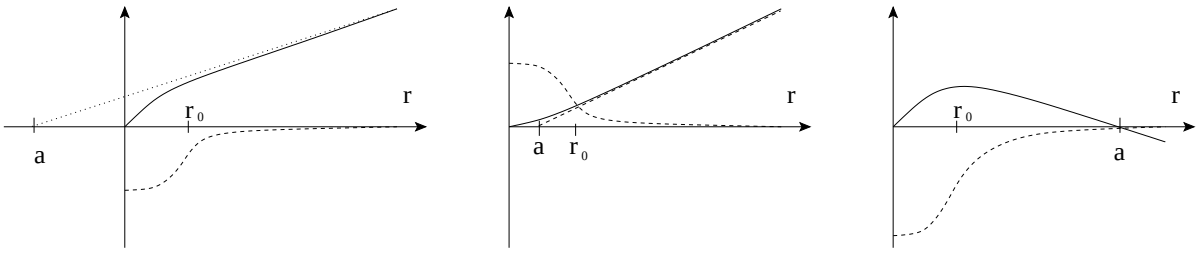
Note that the two length scales, associated with the potential, the range and scattering length, r_0 and a can be different, cf. Fig. 22. The former characterizes the potential alone, the latter is the half of the radius of a sphere which would produce the same scattered particle intensity in classical mechanics.

4. Bound states

A possible bound state, encountered in Fig. 22 (c), can be viewed as the change $k \to i\kappa$ in the s-wave wave function,

$$\psi = \frac{1}{2kri}\left[S_0(k)\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}\right] \sim \frac{e^{-\kappa r}}{r}. \tag{420}$$

The following conditions should be satisfy by $S_\ell(k)$:



(a) (b) (c)

FIG. 22: A qualitative plot of the radial wave function, $u_0(r)$, (solid line), its linear approximation, $u_0(r) \sim r - a$, (dotted line) and the potential, $U(r)$, (dashed line) as functions of r. (a): The potential is attractive, $a < 0$. (b): The potential is repulsive, $a > 0$. (c): The scattering length, a jumps to a large positive value as the attractive strength of the potential (a) is increased and a bound state is formed.

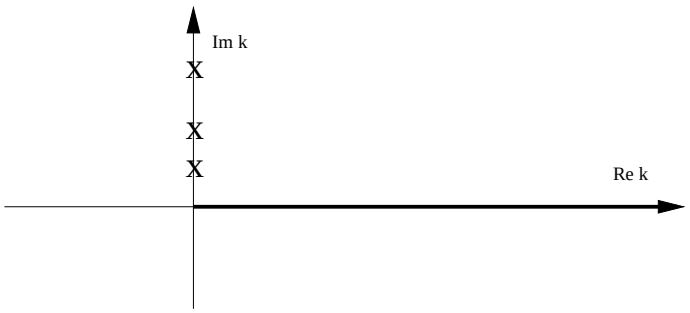


FIG. 23: The poles of the scattering matrix.

1. It should display a pole at $k = i\kappa$. In fact, it is the relative strength of the two terms in the square brackets which matters, hence the emergence of a bound state implies $S = \infty$. One can argue that the divergence of the scattering matrix always corresponds to a simple pole, cf. Fig. 23.

2. The phase shift, $\delta_0(k)$ is real in the physical regime, $|S_\ell(k)| = 1$ for $k > 0$,

3. The limit (419) indicates that $k \cot \delta_0 \to -\frac{1}{a}$ as $k \to 0$. This requires $\delta_0 \to n\pi$ and $S_0(k) = e^{2i\delta_0(k)} \to 1$.

A simple form for $S_0(k)$, satisfying these requirements is

$$S_0(k) = -\frac{k + i\kappa}{k - i\kappa}, \tag{421}$$

giving

$$f_0(k) = \frac{S_0(k) - 1}{2ik} = \frac{i}{k - i\kappa} = \frac{1}{k \cot \delta_0 - ik}, \tag{422}$$

where the bound state parameter, κ is given by

$$\kappa = -\lim_{k\to 0} k\cot\delta_0 = \frac{1}{a}. \tag{423}$$

The analytic structure of the scattering matrix enables one to relate the usually unknown bound state size parameter, κ to the measured scattering length, a.

5. *Resonances*

We mention finally the qualitative behavior of the cross section and the phase shift around a resonance, an "almost" bound state. The effective potential,

$$U_{eff}(r) = U(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}, \tag{424}$$

may support quasi-bound states for sufficiently attractive potential $U(r)$, $\lim_{r\to\infty} U(r) = 0$, at positive energy, $E = E_{\rm ers} > 0$. These states are not really bound, the tunneling through the centrifugal barrier induces a finite life-time.

As the beam energy is increase from zero a partial cross section, corresponding to the most attractive angular momentum ℓ displays a maximum at the $E = E_{\rm ers}$. According to Eq,(403) the phase shift reaches $\delta_\ell = \pi/2$ at this point, cf. Fig. 24. Hence the parametrization

$$\cot\delta_\ell = -c(E - E_{\rm res}) + \mathcal{O}\left((E - E_{\rm res})^2\right) \tag{425}$$

is applicable in the vicinity of the resonance and it yields the scattering amplitude

$$f_\ell = \frac{1}{k\cot\delta_\ell - ik} \approx -\frac{1}{k}\frac{1}{c(E - E_{\rm res}) + i}, \tag{426}$$

written as a simple pole,

$$f_\ell = \frac{\frac{\Gamma}{2}}{k(E - E_{\rm res} + \frac{i\Gamma}{2})}. \tag{427}$$

The cross section turns out

$$\sigma_\ell = \frac{4\pi(2\ell+1)}{k^2}\frac{(\frac{\Gamma}{2})^2}{(E - E_{\rm res})^2 + (\frac{\Gamma}{2})^2} \tag{428}$$

(Breit-Wigner). The phase shift assumes the value $\delta_\ell = \pi/2$, at the resonance and extends approximately over the interval $0 < \delta_\ell < \pi$ as the resonance energy is passed, displaying the fastest variation at the resonance,

$$\frac{d\cot\delta_\ell}{dE}_{|E=E_{\rm res}} = -c = -\frac{2}{\Gamma}. \tag{429}$$

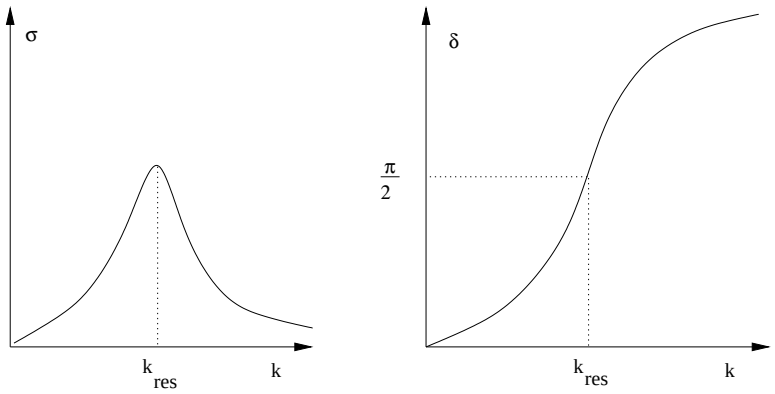


FIG. 24: The cross section, σ_ℓ, and the phase shift, δ_ℓ, around a resonance.

IX. OUTLOOK

Quantum Mechanics has been extended over a large domain, left of the dividing vertical line of Fig. 8 to cover relativistic phenomenas. That extension has two peculiar features, the relativistic invariance holds for the averages of observables and is violated by quantum fluctuations and the space-time can not be continuous. It remains one of the main challenges in Physics to find the true mixture of the principles of Quantum Mechanics and Special Relativity. This issue should obviously be settled before embarking the problem of approaching General Relativity and Quantum Mechanics.

Let us leave these problems for later time and return to non-relativsistic Quantum Mechanics. One expects that this theory serves as the origin of classical mechanics. However the rules, governing quantum and classical mechanics appear too different to reach this goal. Some features of this problem are commented briefly below without attempting of completeness. The guiding principle in visiting the difficulties is a simple theory of the measurement processes due to Neumann. The problems, laid bare by such a simple considerations, are related to determinism, the violation of the rule of interference and the emergence of non-locality.

A. Measurement theory

The quantum level influences the classical world by letting microscopic events "growing" up to the macroscopic scale and simple realization example to guide our intuition is the measuring process. It is described by the help of three components, the measured system, the measuring apparatus and their environment. The latter is needed to generate the macroscopic features of the apparatus. A simple example is the determination of the momentum of a charged particle,

making up the microscopic system. The particle traverses a coil and its velocity can be inferred by measuring the electric current in the coil. The measurement apparatus is therefore an ammeter and the environment consists of the air molecules around the apparatus. The closed dynamics of the full system is governed by the Hamiltonian $H = H_s + H_a + H_{s,a}(t) + H_e + H_{s,a,e}$ where H_s, H_a and H_e denote the Hamiltonian of the system, apparatus and the environment and $H_{s,a} + H_{s,a,e}$ describes the system-apparatus and the system-apparatus-environment interactions. The system-apparatus interaction is time dependent and $H_{s,a}(t) \neq 0$ is assumed only for a short period of time, $t_m - \tau_m < t < t_m + \tau_m$. We consider non-demolishing measurement for the sake of simplicity where the system state does not change during the measurement, $[H_s, H_{s,a}] = 0$.

The whole system starts before t_m within the pure state $|\Psi\rangle = \sum_n c_n |\psi_n\rangle_s \otimes |\phi_0\rangle_a \otimes |\chi\rangle_e$, written as the direct product of the system, apparatus and the environment factors and the measuring process is split into three consecutive steps:

1. *Pre-measurement,* $t_m - \tau_m < t < t_m + \tau_m$*:* The measuring apparatus functions by correlating the microscopic state with the pointer of the ammeter in such a manner that the registration of the pointer state allows us to identify the chosen quantum number n_m of the microscopic system. The measurement process is assumed to be fast enough to ignore the presence of the environment, $\tau_m H_{a,e} \ll \int dt H_{s,a}(t)$, during the measurement and the initial factorized state develops into an entangled one,

$$\sum_n c_n |\psi_n\rangle_s \otimes |\phi_0\rangle_a \otimes |\chi\rangle_e \to \sum_n c_n |\psi_n\rangle_s \otimes |\phi_n\rangle_a \otimes |\chi\rangle_e. \tag{430}$$

   This is the step where the microscopic information spreads over macroscopic distances within the apparatus. However this spread is realized by the unitary time evolution and still shares the fragility of the quantum world.

2. *Decoherence* $t_m + \tau_m < t < t_m + \tau_m + \tau_d$*:* The problem with the state (430) is that it contains the linear superposition of macroscopically different apparatus states since the Schrödinger equation is linear. This is the point where the environment becomes important. The system and the measuring device form together an open system because they interact with their environment and this interaction generates an entangled state,

$$\sum_n c_n |\psi_n\rangle_s \otimes |\phi_n\rangle_a \otimes |\chi\rangle_e \to \sum_n c_n |\psi_n\rangle_s \otimes |\phi_n\rangle_a \otimes |\chi_n\rangle_e, \tag{431}$$

   owing to the different relative environment state, $|\chi_n\rangle_e$. The system-apparatus reduced

density matrix, c.f. appendix A,

$$\rho_{s,a} = \sum_{n,n'} c_n^* c_{n'} \langle \chi_n |_e \chi_{n'} \rangle_e |\psi_n\rangle_s \otimes |\phi_n\rangle_a \langle \psi_{n'}|_s \otimes \langle \phi_{n'}|_a, \tag{432}$$

looses the contributions where the different apparatus states are macroscopically different. This process is called decoherence and its dynamical origin is the same as dissipation, describing the unavoidable loss of information (relative phase of macroscopically different apparatus states) or energy (apparatus energy to the environment). When the apparatus consists of the pointer of the ammeter and the environment contains the surrounding air molecules then the relative environment states of two macroscopically different pointer states, $|\phi_n\rangle$ and $|\phi_{n'}\rangle$ become orthogonal for large environment. A semiclassical argument to show this is to consider the change of the state of a molecules after a reflection from the pointer. If the pointer has different angle in $|\phi_n\rangle$ and $|\phi_{n'}\rangle$ then this molecule will have different momentum after the collision. The further collisions between the molecules generate rapidly different momentum for each molecules. The scalar product $\langle \chi_n |_e \chi_{n'} \rangle_e$ is the product of the overlap of the state of the molecules, each of them has an absolute magnitude less than one hence $\langle \chi_n |_e \chi_{n'} \rangle_e \to 0$.

The decoherence process generates non-unitary time evolution and the arising irreversibility lends some robustness to the information within the apparatus about the microscopic system.

3. *Collapse:* A complicated many-body effect makes a rapid collapse of the mixed state (433) onto

$$\sum_{n,n'} c_n^* c_{n'} \langle \chi_n |_e \chi_{n'} \rangle_e |\psi_n\rangle_s \otimes |\phi_n\rangle_a \langle \psi_{n'}|_s \otimes \langle \phi_{n'}| \to |\psi_{n_m}\rangle_s \otimes |\phi_{n_m}\rangle_a \langle \psi_{n_m}|_s \otimes \langle \phi_{n_m}|_a. \tag{433}$$

Note such a a pure, factorisable system-apparatus density state is a rough approximation, resulting from the omission of the system-apparatus entanglements within microscopically different apparatus states. This step transforms the robust information, stored in the apparatus, into the well defined, deterministic laws of classical physics. A more detailed, microscopic picture of this process is still lacking.

B. (In)Determinism

The choice of the element of the spectrum of the observable, realized by the measurement, is the deepest mystery of Quantum Mechanics because the choice of the quantum number n_m should

be non-deterministic according to the uncertainty principle. In fact, this principle prevents us to obtain all information from a physical system by rendering the observations blurred. Let us consider for instance a particle with spin 3/2, obeying the operator equation

$$\boldsymbol{S}^2 = S_x^2 + S_y^2 + S_z^2 \tag{434}$$

with a state vector which is eigenvector of the left hand side with eigenvalue $\frac{3}{4}$ (in units of $\hbar^2$). The spectrum of the spin component operators is $\{\pm\frac{1}{2}, \pm\frac{3}{2}\}$ and it is a simple exercise to check that eq. (434) can not be satisfied by assigning spectrum elements to each spin component. In other words, information which seems to exists "out there" according to our view of classical physics are non-accessible in the quantum world. This is the basis of distinguishing quantum and classical probabilities, controlling quantum and classical (thermal) fluctuations.

Can it be that such a crushing defeat of our macroscopic world view results only from our insufficient resolution of observing microscopic phenomena? In that case we may hope that the deterministic world view can be extended over the quantum domain when better technology is available. Such a hypothetical classical, deterministic theory contains variables which are at the time being hidden for us.

A simple hidden variable theory has been proposed by David Bohm for a system of N spinless particle where the hidden variable is the N-particle wave function, governed by Schrödinger's equation. Each (classical!) particle obeys a first order differential equation, stating that their velocity is proportional to the gradient of the phase of the wave function with respect to the particle coordinates. It is a matter of trivialities to check that the motion, generated by such an equation of motion produces the desired probability distribution of the particles.

While the construction of hidden variable theories is therefore possible the alternative, offered by them, comes with such a high price which makes this way of refuting the disturbing features of the quantum domain unacceptable for the majority of physicists.

C. Non-locality I. Einsein-Podolksi-Rosen experiment

One of the important difference between the hidden variable and truly classical theories is that the former is non-local. This problem can be approached by considering a thought experiment with a bomb which is cut into two equally massive pieces and glued together. The bomb is then brought to rest in the air and is exploded in such a manner that the two half acquire opposite momentum in the horizontal plane. The two fragments land on a horizontal area and the knowledge of the

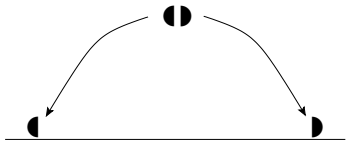


FIG. 25:

identification of the location of one of them allows us to predict immediately the location of the other. Such simple experiment becomes highly non-trivial in the microscopic world.

The thought experiment, proposed by Einstein, Podolsky and Rosen and modified slightly by Bohm, starts with a singlet state of two electrons,

$$|S\rangle = \frac{1}{\sqrt{2}}(|+_z\rangle \otimes |-_z\rangle - |-_z\rangle \otimes |+_z\rangle), \tag{435}$$

where the spin projection on the axis z is shown in units $2/\hbar$. One separates the particles by transporting the electrons to locations 1 and 2 without changing the total spin and measures the projection of the spin of the electron at location 1 on the direction $\boldsymbol{a}$ with the result s. The two particle state collapses to $|s_a\rangle \otimes |-s_a\rangle$ at this moment hence we know without actually performing any observation that the measurement of the spin of the other electron on the same direction, if carried out, must yield the opposite result, $-s$.

The difference between the macroscopic and the microscopic experiments is that while the "other", unobserved part follows a well defined, deterministic path in the former case the real direction of the spin is not defined for neither parts until the measurement in the latter case. Thus the microscopic experiment predicts the instantaneous spread of information, encoded by the spin entanglement in the state (435). Such a violation of Special Relativity has been confirmed by a number of experiments, using entangled two photon states. It was possible to confirm a non-trivial correlation between the spin of a photon, measured along a randomly chosen direction at location 1 and the successive measurement of the spin of the other photon along a fixed direction at location 2. The two measurements have been performed with such a small time delay which excluded that the choice of the direction of the polarization, used at location 1 could have influenced the measurement at location 2.

These are actually the first pair of experiments in the history of science, performed at spatial separation, without causal connection and they lead to a brutal violation of the limiting speed of propagation of signals. Nevertheless there is no explicit violation of Special Relativity because

the latter is stated within the realm of classical physics. The violation is found only on the level of "quantum fluctuations", the choice of one of the factorizable term in the entangled state (435). Since the collapse of the state during the measurement is non-deterministic and can not be influenced by macroscopic means the content of the signal, violating Special Relativity, can not be freely chosen by us. The entangled two-photon state has to be regarded as a non-local state with non-separable photons rather than the combination of two localizable single photon states.

D. Non-locality II. Bell inequality

The hidden variable theory offers a different interpretation of the EPR experiment. Let us denote the hidden variable by λ and its probability distribution by $p(\lambda)$. The result of the measurement of the spin of the electron at location 1 (2) is given by $A(\boldsymbol{a},\lambda)$ ($B(\boldsymbol{a},\lambda)$) where $A(\boldsymbol{a},\lambda), B(\boldsymbol{a},\lambda) = \pm 1$. We assume that the hidden variable theory is local hence the expectation value of the product of the spin, measured along the direction $\boldsymbol{a}$ ($\boldsymbol{b}$) at location 1 (2) is

$$p(\boldsymbol{a},\boldsymbol{b}) = \int d\lambda p(\lambda) A(\boldsymbol{a},\lambda) B(\boldsymbol{b},\lambda). \tag{436}$$

The prediction of Quantum Mechanics for this experiment can easily be fond by exploiting the rotational invariance and choosing $\boldsymbol{a}$ pointing to the z axis,

$$\begin{aligned} p(\boldsymbol{a},\boldsymbol{b}) &= \frac{1}{\sqrt{2}}(\langle +_z| \otimes \langle -_z| - \langle -_z| \otimes \langle +_z|)\sigma_z \otimes \boldsymbol{b\sigma} \frac{1}{\sqrt{2}}(|+_z\rangle \otimes |-_z\rangle - |-_z\rangle \otimes |+_z\rangle) \\ &= \frac{1}{2}(\langle -_z|\boldsymbol{b\sigma}|-_z\rangle - \langle +_z|\boldsymbol{b\sigma}|+_z\rangle) \\ &= \frac{1}{2}\left[\langle -_z| \begin{pmatrix} b_z & b_x - ib_y \\ b_x + ib_y & -b_z \end{pmatrix} |-_z\rangle - \langle +_z| \begin{pmatrix} b_z & b_x - ib_y \\ b_x + ib_y & -b_z \end{pmatrix} |+_z\rangle\right] \\ &= -b_z = -\boldsymbol{ab}. \end{aligned} \tag{437}$$

The results (436) and (437) are incompatible. This can be seen by noting that $A(\boldsymbol{a},\lambda) = -B(\boldsymbol{a},\lambda)$ for a singlet state, choosing a third polarization direction, $\boldsymbol{c}$ and calculating

$$\begin{aligned} p(\boldsymbol{a},\boldsymbol{b}) - p(\boldsymbol{a},\boldsymbol{c}) &= -\int d\lambda p(\lambda)[A(\boldsymbol{a},\lambda)A(\boldsymbol{b},\lambda) - A(\boldsymbol{a},\lambda)A(\boldsymbol{c},\lambda)] \\ &= \int d\lambda p(\lambda) A(\boldsymbol{a},\lambda)A(\boldsymbol{b},\lambda)[A(\boldsymbol{b},\lambda)A(\boldsymbol{c},\lambda) - 1]. \end{aligned} \tag{438}$$

The bound $|A(\boldsymbol{a},\lambda)| \leq 1$ yields Bell's inequality,

$$\begin{aligned} |p(\boldsymbol{a},\boldsymbol{b}) - p(\boldsymbol{a},\boldsymbol{c})| &\leq \int d\lambda p(\lambda)[1 - A(\boldsymbol{b},\lambda)A(\boldsymbol{c},\lambda)] \\ &= 1 + p(\boldsymbol{b},\boldsymbol{c}). \end{aligned} \tag{439}$$

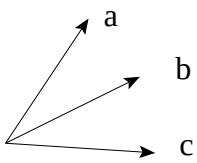


FIG. 26: The directions $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$, with $\boldsymbol{ab} = \boldsymbol{bc} = \frac{\sqrt{3}}{2}$ to show the incompatibility of the inequalities (436) and (437).

It is easy to check that this inequality is violated by (437) say by choosing the directions $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ in the same plane as in Fig. One way to bring Quantum Mechanics and the hidden variable theory compatible is to make the latter non-local, i.e renouncing (436) and loosing a decisive feature of classical physics.

E. Contextuality

Another possibility to save the deterministic hidden variable scheme is to renounce a tacit assumption about the well definiteness of physical quantity and accept contextuality. This concept is unusual in Quantum Mechanics on two counts. First, it characterizes the result of single observations rather than averages. Second, the deterministic structure of the hidden variable theories allows us to consider dynamical variables which are actually not measured but could be measured and their value happened to be well defined. The contextuality covers such kind of imaginary measurements.

Let us consider three observables, A, B and C such that $[A, B] = [A, C] = 0$ and $[B, C] \neq 0$. We may measure either the pair A, B or A, C and the result is contextual if the value of A is different in the two cases. The contextual hidden variable theories are consistent with the restriction of observations to compatible (commuting) observables however they explain the uncertainty of non-compatible observable by statistical fluctuations of hidden variables rather than the quantum state.

The contextuality of any hidden variable theory theory can be seen in the case of the simultaneous measure of the spin of two electrons. Consider the rearrangement of the spin observables,

$$\begin{array}{ccc} \mathbb{1} \otimes \sigma_z & \sigma_z \otimes \mathbb{1} & \sigma_z \otimes \sigma_z \\ \sigma_x \otimes \mathbb{1} & \mathbb{1} \otimes \sigma_x & \sigma_x \otimes \sigma_x \\ \sigma_x \otimes \sigma_z & \sigma_z \otimes \sigma_x & \sigma_y \otimes \sigma_y \end{array} \tag{440}$$

where each row and column contains commuting observables which can be measured simultaneously and therefore have well defined values in any hidden variable theory. The product of two observables in each row and column gives the third one except in the third column where a -1 sign occurs hence there is no way to assign a spectral values, ± 1, to all operators.

F. Instead of conclusion

The fundamental equations of physics can never be proven mathematically, they represent our way to summarize our knowledge about Nature. In a similar manner there is no way to prove any interpretation of Quantum Mechanics. Nevertheless it seems to me that the most reasonable interpretation is based on the view that Quantum Mechanics provides us consistent and optimized rules in dealing with the partial information we can have about the world around us and within us.

This impression has already been expressed by Heisenberg in 1958: *"We are finally led to believe that the laws of nature that we formulate mathematically in quantum theory deal no longer the particles themselves but with our knowledge of the elementary particles. ... The conception of the objective reality of the particles has thus evaporated in a curious way, not in the fog of some new, obscure, or not yet understood reality concept, but into the transparent clarity of a mathematics that represents no longer the behavior of the elementary particles but rather our knowledge of this behavior."* It remains for the next generations to refine this view or to find a more convincing one.

APPENDIX A: DENSITY MATRIX

The probability theory, a chapter of mathematics, describes the rules of using the probability without defining probability. The interpretation of the probability is provided by the law of large numbers. It is based on the empirical frequency of the realization of an event, $\nu(N_{tot}) = N_r/N_{tot}$, the ratio of the realization of the event and the number of trials and states that the probability of any finite deviation between ν and p, the probability of the event, is vanishing in the limit $N_{tot} \to \infty$, $P(|\nu(N_{tot}) - p| > \epsilon) = 0$ for any $\epsilon > 0$ as $N_{tot} \to \infty$. This is a circular definition without any hint about the origin or meaning of probability. The only discipline of natural science claiming to possess a constructive definition of probability is quantum mechanics and even that leaves the interpretation open.

1. Gleason theorem

The indeterministic nature of the microscopic world leaves us the possibility to use only probabilities in describing phenomena. The probability is defined in the classical world as a measure p, defined on a σ-algebra, $\mathcal{H}$. The σ-algebra is a collection of the measurable subsets of a set of elementary events, $\mathcal{M}$, and is closed under

1. forming the union of countable many subsets, $\cup_n a_n \in \mathcal{M}$ if $a_n \in \mathcal{M}$ and
2. the making the complement, $\mathcal{H} \backslash a \in \mathcal{M}$ if $a \in \mathcal{M}$.

A probability measure, a real valued function on the subspaces, $\mu : \mathcal{M} \to R$, satisfies the conditions

1. $0 \leq p(a) < \infty$ ($p(a) < 1$ for discrete values of a)
2. $p(\emptyset) = 0$
3. $p(\cup_n a_n) = \sum_n p(a_n)$ for $a_n \in \mathcal{M}$ and $a_m \cap a_n = \emptyset$.

The probability of quantum theory is defined by the help of a set $\mathcal{H}$, consisting of the linear space of states, and $\mathcal{M}$ containing the closed linear subspaces to which probability can be assigned. The set of measurable linear subspaces, $\mathcal{M}$, is closed under forming

1. the linear superposition of countable many states of the measurable subspaces, $\sum_n c_n a_n \in \mathcal{M}$ if $a_n \in \mathcal{M}$ and
2. the orthogonal complement, $\{v | \langle v | w \rangle = 0, \forall w \in a\} \in \mathcal{M}$.

A probability measure, a real valued function on the subspaces, $\mu : \mathcal{M} \to R$, satisfies the conditions

1. $0 \leq p(a) < \infty$
2. $p(\emptyset) = 0$
3. $p(\{\sum_n c_n a_n\}) = \sum_n p(a_n)$ for $a_n \in \mathcal{M}$ and $a_m \perp a_n = 0$.

Gleason theorem states that for any measure, p in a separable Hilbert space of at least 3 dimensions, either above real or complex numbers, one can find a linear operator ρ, called density matrix, such that

$$p(a) = \mathrm{Tr}[\rho \Lambda(a)], \tag{A1}$$

where

$$\Lambda(a) = \sum_n |n\rangle\langle n|, \tag{A2}$$

is the projector onto a, constructed by the help of a basis, $\{|n\rangle\}$, within the linear subspace, $|n\rangle \in a$.

The observable

$$A = \sum_n |\psi_n\rangle\lambda_n\langle\psi_n| \tag{A3}$$

consists of a correspondence, $|\psi_n\rangle \leftrightarrow \lambda_n$, between a basis in the Hilbert space and real numbers, and the result of the measurement of the observable in question in case when the state of the system is the corresponding basis vector. Therefore the average of the observable,

$$\langle A\rangle = \sum_n p_n\lambda_n, \tag{A4}$$

with $p_n = \mathrm{Tr}[\rho\Lambda(|n\rangle)]$ can be written in the form

$$\langle A\rangle = \mathrm{Tr}\rho A. \tag{A5}$$

There is no indication in quantum mechanics whether the probability is meaningful in case of the observation of an individual event.

2. Properties

The density matrix possesses the following properties:

1. $\rho^\dagger = \rho$: Any operator can be written as the sum of a Hermitian and an anti-Hermitian piece, $\rho = \rho_h + \rho_{ah}$, with $\rho_h = \frac{1}{2}(\rho + \rho^\dagger)$ and $\rho_{ah} = \frac{1}{2}(\rho - \rho^\dagger)$. The probability $\mathrm{Tr}P_\psi\rho = \langle\psi|\rho|\psi\rangle$ is real $|\psi\rangle$ hence $\langle\psi|\rho|\psi\rangle = \langle\psi|\rho^\dagger|\psi\rangle$. This equation holds for an arbitrary vector $|\psi\rangle$ therefore $\rho_{ah} = 0$.

2. The density matrix is a positive operator because its expectation value in any state is non-negative, $\langle\psi|\rho|\psi\rangle = \mathrm{Tr}[\Lambda(\psi)\rho] \geq 0$.

3. $\mathrm{Tr}\rho = 1$: The probability of the whole space of events, $\mathrm{Tr}\mathbb{1}\rho$ is unity.

4. The density matrix, being a Hermitian operator, is diagonalizable and can be written as

$$\rho = \sum_n |\psi_n\rangle p_n\langle\psi_n|, \tag{A6}$$

$\{|\psi_n\rangle\}$ being an orthonormal base. The eigenvalues are real, $0 \leq p_n$, and the diagonalization preserves the trace, $\sum_n p_n = 1$. The spectrum, $\{p_n\}$, can be interpreted as the probability of finding the system in one of the states, $|\psi_n\rangle$ since

$$\mathrm{Tr}A\rho = \sum_n p_n \langle\psi_n|A|\psi_n\rangle. \tag{A7}$$

5. The inequality

$$\mathrm{Tr}p^2 = \sum_n p_n^2 \leq \sum_n p_n = \mathrm{Tr}\rho \tag{A8}$$

becomes an equality only for pure states, $\rho = |\psi\rangle\langle\psi|$. The states with strict inequality are called mixed. The decomposition of the density matrix as a sum over pure state projectors is not unique, there are different systems of non-orthogonal states which yield the same density matrix.

Example: The most general density matrix of a two-state system is

$$\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{p}\boldsymbol{\sigma}) \tag{A9}$$

where the Pauli-matrices are

$$\boldsymbol{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right). \tag{A10}$$

This corresponds to the mixture of two states with probabilities $\frac{1}{2}(1 \pm |\boldsymbol{p}|)$ and

$$\langle\boldsymbol{\sigma}\rangle = \mathrm{tr}[\rho\boldsymbol{\sigma}] = \boldsymbol{p}. \tag{A11}$$

3. Composite systems

We make a little detour in discussing the way composite quantum systems can be represented before discovering the physical origin of the mixed states. Let suppose that we have two systems and use the the linear spaces, $\mathcal{H}_j$, $j = 1, 2$ for the description of their states. How to describe the composite systems of the two subsystems? It is clear that we have to use a linear space, $\mathcal{H}_{12}$, constructed by the help of the pairs, $(|\psi_1\rangle, |\psi_2\rangle) \in \mathcal{H}_{12}$, $|\psi_j\rangle \in \mathcal{H}_j$. The structure of the linear space, the definition of the addition, multiplication and the scalar product, remains to be defined. The following two possibilities are used in linear algebra:

Direct product: The elements of $\mathcal{H}_{1\otimes 2} = \mathcal{H}_1 \otimes \mathcal{H}_2$, are denoted by $|\psi_1\rangle \otimes |\psi_2\rangle$ and the structure is defined by:

1. Multiplication:

$$(c|\psi_1\rangle) \otimes |\psi_2\rangle = |\psi_1\rangle \otimes (c|\psi_2\rangle) = c(|\psi_1\rangle \otimes |\psi_2\rangle). \tag{A12}$$

2. Addition: $\mathcal{H}_1 \otimes \mathcal{H}_2$ is closed with respect to addition, $|\psi_1\rangle \otimes |\psi_2\rangle, |\psi_1'\rangle \otimes |\psi_2'\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ implies $|\psi_1\rangle \otimes |\psi_2\rangle + |\psi_1'\rangle \otimes |\psi_2'\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$.

3. Scalar product:

$$(\langle\psi_1| \otimes \langle\psi_2|)(|\psi_1'\rangle \otimes |\psi_2'\rangle) = \langle\psi_1|\psi_1'\rangle\langle\psi_2|\psi_2'\rangle. \tag{A13}$$

4. A pair of operators, $A_j : \mathcal{H}_j \to \mathcal{H}_j$ defines $A_1 \otimes A_2 : \mathcal{H}_{1\otimes 2} \to \mathcal{H}_{1\otimes 2}$, as

$$\langle\psi_1| \otimes \langle\psi_2|A_1 \otimes A_2|\psi_1'\rangle \otimes |\psi_2'\rangle = \langle\psi_1|A_1|\psi_1'\rangle\langle\psi_2|A_2|\psi_2'\rangle. \tag{A14}$$

These properties suggest to represent the direct product of vectors by multiplying their components, $\langle j_1, j_2|\psi_1\rangle \otimes |\psi_2\rangle = \langle j_1|\psi_1\rangle\langle j_2|\psi_2\rangle$, and $(\psi_1 \otimes \psi_2)(x_1, x_2) = \psi_1(x_1)\psi_2(x_2)$ with $\psi(x) = \langle x|\psi\rangle$, in terms of the bra-kets and the wave functions, respectively. If the set $\{|n_j\rangle\}$ is a basis for $\mathcal{H}_j$ then $\{|m_1\rangle \otimes |n_2\rangle|$ is a basis for $\mathcal{H}_{1\otimes 2}$ and $\dim \mathcal{H}_{1\otimes 2} = \dim \mathcal{H}_1 \dim \mathcal{H}_2$.

Direct sum: The linear spaces, $\mathcal{H}_{1\oplus 2} = \mathcal{H}_1 \oplus \mathcal{H}_2$, consisting of the pairs $|\psi_1\rangle \oplus |\psi_2\rangle$ is defined by

1. Multiplication: $\mathcal{H}_1 \oplus \mathcal{H}_2$ is closed with respect to the multiplication, $|\psi_1\rangle \oplus |\psi_2\rangle \in \mathcal{H}_1 \oplus \mathcal{H}_2$ implies $(c|\psi_1\rangle) \oplus |\psi_2\rangle, |\psi_1\rangle \oplus (c|\psi_2\rangle) \in \mathcal{H}_1 \oplus \mathcal{H}_2$.

2. Addition:

$$|\psi_1\rangle \oplus |\psi_2\rangle + |\psi_1'\rangle \oplus |\psi_2'\rangle = (|\psi_1\rangle + |\psi_1'\rangle) \oplus (|\psi_2\rangle + |\psi_2'\rangle), \tag{A15}$$

3. Scalar product:

$$(\langle\psi_1| \oplus \langle\psi_2|)(|\psi_1'\rangle \oplus |\psi_2'\rangle) = \langle\psi_1|\psi_1'\rangle + \langle\psi_2|\psi_2'\rangle, \tag{A16}$$

4. A pair of operators, $A_j : \mathcal{H}_j \to \mathcal{H}_j$ defines $A_1 \oplus A_2 : \mathcal{H}_{1\oplus 2} \to \mathcal{H}_{1\oplus 2}$, as

$$\langle\psi_1| \oplus \langle\psi_2|A_1 \oplus A_2|\psi_1'\rangle \oplus |\psi_2'\rangle = \langle\psi_1|A_1|\psi_1'\rangle + \langle\psi_2|A_2|\psi_2'\rangle. \tag{A17}$$

It is natural to represent the direct sum of vectors by a simple sum, $\langle j|(|\psi_1\rangle \oplus |\psi_2\rangle) = \langle j|\psi_1\rangle + \langle j|\psi_2\rangle$, and $(\psi_1 \oplus \psi_2)(x) = \psi_1(x) + \psi_2(x)$. If the set $\{|n_j\rangle\}$ is a basis for $\mathcal{H}_j$ then $\{|m_1\rangle \oplus |n_2\rangle|$ is a basis for $\mathcal{H}_{1\oplus 2}$ and $\dim \mathcal{H}_{1\oplus 2} = \dim \mathcal{H}_1 + \dim \mathcal{H}_2$.

Either procedure can in principle be followed to define a composite quantum system, the thumb rule is to use the direct product or the direct sum in describing simultaneously or exclusively existing components, respectively, for instance a spinless electronic state of the Hydrogen atom is $\psi(\boldsymbol{x}) = \sum_{nml} c_{nml}\psi_{nml}(\boldsymbol{x})$ and a factorisable two (distinguishable) particle wave function can be written in the form $\psi(\boldsymbol{x}_1, \boldsymbol{x}_2) = \psi_1(\boldsymbol{x}_1)\psi_2(\boldsymbol{x}_2)$.

Multi-particle systems with variable particle number require a unification of the two schemes, resulting the **Fock space**, $\mathcal{H}_{F12} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus (\mathcal{H}_1 \otimes \mathcal{H}_2)$.

4. Physical origin

Two, superficially different circumstances, loss of information and entanglement require the use of mixed states.

a. Loss of classical information

One has to distinguish classical and quantum probabilities. Probability appears in deterministic classical physics only if we lack some information. Such a probability characterizes our limited knowledge in an otherwise completely determined world. The information loss, behind the probability, given by the quantum mechanical Born's rule, is different.

On the one hand, the Heisenberg uncertainty relation implies a fuzziness which can not be recovered by improving our measuring device. One can find the origin of the unavoidable loss of information by noting that the equation of motion is a differential equation of order 2 and 1 in the classical and the quantum case, respectively. Hence a state say of a free particle is represented by twice as much numbers in the classical (coordinate and momentum) than in quantum mechanics (coordinate or momentum). Therefore the probability distribution of an observable in a pure state, p_n in (A4), always represents some uncertainty, compared to the classical description. The limitation of the available information by the uncertainty principle induces a loss of information, represented by quantum probability, the probability distribution of the spectrum variables of the observables, given by Born's rule.

On the other hand, the classical probability arises from the lack of the definite knowledge of the actual (pure) state of the system. We perform a number of measurements on a family of equivalently prepared systems to determine its quantum state. If the result is not certain then all we have at the end is a probability distribution of possible states, $|\psi_n\rangle \leftrightarrow p_n$. This gives rise to

the probability distribution $\{p_n\}$, represented by the density matrix in the expectation value (A7). Such a classical probability distribution enters in an additive manner in the expectation value.

The quantum probability of the observable A in the pure state, $|\psi\rangle = \sum_n \sqrt{p_n}|\psi_n\rangle$,

$$\langle\psi|A|\psi\rangle = \sum_{m,n} \sqrt{p_m p_n}\langle\psi_m|A|\psi_n\rangle, \tag{A18}$$

is not additive anymore in p_n owing to the interference between the different components of $|\psi\rangle$. The non-additivity results from the interference of the components of the state $|\psi\rangle$. It can be argued that the coherence between macroscopically different components is lost. Let us suppose for the sake of simplicity that the states $|\psi_n\rangle$, contributing to $|\psi\rangle$, are macroscopically different. Then the decoherence, a necessary condition of the emergence of the classical world from quantum mechanics, is the change

$$\langle\psi|A|\psi\rangle = \sum_{mn} \sqrt{p_m p_n}\langle\psi_m|A|\psi_n\rangle \to \sum_n p_n\langle\psi_n|A|\psi_n\rangle, \tag{A19}$$

which can be achieved by the change

$$\rho = \sum_{m,n} \sqrt{p_m p_n}|\psi_m\rangle\langle\psi_n| \to \sum_n p_n|\psi_n\rangle\langle\psi_n|. \tag{A20}$$

The destruction of the coherence among macroscopically different states generates classical probabilities for macroscopically different quantum states. That is not only the driving force in reaching the macroscopic physics from the microscopic one but it presumably serves as the origin of the universal laws of Statistical Physics.

b. Entangled states

Let us suppose that a closed system consists of two sub-systems with bases $|\phi_m\rangle$ and $|\chi_n\rangle$ and we can observe sub-system 1 only. We shall call the sub-system 1 and 2 as the observed system and its environment, respectively. Any pure state of the complete system can then be written as a linear superposition,

$$|\psi\rangle = \sum_{m,n} c_{m,n}|\phi_m\rangle \otimes |\chi_n\rangle. \tag{A21}$$

Such a decomposition is not unique and the Schmidt decomposition of $|\psi\rangle$ gives a specially useful representation,

$$|\psi\rangle = \sum_{n=1}^{N} c_n|u_n\rangle \otimes |v_n\rangle, \tag{A22}$$

because its states are orthogonal, $\langle u_m|u_{m'}\rangle = \delta_{m,m'}$, $\langle v_n|v_{n'}\rangle = \delta_{n,n'}$. A state with $N = 1$ consists of a single contribution, $|\psi\rangle = |u\rangle| \otimes |v\rangle$, and is called factorisable and the states with $N \geq 2$ are called entangled.

The properties of a sub-system are well defined only if the whole system is in a factorisable state. In fact, let us consider an observable A_1 of our system, represented by the operator $A = A_1 \otimes \mathbb{1}_2$. The expectation values in a factorisable state, $|\psi\rangle = |\phi\rangle| \otimes |\chi\rangle$,

$$\langle\psi|A|\psi\rangle = \langle\phi| \otimes \langle\chi|A_1 \otimes \mathbb{1}_2|\phi\rangle \otimes |\chi\rangle = \langle\phi|A_1|\phi\rangle, \tag{A23}$$

is indeed determined by the state $|\phi\rangle$.

This is not possible anymore for entangled states, there is no pure state of the observed system which reproduces all the expectation value of an entangled (pure!) state. In fact, let us suppose that the contrary is true, i.e. $N \geq 2$ in (A22) and any the system expectation values can be calculated by using the system state $|\phi_{obs}\rangle$. We inquire about the probability of finding the system in the state $|\phi_{obs}\rangle$. That probability can be obtained in two different manner: On the one hand, we have in linear space of the the observed system,

$$p(|\phi_{obs}\rangle\langle\phi_{obs}|) = \langle\phi_{obs}|\phi_{obs}\rangle\langle\phi_{obs}|\phi_{obs}\rangle = 1. \tag{A24}$$

On the other, the calculation on the level of the full, closed system yields

$$\begin{aligned} p(|\phi_{obs}\rangle\langle\phi_{obs}|) &= \langle\psi|(|\phi_{obs}\rangle\langle\phi_{obs}| \otimes \mathbb{1}_2)|\psi\rangle \\ &= \sum_{n,n'} c^*_{n'} c_n \langle u_{n'}| \otimes \langle v_{n'}|(|\phi_{obs}\rangle\langle\phi_{obs}| \otimes \mathbb{1})|u_n\rangle \otimes |v_n\rangle \\ &= \sum_{n=1}^{N} |c_n|^2 |\langle u_n|\phi\rangle|^2 < 1. \end{aligned} \tag{A25}$$

In the case of $N \geq 2$ the inequality follows from the normalization $\sum_n |c_n|^2 = 1$, and the bound $|\langle u_n|\phi_{obs}\rangle| \leq 1$. The expectation value of system observable in an entangled state (A21)

$$\begin{aligned} \langle A\rangle &= \sum_{n,n'} c^*_n c_{n'} \langle u_n| \otimes \langle v_n|A_1 \otimes \mathbb{1}_2|u_{n'}\rangle \otimes |v_{n'}\rangle \\ &= \sum_n |c_n|^2 \langle u_n|A_1|u_n\rangle, \end{aligned} \tag{A26}$$

is of a mixed state, described by the density matrix

$$\rho_1 = \sum_n |u_n\rangle |c_n|^2 \langle u_n|. \tag{A27}$$

The density matrix (A27), defining the mixed state of the observed system is called the reduced density matrix. The reduced density matrix of the subsystem 1, ρ_1, and can be obtained from the density matrix of the full system,

$$\rho_{12} = \sum_{n,n'} c_n c_{n'}^* |u_n\rangle \otimes |v_n\rangle\langle u_{n'}| \otimes \langle v_{n'}|, \tag{A28}$$

by "tracing out" the unobserved environment space,

$$\begin{aligned} \rho_1 &= \mathrm{Tr}_2[\rho_{12}] \\ &= \sum_{\bar{n}} \langle \chi_{\bar{n}} | \rho_{12} | \chi_{\bar{n}} \rangle \\ &= \sum_{\bar{n},n,n'} c_n c_{n'}^* \langle \chi_{\bar{n}} | (|u_n\rangle \otimes |v_n\rangle\langle u_{n'}| \otimes \langle v_{n'}|) | \chi_{\bar{n}} \rangle \\ &= \sum_{\bar{n},n,n'} c_n c_{n'}^* |u_n\rangle\langle u_{n'}| \langle v_n | \chi_{\bar{n}} \rangle \langle \chi_{\bar{n}} | v_{n'} \rangle. \end{aligned} \tag{A29}$$

The closing relation $\mathbb{1}_2 = \sum_{\bar{n}} |\chi_{\bar{n}}\rangle\langle\chi_{\bar{n}}|$ completes the demonstration of the equivalence of the expressions (A27) and (A29),

$$\begin{aligned} \rho_1 &= \sum_{n,n'} c_n c_{n'}^* |u_n\rangle\langle u_{n'}| \langle v_n | v_{n'} \rangle \\ &= \sum_{n} |c_n|^2 |u_n\rangle\langle u_n|. \end{aligned} \tag{A30}$$

The lesson of the above steps is:

1. A sub-system which is entangled with its environment has mixed state and possesses no unique properties, the expectation values are given in terms of the amplitudes of the full system state.

2. If the full system starts in a factorisable pure state then the interaction between the two sub-systems generates entanglement except of the unimportant special case where the interaction Hamiltonian is diagonal in the Schmidt decomposition basis. Hence entanglement arises from interactions. However entanglement is more general than interactions because the latter assumes an interaction Hamiltonian while the former is a property of the state of the complete system, without any reference to the interaction between the sub-systems.

3. Both the loss of classical information and the entanglement are represented by the same mathematical device, a mixed state. Therefore one tends to consider entanglement as the physical origin of mixed states and the modelization of lost classical information at the more fundamental quantum level.

c. Relative states

The correlation between the system and its environment can better be seen by relaxing the orthogonality condition of the Schmidt decomposition because it shows in a clearer manner the correlation between the two subsystems. For any pure complete system state $|\psi\rangle$ the relative state of an environment state vector, $|\chi\rangle$, is defined by

$$|R(\chi)\rangle = N \sum_m |\phi_m\rangle\langle\phi_m, \chi|\psi\rangle, \tag{A31}$$

where the notation $|\phi_m, \chi\rangle = |\phi_m\rangle \otimes |\chi\rangle$ is introduced and $N = 1/\sqrt{p}$ denotes the normalization, defined by the marginal probability distribution,

$$\begin{aligned} p(\chi) &= \sum_m |\langle\phi_m, \chi|\psi\rangle|^2 \\ &= \langle\psi|(\mathbb{1} \otimes |\chi\rangle\langle\chi|)|\psi\rangle, \end{aligned} \tag{A32}$$

of the environment states in $|\psi\rangle$. One can prove that the relative state and the marginal probabilities are independent of the choice of the system basis, $|\phi_m\rangle$.

Let us consider a system observable which is diagonal in our basis, $A_s = \sum_m |\phi_m\rangle\lambda_m\langle\phi_m|$. Its expectation value in a relative state, assuming that the environment is in the pure state $|\chi\rangle$,

$$\langle R(\chi)|A_s|R(\chi)\rangle = \frac{1}{p(\chi)} \sum_m \langle\psi|\phi_m, \chi\rangle\langle\phi_m, \chi|A_s \otimes \mathbb{1}|\phi_m, \chi\rangle\langle\phi_m, \chi|\psi\rangle, \tag{A33}$$

can be written as

$$\langle R(\chi)|A_s|R(\chi)\rangle = \sum_m \lambda_m \frac{\langle\phi_m, \chi|\psi\rangle|^2}{p(\chi)}. \tag{A34}$$

Since the factor $p(\phi_m|\chi) = \langle\phi_m, \chi|\psi\rangle|^2/p(\chi)$ is just the conditional probability of finding the system state $|\phi_m\rangle$, assuming that the environment is in the state $|\chi\rangle$, we have

$$\langle R(\chi)|A_s|R(\chi)\rangle = \sum_m \lambda_m p(\phi_m|\chi), \tag{A35}$$

indicating that the knowledge of the environment state translates itself into the relative system states, as far as the system observables are concerned. The pure complete system state can be written as

$$|\psi\rangle = \sum_{m,n} |\phi_m, \chi_n\rangle\langle\phi_m, \chi_n|\psi\rangle = \sum_n \sqrt{p(\chi_n)}|R(\chi_n)\rangle \otimes |\chi_n\rangle \tag{A36}$$

We now return to the discussion of the density matrix and write the expectation value of the system observable, A_s, in the pure complete system state, $|\psi\rangle$, as

$$\begin{aligned}\langle\psi|A_s|\psi\rangle &= \sum_{n,n'}\sqrt{p(\chi_n)p(\chi_{n'})}\langle R(\chi_{n'})|\otimes\langle\chi_{n'}|A_s\otimes\mathbb{1}|R(\chi_n)\rangle\otimes|\chi_n\rangle \\ &= \sum_n p(\chi_n)\langle R(\chi_n)|A_s|R(\chi_n)\rangle. \end{aligned} \tag{A37}$$

In other words, the reduced density matrix is

$$\rho=\sum_n |R(\chi_n)\rangle p(\chi_n)\langle R(\chi_n)|. \tag{A38}$$

The lesson is that entanglement arises if different environment states can condition linearly independent system states in the given pure complete system state.

APPENDIX B: QUANTUM ANOMALIES

The trajectory of a classical free point particle has analytical, more precisely linear, time dependence. There are no trajectories in quantum mechanics but the propagation of a free point particle displays singular features for short time. Such singularities introduce unexpected modification to a thumb rule, introduced in the early days of quantum mechanics, namely that the commutators of dynamical quantities can be obtained from their classical counterparts, the Poisson bracket, by inserting a multiplicative factor $i\hbar$ into the right hand side, e.g.

$$\{x_j,p_k\}=\delta_{j,k} \qquad \Longrightarrow \qquad [x_j,p_k]=i\hbar\delta_{j,k}. \tag{B1}$$

It will be pointed out that the short time singularities of the transition amplitude of a free particle between two space points is the result of Heisenberg's canonical commutation relation. Since the use of the Poisson bracket in classical mechanics is based on regular, differentiable functions the short time singularities generate unexpected, so called Schwinger terms to the commutators. These corrections violate the above mentioned simple quantization rule and are given the rather unfortunate name "anomaly".

1. Singular time dependence

The amplitude of propagation $\boldsymbol{x}\to\boldsymbol{y}$ within time t of a three dimensional free particle,

$$\langle\boldsymbol{x}|e^{-\frac{i}{\hbar}\frac{\boldsymbol{p}^2}{2m}t}|\boldsymbol{y}\rangle=\Big(\frac{m}{2\pi i\hbar t}\Big)^{\frac{3}{2}}e^{i\frac{m}{2\hbar t}(\boldsymbol{x}-\boldsymbol{y})^2} \tag{B2}$$

gives us the wave function

$$\psi(t,\boldsymbol{x}) = \langle \boldsymbol{x}|e^{-\frac{i}{\hbar}\frac{\boldsymbol{p}^2}{2m}t}|\boldsymbol{y}\rangle, \tag{B3}$$

satisfying the initial condition

$$\psi(0,\boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y}). \tag{B4}$$

In fact, it is easy to check that the wave function satifies Schrödinger's equation,

$$i\hbar\partial_t\psi(t,\boldsymbol{x}) = -\frac{\hbar^2}{2m}\Delta\psi(t,\boldsymbol{x}), \tag{B5}$$

and the initial condition arises from the orthogonality of the coordinate eigenstates, $\langle \boldsymbol{x}|\boldsymbol{y}\rangle = \delta(\boldsymbol{x}-\boldsymbol{y})$.

The phase difference of the wave function at different space points is measurable and the distance of points with a given phase difference Φ is

$$|\Delta\boldsymbol{x}| = \sqrt{\frac{2\hbar t\Phi}{m}}. \tag{B6}$$

The velocity of the spread of the pair of points, corresponding to a fixed phase difference,

$$v = \frac{|\Delta\boldsymbol{x}|}{t} = \sqrt{\frac{2\hbar\Phi}{mt}}, \tag{B7}$$

diverges at short time, $t \to 0$. The singularity results from Heisenberg's uncertainty principle and is the dynamical origin of the spread of the wave packet. In fact, the initial condition (B4) amounts ot the perfect knowledge of the coordinate hence the observation of the momentum, the mass time the velocity, produces diverging fluctuations.

The short time singularity of the propagation leaves two important fingerprints in quantum theory:

1. The regular time dependence in classical mechanics allows us to change the coordinate system by following the standard rules of calculus. The short time singularity in quantum mechanics generates $\mathcal{O}(\hbar)$ corrections to these rules. In particular, the Legendre transformation, connecting the classical Lagrangian and Hamiltonian has to be modified in quantum mechanics. This amounts to an $\mathcal{O}(\hbar)$ violation of the canonical symmetry of quantum mechanics and the change of the quantization rules when a non-linear coordinate transformation is performed.

2. The Poisson bracket structure of classical mechanics implies regular time dependence. However the singular time dependence produces Schwinger terms to certain commutators. Hence

certain classical conservation laws and symmetries, expressed by the vanishing of the Poisson bracket between the Hamiltonian and a dynamical quantity may be violated by $\mathcal{O}(\hbar)$ quantum effects.

These issues are best understood within the framework of Feynman's path integral formalism of quantum mechanics where they result from the fractal nature of the typical trajectories of a particle. However the argument would lead us beyond the scope of these lectures. Thus the demonstration of the modification of the quantization rules in polar coordinate system is presented below within the operator formalism.

2. Quantization rules in polar coordinates

The quantization rules define the Hamiltonian and the equation of motion by starting the Lagrangian. In case of a free particle, described by the Cartesian coordinates $\boldsymbol{x} = (x_1, x_2, x_3)$, one starts with the Lagrangian

$$L = \frac{m}{2}\dot{\boldsymbol{x}}^2, \tag{B8}$$

defines the momentum

$$\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{x}}} = m\dot{\boldsymbol{x}}, \tag{B9}$$

and construct the Hamiltonian,

$$H = \dot{\boldsymbol{x}}\boldsymbol{p} - L, \tag{B10}$$

expressed in terms of the momentum

$$H = \frac{\boldsymbol{p}^2}{2m}. \tag{B11}$$

The canonical commutation relations,

$$[x_j, p_k] = i\hbar\delta_{j,k}, \tag{B12}$$

give rise to the representation $p_j = \frac{\hbar}{i}\partial_{x_j}$ and the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2, \tag{B13}$$

which possesses translational and rotational symmetry,

$$[H, \boldsymbol{p}] = [H, \boldsymbol{L}] = 0, \tag{B14}$$

where the momentum $\boldsymbol{p}$ and angular momentum $\boldsymbol{L}$ generates translations and rotations, respectively.

The quantization in polar coordinates is carried out by the help of the parametrization

$$\boldsymbol{x} = \begin{cases} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{cases} \tag{B15}$$

and the free Lagrangian

$$L = \frac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) \tag{B16}$$

yields the momenta

$$\begin{aligned} p_r &= \frac{\partial L_0}{\partial \dot{r}} = m\dot{r}, \\ p_\theta &= \frac{\partial L_0}{\partial \dot{\theta}} = mr^2\dot{\theta}, \\ p_\phi &= \frac{\partial L_0}{\partial \dot{\phi}} = mr^2\sin^2\theta\dot{\phi}. \end{aligned} \tag{B17}$$

The classical Hamiltonian is therefore of the form

$$\begin{aligned} H_{cl} &= p_r\dot{r} + p_\theta\dot{\theta} + p_\phi\dot{\phi} - L \\ &= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2\sin^2\theta}. \end{aligned} \tag{B18}$$

The canonical commutation relations,

$$[r, p_r] = [\theta, p_\theta] = [\phi, p_\phi] = i\hbar \tag{B19}$$

are satisfied by

$$p_r = \frac{\hbar}{i}\frac{\partial}{\partial r}, \quad p_\theta = \frac{\hbar}{i}\frac{\partial}{\partial \theta}, \quad p_\phi = \frac{\hbar}{i}\frac{\partial}{\partial \phi}. \tag{B20}$$

The insertion of these operators into the classical Hamiltonian yields

$$H_{naive} = -\frac{\hbar^2}{2m}\left[\partial_r^2 + \frac{1}{r^2}\left(\partial_\theta^2 + \frac{1}{\sin^2\theta}\partial_\phi^2\right)\right]. \tag{B21}$$

It is not difficult to see that this operator does not possess the usual symmetries, namely $[H_{naive}, \boldsymbol{p}] \neq 0$, $[H_{naive}, \boldsymbol{L}] \neq 0$, i.e. Schwinger terms arise in these commutators.

It is well known that the correct Hamiltonian is obtained by starting with the Cartesian result (B13) involving the Laplace-Beltrami operator,

$$H = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\phi^2\right)\right], \tag{B22}$$

which differs from H_{naive},

$$H = H_{naive} + i\frac{\hbar}{2m}\left(\frac{2}{r}p_r + \cot\theta p_\theta\right), \tag{B23}$$

and the difference, an $\mathcal{O}(\hbar)$ term, is called Îto potential.