Elements of Advanced Quantum Mechanics

Quantenmechanik II

— Lecture script, internal version —

WS 2016/17

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→ Teaching → Fortgeschrittene Quantenmechanik

(Script and additional material)

Stephan Fritzsche

Helmholtz-Institut Jena &

Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, Fröbelstieg 3, D-07743 Jena, Germany

(Email: s.fritzsche@gsi.de, Telefon: +49-3641-947606, Raum 204)

Please, send information about misprints, etc. to s.fritzsche@gsi.de.

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0. Preliminary remarks

0.1. Schedule and agreements

Lecture period:	17. 10. 2016 – 03. 2. 2017
Lecture:	We & Thu, 8 – 10, Abbeanum, HS 2
Tutorials:	Tue, 10 – 12, Abbeanum, SR 102
	Fr, 8 – 10, HW 4, SR 1
Language:	German / English ??
ECTS points:	8 (inclusive the tasks and exam).
Exam:	Tasks (40 %), written exam.
Requirements for exam:	*Modulanmeldung* within the first 6 weeks; at least 50 % of points from tutorials.
Klausur:	Thursday, 9. February 2017, 8 – 11; Abbeanum, HS 2

0.2. Further reading

- C. Cohan-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics: Fundamentals* (Springer, 2003).
- J. Sakurai, *Modern Quantum Mechanics* (Pearson, 1993).
- A. S. Davidow, *Quantenmechanik* (J. A. Barth, 1992).
- B. Thaller, *Advanced Visual Qantum Mechanics* (Springer, 2005).
- K. Konishi and G. Paffuti, *Quantum Mechanics: A New Introduction* (Oxford, 2009).

Other texts: ... (Blackboard)

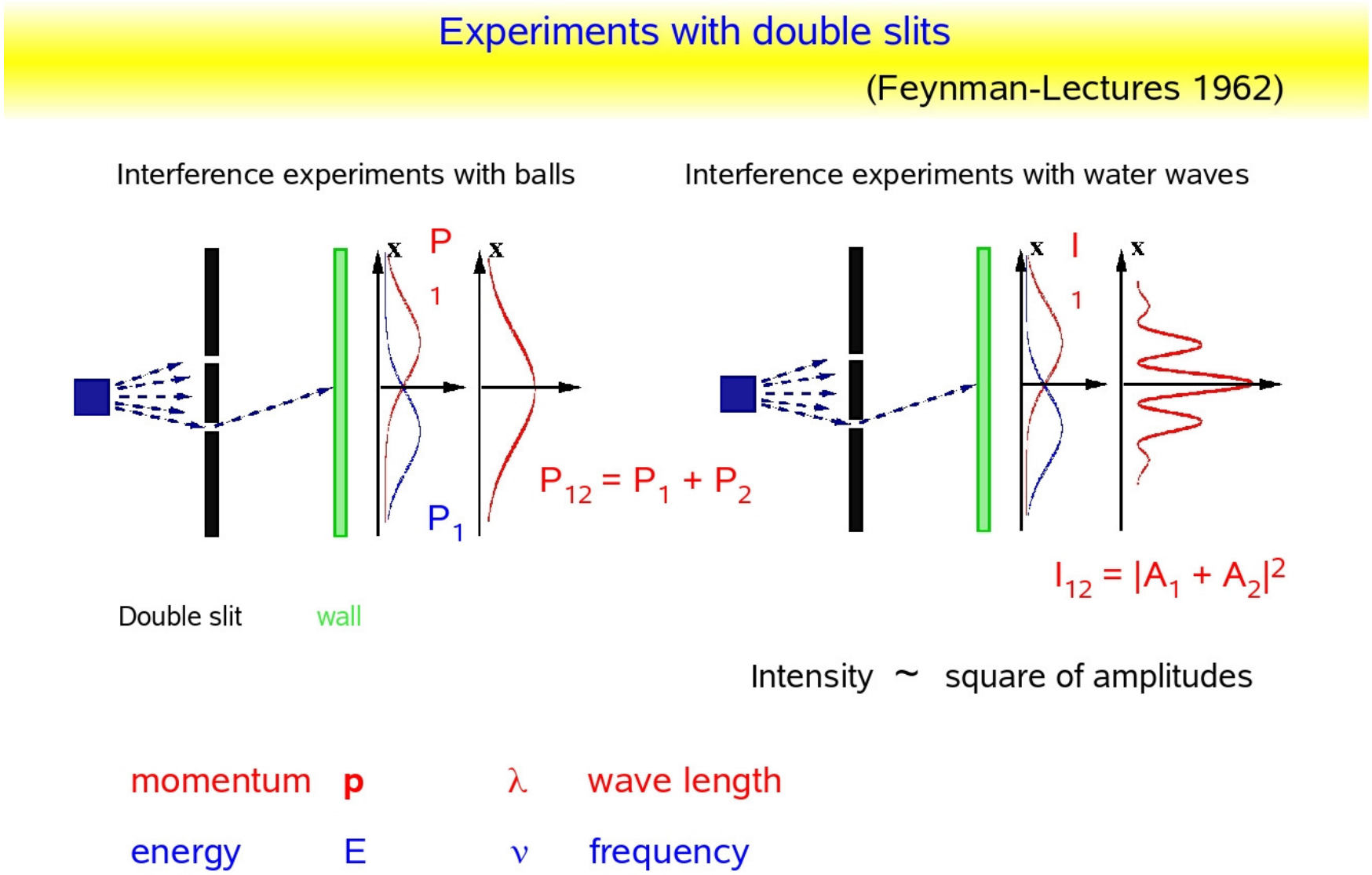


Figure 0.1.: Young's double-slit experiment: classical particles vs. waves; cf. Feynman Lectures (1963).

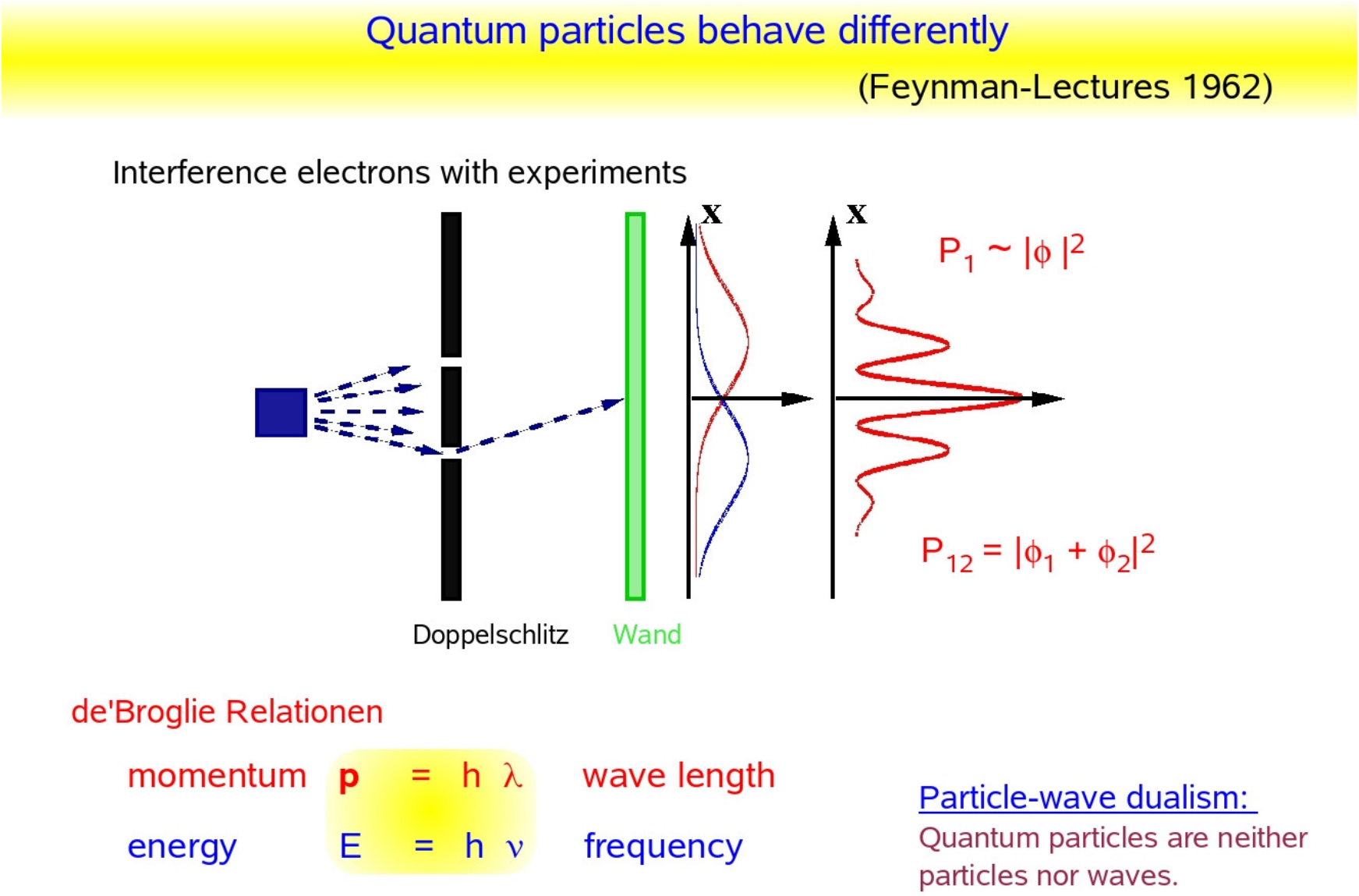
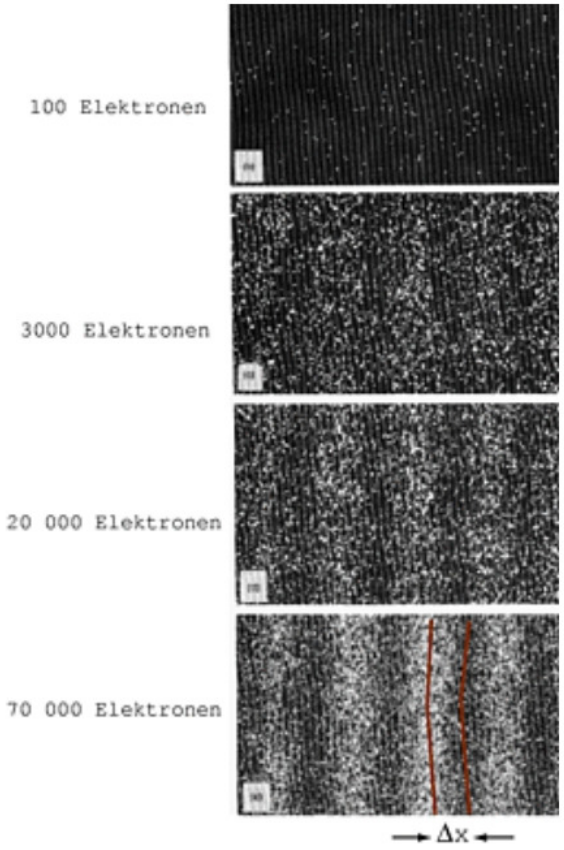
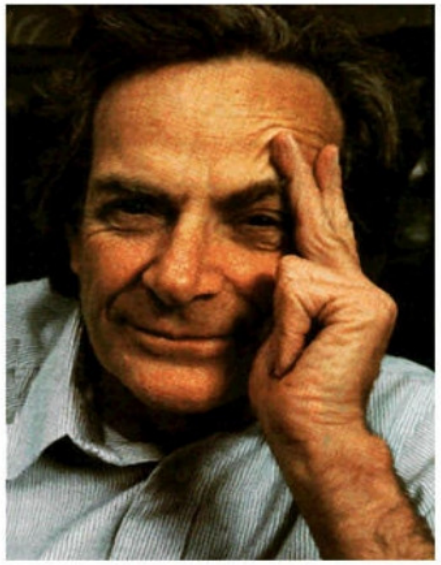


Figure 0.2.: Young's double-slit experiment: Quantum particles behave differently; cf. Feynman Lectures (1963).

Doppelspaltexperiment mit Elektronen

A. Tanamura et al., Am. J. Phys. 57 (1989) 117





Richard Feynman (1918–1988)

"...Wir können das Geheimnis (dieses Versuchs) nicht aufdecken, indem wir "erklären" wie es funktioniert. Wir können nur berichten wie es funktioniert, und indem wir dies tun, erörtern wir die grundlegenden Eigentümlichkeiten der ganzen Quantenmechanik."

Figure 0.3.: Young's double-slit experiment in practice ... here with electrons and 25 years later after the famous Feynman lectures.

1. Quantum theory: A short reminder

1.1. Young's double-slit experiment for quantum particles

A very few remarks :

- ➢ Particle-wave dualism: Quantum particles are neither particles nor waves.
- ➢ First described (so clearly !!) by Richard Feynman, although experiments with electrons were realized only about 25 years later.
- ➢ This experiment shows very nicely (almost all) essential details and problems with quantum mechanics.
- ➢ Similar experiments have been realized meanwhile also with atoms, molecules, bucky balls, ...
- ➢ Which-path information: Quantum interference disappears (gradually) as more information is obtained about the actual path of the particles.

1.2. Mach-Zehnder interferometer

= pair of spatial pathes

The Mach-Zehnder interferometer setup is another one (out of many further experimental set-ups) which have convinced

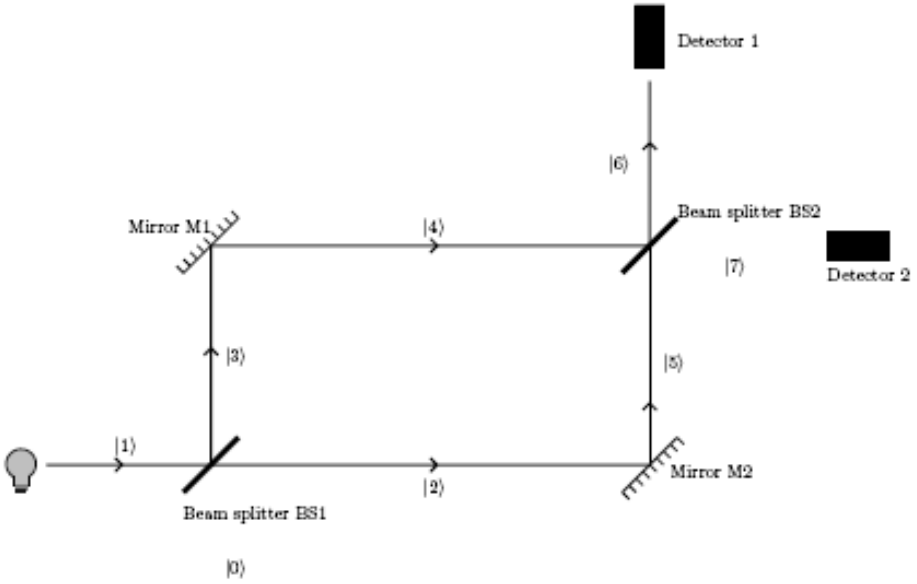


Figure 1.1.: The Mach-Zehnder interferometer. A photon is sent through a beam splitter and bounced off at two mirrors into another beam splitter. Mysteriously, only one of the detectors registers a photon.

the physicists that the behaviour of quantum particles can – by no means – be described by classical mechanics.

Set-up and properties: ... (Blackboard)

1.3. Postulates of QM

1.3.a. Postulate I (State space & state vectors)

For each quantum-mechanical systems, there is associated a scalar product space (Hilbert space), $\mathcal{H}$, whose unit vectors describe the system uniquely, i.e. all these states (superpositions) represent possible states of the system.

1.3.b. Postulate II (Time evolution of closed systems):

The time evolution of the system is described by a unitary transformation

$$|\psi'(t_2)\rangle \;=\; U(t_2,\, t_1)\;\, |\psi(t_1)\rangle$$

U ... time evolution operator; discrete time evolution

A strict unitary time evolution applies only for closed systems; although this is an idealization, it is often quite well fulfilled (discrete time evolution).

Schrödinger equation: alternative description with contineous time evolution

$$-i\hbar \frac{d\;|\psi\rangle}{dt} \;=\; H\;\, |\psi\rangle$$

... hermitian Hamilton operator H

The knowledge of the Hamilton operator typically requires physical intuition and experimental information; in nuclear and solid-state physics, the form of the (effective) Hamiltonian is still an issue of research due to unknown interactions. In AMO and QI, in contrast, the Hamiltonian is typically assumed to be a known. Then, we are interested in good (many-particle) approximations as well as the time-evolution and the coupling of different subsystems.

Spectral decomposition: $H \;=\; \sum_E E\;\, |E\rangle\,\langle E|$

... eigenvalues and eigenvectors of H

Relation for $H \neq H(t)$:

$$|\psi(t_2)\rangle = \exp\left(\frac{-iH(t_2-t_1)}{\hbar}\right)|\psi(t_1)\rangle = U(t_2,t_1)\,|\psi(t_1)\rangle$$

$$K \text{ hermitian} \qquad \Longleftrightarrow \qquad U = \exp(iK) \quad \text{is unitary}$$

Experiment: Interactions with external systems can often be described by means of some time-dependent Hamiltonian, $H = H(t)$.

Exceptions:

- ➢ Quantum measurements.
- ➢ Coupling to some bath or environment.

1.3.c. Postulate III (Quantum measurements and measurement operators):

Quantum measurements can be formally described by a set of measurement operators $\{M_m\}$ that act within the state space of the system and where m denotes one of the possible outcomes of the measurement.

Set of measurement operators $\{M_m\}$ ..... linear operators $\mathcal{H} \rightarrow \mathcal{H}$.

Consider a system in the state $|\psi\rangle$ before the measurement, then the probability for the outcome m is

$$p(m) = \langle\psi\,|M_m^+ M_m|\,\psi\rangle$$

and the state (just) after the measurement

$$\frac{M_m\,\psi}{\sqrt{p(m)}} = \frac{M_m\,\psi}{\sqrt{\langle\psi\,|M_m^+ M_m|\,\psi\rangle}}\,.$$

Completeness relation:

$$1 = \sum_m p(m) = \sum_m \langle\psi\,|M_m^+ M_m|\,\psi\rangle \qquad \forall\ |\psi\rangle \qquad \Longleftrightarrow \qquad I = \sum_m M_m^+ M_m$$

Blackboard example (Measurement of a spin-1/2 particle in the standard basis):

1.3.d. Postulate IV (Composite systems and entanglement):

For composite systems, the state space is given by the tensor product of the state space of all subsystems. Especially for N systems in state $\{|\psi_i\rangle\,,\ i = 1, ..., N\}$, the overall states is:

$$|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ ... \ \otimes |\psi_N\rangle$$

... total state in the interaction free case

In general, however, such systems will not reside in such a product state due to internal interactions or interactions with some environement.

Notations: There are many different forms to describe many-particle; in QI, for example, one often uses an 'index' to denote the subsystem, $X_2,\ Z_5,\ ...$

Entanglement: Composite systems can be in (superposition of) states that cannot be written as 'product states'. This has been recognized also as an important resource in QI and can lead to very unexpected results.

Further reading (On the foundation of quantum mechanics):

➢ Read the article The Oxford Questions on the foundations of quantum physics by G. A. D. Briggs, J. N. Butterfield and A. Zeilinger, Proc. R. Soc. A 469 (2013); cf. 1.3-Oxford-questions.pdf on the web page of the lecture.

2. Scattering theory

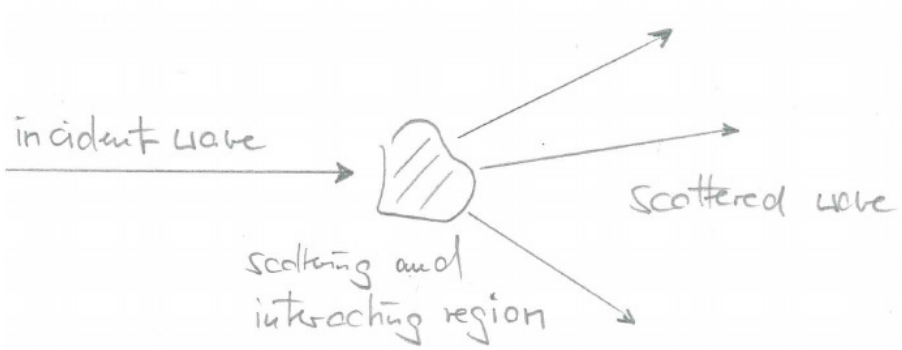


Figure 2.1.: Scattering of an incident wave in some given (fixed) potential.

2.1. Scattering in short-range potentials

We shall start with the scattering of a particle in a short-range potential; here, the incident particles are usually described by either a (monochromatic) plane-wave or wave packet.

Short-range potential $V(\mathbf{r})$**:** ... decays faster than $1/r \equiv 1/|\mathbf{r}|$ for $r \to \infty$, or:

$$\lim_{r\to\infty} r\, V(\mathbf{r}) = 0\,,$$

and where we assume a characteristic extent R, so that $V(\mathbf{r})$ is negligible for $r \gg R$.

Time-independent SE: ... we are looking for a (stationary) wave function as solution of

$$\left(\frac{\hbar^2}{2m}\,\nabla^2 \,+\, E_k\right)\,\psi_{\mathbf{k}}(\mathbf{r}) \;=\; V(\mathbf{r})\,\psi_{\mathbf{k}}(\mathbf{r})\,, \qquad E_k \;=\; \frac{\hbar^2\,k^2}{2m}\,, \qquad k \;=\; |\mathbf{k}|\,, \qquad \mathbf{k} \text{ ... wave vector}$$

and with the wave vector $\mathbf{k}$ of the indicent particle (wave packet) as parameter. For a proper potential $V(\mathbf{r})$, there exist a solution for each wave vector $\mathbf{k}$.

2.1.a. Lippman-Schwinger equation

We can formally solve the time-independent SE from above by means of a Greens function $G(\mathbf{r}, k)$ for a δ-like potential

$$\left(\frac{\hbar^2}{2m}\,\nabla_{\mathbf{r}}^2 \,+\, E_k\right)\,G(\mathbf{r}, k) \;=\; \delta(\mathbf{r})$$

$$\psi_{\mathbf{k}}(\mathbf{r}) \;=\; \underbrace{\phi_{\mathbf{k}}(\mathbf{r})}_{e^{i\mathbf{k}\cdot\mathbf{r}}} + \int d^3\mathbf{r}'\,G(\mathbf{r}-\mathbf{r}', k)\,V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}')$$

Indeed:

$$\left(\frac{\hbar^2}{2m}\,\nabla_{\mathbf{r}}^2 \,+\, E_k\right)\,\psi_{\mathbf{k}}(\mathbf{r}) \;=\; \underbrace{\left(\frac{\hbar^2}{2m}\,\nabla_{\mathbf{r}}^2 \,+\, E_k\right)\,\phi_{\mathbf{k}}(\mathbf{r})}_{=0} + \int d^3\mathbf{r}'\,\left[\underbrace{\left(\frac{\hbar^2}{2m}\,\nabla_{\mathbf{r}}^2 \,+\, E_k\right)\,G(\mathbf{r}-\mathbf{r}', k)}_{=\,\delta(\mathbf{r}-\mathbf{r}')}\right]\,V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}')$$

$$=\; 0 \,+\, \int d^3\mathbf{r}'\,\delta(\mathbf{r}-\mathbf{r}')\,V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}') \;=\; V(\mathbf{r})\,\psi_{\mathbf{k}}(\mathbf{r})$$

2.1.b. Finding the Greens function

Explicit solution can be obtained with help of the Fourier transform

$$G(\mathbf{r},k) \;=\; \frac{1}{(2\pi)^3}\int d^3\mathbf{q}\;\tilde{G}(\mathbf{q},k)\,e^{i\mathbf{q}\cdot\mathbf{r}} \tag{2.1}$$

$$\left(\frac{\hbar^2}{2m}\,\nabla^2_{\mathbf{r}}\;+\;E_k\right)\;G(\mathbf{r},k) \;=\; \frac{1}{(2\pi)^3}\int d^3\mathbf{q}\;\underbrace{\left(-\frac{\hbar^2\,\mathbf{q}^2}{2m}\;+\;E_k\right)\;\tilde{G}(\mathbf{q},k)}_{=1\;!!}\;e^{i\mathbf{q}\cdot\mathbf{r}} \;=\; \delta(\mathbf{r})$$

$$\tilde{G}(\mathbf{q},k) \;=\; \frac{1}{E_k\;-\;\frac{\hbar^2\,\mathbf{q}^2}{2m}} \;=\; \frac{2m}{\hbar^2}\;\frac{1}{k^2\;-\;\mathbf{q}^2}$$

Substitution into the (definition of the) Fourier transform (2.1) then gives rise to:

$$G(\mathbf{r},k) = \frac{1}{(2\pi)^3}\int d^3\mathbf{q}\,\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{E_k - \frac{\hbar^2\,\mathbf{q}^2}{2m}} \qquad \Longrightarrow \qquad \mathbf{q} = (q,\vartheta,\varphi) \qquad \text{spherical coordinates}$$

$$= -\frac{m}{2\pi^2\,\hbar^2}\int_0^\infty dq\,q^2\int_1^{-1} d\,(\cos\vartheta)\,\frac{e^{iqr\,\cos\vartheta}}{k^2-q^2}$$

$$= \frac{m}{2ir\,\pi^2\,\hbar^2}\int_{-\infty}^{\infty} dq\,q\,\frac{e^{iqr}}{k^2-q^2} \qquad \text{Bronstein or contour integration}$$

$$= -\frac{m}{2\pi\,\hbar^2}\,\frac{e^{ikr}}{r} =: G^+(\mathbf{r},k) \qquad G^\pm(\mathbf{r}-\mathbf{r}',k) = -\frac{m}{2\pi\,\hbar^2}\,\frac{e^{\pm ik\,|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

two linear-independent solutions $G^\pm(\mathbf{r}-\mathbf{r}',k)$

Technical remarks: ... (Blackboard)

2.1.c. Stationary wave function for $r \gg R$; scattering amplitude

Lippmann-Schwinger equation: ... substitution of the Greens function into LS equation gives rise to the integral equation

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{m}{2\pi\,\hbar^2}\int d^3\mathbf{r}'\,\frac{e^{ik\,|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\,V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}')$$

Remarks: ... (Blackboard)

Approximation for $r \gg R$:

➢ We search for the behaviour at the detectors if the potential is centered around the origin of coordinates

$$k\,|\mathbf{r}-\mathbf{r}'| \;=\; k\,\sqrt{\mathbf{r}^2+\mathbf{r}'^2-2\mathbf{r}\cdot\mathbf{r}'}$$

$$\approx\; kr\,\sqrt{1-2\,\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}} \;=\; kr-k\,\frac{\mathbf{r}}{r}\cdot\mathbf{r}' \;=\; kr-\mathbf{k}'\cdot\mathbf{r}' \qquad\qquad \mathbf{k}'=k\,\frac{\mathbf{r}}{r}, \qquad r'<R$$

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} \;\approx\; \frac{1}{r-\frac{\mathbf{r}\cdot\mathbf{r}'}{r}} \;\approx\; \frac{1}{r} \qquad\Longrightarrow\qquad \frac{e^{ik\,|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \;\approx\; \frac{e^{ikr}}{r}\,e^{i\mathbf{k}'\cdot\mathbf{r}'} \qquad r\;\gg\;R$$

Lippmann-Schwinger equation for $r \gg 0$: With this approximation, we can write this equation as

$$\psi_{\mathbf{k}}(\mathbf{r}) \;=\; e^{i\mathbf{k}\cdot\mathbf{r}}+\frac{e^{ikr}}{r}\,f(\mathbf{k},\mathbf{k}')\,, \qquad\qquad f(\mathbf{k},\mathbf{k}') \;=\; -\frac{m}{2\pi\,\hbar^2}\int d^3\mathbf{r}'\,e^{-i\mathbf{k}'\cdot\mathbf{r}'}\,V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}') \qquad \mathbf{k}'=k\,\frac{\mathbf{r}}{r}$$

For $r \gg R$, (complex) scattering amplitude $f(\mathbf{k},\mathbf{k}')$ only depends on the direction of $\mathbf{r}$.

Since $f(\mathbf{k},\mathbf{k}') = f(\vartheta,\varphi)$ only depends on $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\vartheta,\varphi)$, we only need to know and describe the position of the detectors in terms of the spherical angles (ϑ,φ).

2.1.d. Current density of probability

We also wish to evaluate the current density for $r \gg R$, independent for the incident (in, incoming) and scattered part (out, outgoing) of the wave functions, $\psi_{\mathbf{k}} = \psi_{\mathbf{k}}^{(in)} + \psi_{\mathbf{k}}^{(out)}$

$$
\begin{aligned}
\psi_{\mathbf{k}}(\mathbf{r}) &= e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f(\mathbf{k},\mathbf{k}') \\
\mathbf{j} &= \frac{\hbar}{2mi} \left(\psi^* \nabla\psi - \psi \nabla\psi^*\right) \\
\mathbf{j}^{(in)} &= \frac{\hbar\,\mathbf{k}}{m} \\
\mathbf{j}^{(out)}(r \gg 0) &\approx \frac{\hbar}{2mi} \left(f^* \frac{e^{-ikr}}{r} \nabla f \frac{e^{ikr}}{r} - f \frac{e^{ikr}}{r} \nabla f^* \frac{e^{-ikr}}{r} \right) \\
&= \frac{\hbar}{2mi} \left[\mathbf{e}_r \left(f^* f \frac{e^{-ikr}}{r} \frac{\partial}{\partial r} \frac{e^{ikr}}{r} - f f^* \frac{e^{ikr}}{r} \frac{\partial}{\partial r} \frac{e^{-ikr}}{r} \right) + \mathbf{e}_\vartheta\,() + \mathbf{e}_\varphi\,() \right] \\
\mathbf{e}_r \cdot \mathbf{j}^{(out)}(r \gg 0) &= \frac{\hbar\,k}{2mi} |f|^2 \left(\frac{ik}{r^2} - \frac{1}{r^3} + \frac{ik}{r^2} + \frac{1}{r^3} \right) = \frac{\hbar\,k}{m} \frac{|f(\mathbf{k},\mathbf{k}')|^2}{r^2} + \mathcal{O}(r^{-3})
\end{aligned}
$$

with $k = k'$ (elastic scattering) and where the term $\mathcal{O}(r^{-3})$ arises from the $\nabla_{\mathbf{r}}$ operator when acting upon $f(\mathbf{k},\mathbf{k}')$.

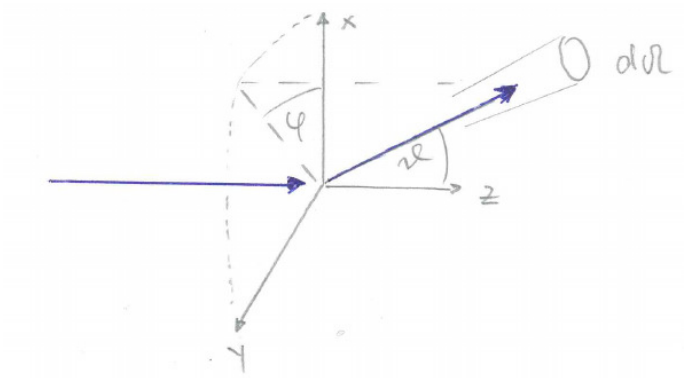


Figure 2.2.: Definition of the angle-differential cross section.

Differential scattering cross section: For a sphere with $r \gg R$, the (probability) current of the scattered wave into the spherical element $d\Omega$ does not depend on r and can be written

$$|\mathbf{j}^{(out)}|\, r^2\, d\Omega \;=\; \frac{\hbar \mathbf{k}'}{m}\, |f(\mathbf{k},\mathbf{k}')|^2 d\Omega \;=\; |\mathbf{j}_i|\, |f(\mathbf{k},\mathbf{k}')|^2\, d\Omega \qquad\qquad k' \;=\; k$$

$$\frac{d\sigma}{d\Omega}\,(\mathbf{k},\mathbf{k}') \;=\; \frac{\text{scattered current density through } d\Omega}{\text{incident current density per area}} \;=\; \frac{|\mathbf{j}^{(out)}|\, r^2}{|\mathbf{j}^{(in)}|} \;=\; |f(\mathbf{k},\mathbf{k}')|^2$$

(angle-) differential scattering cross section

This differential cross sections describes the probability that am incident particle with momentum $\mathbf{k}$ is scattered by the potential into the solid angle element $d\Omega$ around the direction of $\mathbf{k}' \;=\; k\,\mathbf{r}/r \;=\; k\,\hat{\mathbf{r}}(\vartheta,\varphi)$.

Total scattering cross section: ... obtained by integration of the differential cross section over all solid angles

$$\sigma \;=\; \int d\Omega\, |f(\mathbf{k},\mathbf{k}')|^2$$

Probability that the particle is deflected to due its interaction with the scattering potential; typically measured in *barn* $= 10^{-28}\,\mathrm{cm}^2$.

Blackboard example (Beam attenuation & mean-free path:):

2.1.e. Short summary

In (standard) potential scattering theory, we are always looking for scattering states with the correct asymptotic behaviour $r \to \infty$:

$$\psi_{\mathbf{k}}(\mathbf{r}) \;=\; e^{i\mathbf{k}\cdot\mathbf{r}} \;+\; \frac{e^{+ikr}}{r}\, f(\mathbf{k},\mathbf{k}')$$

Frequently applied methods:

- ➢ Born's approximation: Perturbative approach to the scattering, typically applied at high energies.
- ➢ Eikonal approximation: Use of classical action and Hamilton-Jacobi formalism.
- ➢ Low-energy approximation.
- ➢ Resonance approximation.
- ➢ Semi-classical approaches.

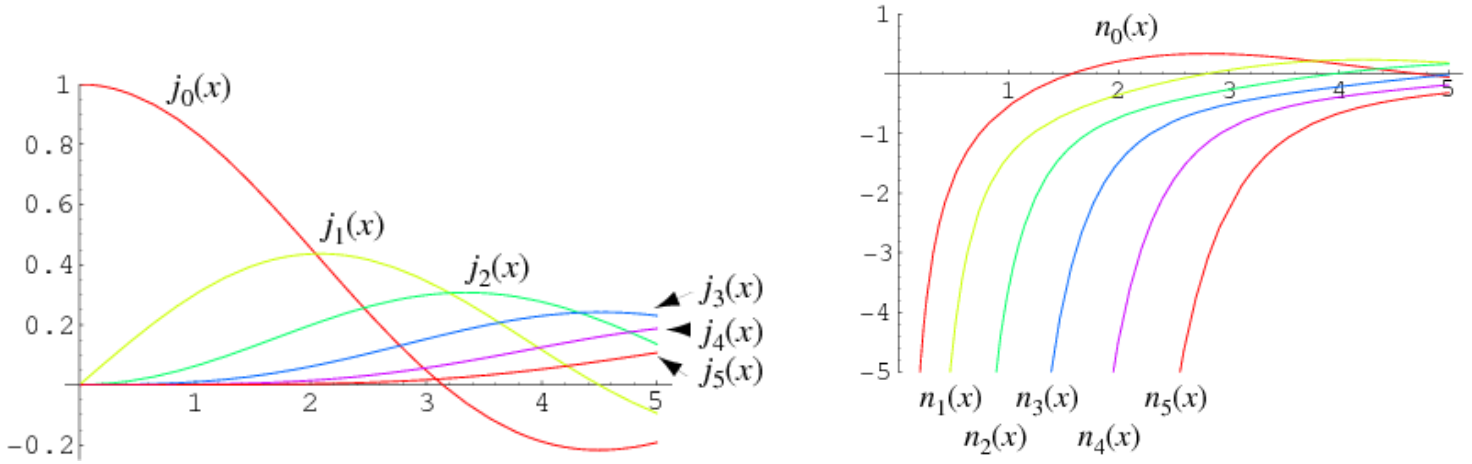


Figure 2.3.: Low-order spherical Bessel and sperical Neumann functions; taken from Wolfram MathWorld.

2.2. Spherical Bessel functions

Radial SE for a free particle:

➢ We define the wave number and re-write the SE in the form with $\rho = kr$; cf. H-atom

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right] R(r) = 0, \qquad k = \frac{\sqrt{2m\,E}}{\hbar}$$

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{\ell(\ell+1)}{\rho^2} + 1\right] R(\rho) = 0$$

defining equation for spherical Bessel functions

Solutions to this eq. are the spherical Bessel, Neumann and Hankel with simple algebraic relations to the standard Bessel and Neumann functions. The Neumann functions are sometimes also called the Bessel functions of second kind.

Spherical Bessel, Neumann and Hankel functions:

➢ Bessel functions of order $\ell = 0$:

$$\frac{d^2}{d\rho^2}(\rho R_0) + (\rho R_0) = 0 \qquad \text{harmonic oscillator for} \quad (\rho R_0)$$

$$R_0 = \begin{cases} \frac{\sin\rho}{\rho} & \text{regular at} \quad \rho = 0 \\ \frac{\cos\rho}{\rho} & \text{irregular (singular) at} \quad \rho = 0 \end{cases}$$

For $\ell \neq 0$, the Bessel functions can be determined via recursion relations.

➢ Spherical Bessel functions $j_\ell(\rho)$ and Neumann functions $n_\ell(\rho)$:

$$j_\ell(\rho) = (-\rho)^\ell \left(\tfrac{1}{\rho}\tfrac{d}{d\rho}\right)^\ell \tfrac{\sin\rho}{\rho} \qquad n_\ell(\rho) = -(-\rho)^\ell \left(\tfrac{1}{\rho}\tfrac{d}{d\rho}\right)^\ell \tfrac{\cos\rho}{\rho}$$

$$j_0(\rho) = \tfrac{\sin\rho}{\rho} \qquad n_0(\rho) = -\tfrac{\cos\rho}{\rho}$$

$$j_1(\rho) = \tfrac{\sin\rho - \rho\cos\rho}{\rho^2} \qquad n_1(\rho) = -\tfrac{\cos\rho + \rho\sin\rho}{\rho^2}$$

$$j_2(\rho) = \tfrac{(3-\rho^2)\,\sin\rho - 3\rho\cos\rho}{\rho^3} \qquad n_2(\rho) = -\tfrac{(3-\rho^2)\,\cos\rho + 3\rho\sin\rho}{\rho^3}$$

$$j_\ell(\rho \to 0) = \tfrac{\rho^\ell}{1\cdot 3\cdot 5\ldots\cdot(2\ell+1)} \qquad n_\ell(\rho \to 0) = -\tfrac{1\cdot 3\cdot 5\ldots\cdot(2\ell-1)}{\rho^{\ell+1}}$$

$$j_\ell(\rho \to \infty) = \tfrac{1}{\rho}\sin(\rho - \pi\,\ell/2) \qquad n_\ell(\rho \to \infty) = -\tfrac{1}{\rho}\cos(\rho - \pi\,\ell/2)$$

➢ Spherical Hankel functions $h_\ell^{(1,2)}(\rho)$ of first and second kind:

$$h_\ell^+(\rho) = j_\ell(\rho) + i\, n_\ell(\rho) \qquad h_\ell^-(\rho) = h_\ell^{+*}(\rho)$$

$$j_\ell(\rho) = \Re\, h_\ell^+ \qquad n_\ell(\rho) = \Im\, h_\ell^+$$

$$h_\ell^+(\rho \to \infty) = -\tfrac{i}{\rho}\, e^{i\,(\rho\, -\, \pi\,\ell/2)}$$

Expansion of plane-waves in spherical Bessel functions:

➢

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell\, j_\ell(kr)\, Y_{\ell m}^*(\Omega_\mathbf{k})\, Y_{\ell m}(\Omega_\mathbf{r}) = \sum_{\ell=0}^{\infty} i^\ell\, (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\vartheta)$$

Proof:

➢ This expansion can be obtained by the following ansatz, if first taken for $\mathbf{k}\,||\mathbf{e}_z$:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m}(\mathbf{k})\, j_\ell(kr)\, Y_{\ell m}(\vartheta,\varphi)$$

$$e^{ikr\,\cos\vartheta} = \sum_{\ell=0}^{\infty} a_{\ell 0}(\mathbf{k})\, j_\ell(kr)\, Y_{\ell 0}(\vartheta,\varphi) = \sum_{\ell=0}^{\infty} \left(\frac{2\ell+1}{4\pi}\right)^{1/2} a_{\ell 0}(\mathbf{k})\, j_\ell(kr)\, P_\ell(\cos\vartheta)$$

Since the left-hand side does not depend on φ, only terms with $m = 0$ can contribute to the expansion because $Y_{\ell m} \propto e^{im\,\varphi}$.

➢ We can multiply this equation by $P_{\ell'}(\cos\vartheta)$ and integrate over $\int_{-1}^{1} d(\cos\vartheta)\ldots$:

$$\int_{-1}^{1} d(\cos\vartheta)\, P_{\ell'}(\cos\vartheta)\, e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} \left(\frac{2\ell+1}{4\pi}\right)^{1/2} a_{\ell 0}(\mathbf{k})\, j_\ell(kr) \underbrace{\int_{-1}^{1} d(\cos\vartheta)\, P_{\ell'}(\cos\vartheta)\, P_\ell(\cos\vartheta)}_{\frac{2\,\delta_{\ell\ell'}}{2\ell+1}}$$

$$= \left(\frac{1}{(2\ell+1)\,\pi}\right)^{1/2} a_{\ell 0}(\mathbf{k})\, j_\ell(kr)$$

$$a_{\ell 0}(\mathbf{k})\, j_\ell(kr) = \sqrt{\pi(2\ell+1)} \int_{-1}^{1} dt\, P_{\ell'}(t)\, e^{ikr\,t} \qquad t = \cos\vartheta$$

➢ Because $a_{\ell 0}(\mathbf{k})$ is independent of r, the expansion must apply also for $kr \to 0$; from the expansion of the lhs and rhs and comparison of the leading terms, one finds:

$$e^{ikr\,\cos\vartheta} = \sum_{\ell=0}^{\infty} i^l\, (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\vartheta)$$

➢ To find the same expansion for a general direction, one can use the addition theorem of the spherical harmonics

$$P_\ell(\cos\vartheta) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\Omega_{\mathbf{k}})\, Y_{\ell m}(\Omega_{\mathbf{r}}) \qquad \cos\vartheta = \frac{\mathbf{k}\cdot\mathbf{r}}{kr}$$

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell\, j_\ell(kr)\, Y^*_{\ell m}(\Omega_{\mathbf{k}})\, Y_{\ell m}(\Omega_{\mathbf{r}})$$

2.3. Simplest case: Scattering and solutions for a spherical box potential

2.3.a. Radial SE in a sphericalbox potential

For a central-field potential $V = V(r)$, we can simplify the time-independent SE with the ansatz $\psi(\mathbf{r}) = R(r)\,Y_{lm}(\vartheta,\varphi)$ to the radial SE, i.e. to just an ordinary differential equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right) + V(r)\right] R(r) = E\,R(r)$$

Spherical box potential:

$$V(r) = \begin{cases} -V_o & r < a \\ 0 & r > a \end{cases}$$

We saw that solutions to this eq. are the spherical Bessel, Neumann and Hankel, and with quite simple algebraic relations to the standard Bessel and Neumann functions.

2.3.b. Bound states

Solutions for $-V_o < E < 0$: ... (Blackboard)

2.3.c. Scattering solutions

Solutions for $E > 0$:

➢ Radial SE inside and outside the box

$$\begin{array}{ll} \text{inside} \\ \text{outside} \end{array} \qquad \left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + \begin{pmatrix} q^2 \\ k^2 \end{pmatrix}\right] R(r) = 0 \qquad \begin{array}{l} q = \frac{\sqrt{2m(E+V_o)}}{\hbar} \\ k = \frac{\sqrt{2m\,E}}{\hbar} \end{array}$$

➢ Regular solution at the origin:

$$R(r) = \begin{cases} A\, j_\ell(qr) & 0 \le r < a \\ B\, j_\ell(kr) + C\, \eta_\ell(kr) & r > a \end{cases} \qquad q\,\frac{d\,j_\ell/d\rho}{j_\ell}\Big|_{qa} = k\left[\frac{B\,d\,j_\ell/d\rho + C\,d\,\eta_\ell/d\rho}{B\,j_\ell + C\,\eta_\ell}\right]\Big|_{\kappa a}$$

➢ Scattering phase $\tan\,\delta_\ell(k) := C/B$ from asymptotic behavior.

$$\begin{aligned} R(r\to\infty) &\approx \frac{B}{\kappa\, r}\left[\sin\left(kr - \frac{\ell\,\pi}{2}\right) - \frac{C}{B}\cos\left(kr - \frac{\ell\,\pi}{2}\right)\right] \\ &= \frac{B}{\cos\,\delta_\ell(k)}\,\frac{1}{kr}\,\sin\left(kr - \frac{\ell\,\pi}{2} + \delta_\ell(k)\right) \end{aligned}$$

Spherical wave with phase shift $\delta_\ell(k)$.

➢ Especially, phase shift $\delta_0(k)$ of a-waves:

$$q\,\cot(qa) \;=\; k\,\frac{B\,\cos(ka)\;+\;C\,\sin(ka)}{B\,\sin(ka)\;-\;C\,\cos(ka)} \;=\; k\,\frac{\cos ka\;\cos\delta_o\;-\;\sin ka\;\sin\delta_o}{\sin ka\;\cos\delta_o\;+\;\cos ka\;\sin\delta_o}$$

$$\delta_0(k) \;=\; \arctan\left(\frac{k}{q}\,\tan(qa)\right)\;-\;ka \qquad\qquad q \;=\; \frac{\sqrt{2m(E+V_o)}}{\hbar}$$

Phase shift as function of the energy of the incident particles as well as the strength and size (a) of the spherical box.

➢ Attractive *vs.* repulsive potentials:

$$V \;=\; \begin{cases} -\,V_o \;<\; 0 & \text{... attractive} \qquad \delta_0 \;>\; 0 \\ \;\;V_o \;>\; 0 & \text{... repulsive} \qquad \delta_0 \;<\; 0 \end{cases}$$

2.3.d. Hard spheres

cf. tutorial.

2.4. Partial-wave expansions

2.4.a. Scattering amplitudes for central-field potentials & optical theorem

Radial SE for a central-field potential $V(r)$: ... (Blackboard)

Scattering amplitude for a central-field potential $V(r)$ & optical theorem:

➢ Comparison of coefficients gives us:

$$c_\ell \;=\; \frac{i^\ell}{k}\,(2\ell+1)\,e^{i\delta_\ell}, \qquad\qquad \psi(\mathbf{r}) \;=\; \frac{1}{kr}\sum_{\ell=0}^{\infty} i^\ell\,(2\ell+1)\,e^{i\delta_\ell}\,u_\ell(r)\,P_\ell(\cos\vartheta)$$

$$f(k,\vartheta) \;=\; \frac{1}{k}\sum_{\ell=0}^{\infty} a_\ell\,(2\ell+1)\,P_\ell(\cos\vartheta), \qquad\qquad a_\ell(k) \;=\; \frac{e^{2i\,\delta_\ell}\,-\,1}{2i} \;=\; e^{i\delta_\ell}\,\sin\delta_\ell$$

$$f(k,\vartheta) \;=\; \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2ik}\,P_\ell(\cos\vartheta)\,\left(e^{2i\,\delta_\ell}\,-\,1\right)$$

➢ In a (short-range) central-field potentials, the scattering phases $a_\ell(k)$ already contain all information about the scattering (amplitude).

➢ Total scattering cross section for a central-field potential takes a simple form by the summation over the partial waves, and especially in forward direction $\vartheta = 0 \rightsquigarrow P_\ell(\cos\vartheta = 1) = 1]$:

$$\sigma(k) = \int d\varphi\, d\vartheta\, \sin\vartheta\, |f(\vartheta,\varphi)|^2 = \frac{2\pi}{k^2} \sum_{\ell\ell'} (2\ell+1)\,(2\ell'+1)\, a_\ell^*\, a_{\ell'} \underbrace{\int_{-1}^{1} dt\, P_\ell^*(t)\, P_{\ell'}(t)}_{=\,2\delta_{\ell\ell'}/(2\ell+1)}$$

$$= \sum_{\ell=0}^{\infty} \sigma_\ell = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1)\, \sin^2\delta_\ell(k)$$

$$f(k,\,0) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\,\delta_\ell}\, \sin\delta_\ell = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1)\, \sin\delta_\ell\, (\cos\delta_\ell + i \sin\delta_\ell)$$

$$\Im\,(f(k,\,0)) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1)\, \Im\,(a_\ell(k))) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1)\, \sin^2\delta_\ell(k)$$

$$\sigma(k) = \frac{4\pi}{k}\, \Im\,(f(k,\,0))$$

(so-called) optical theorem

This theorem is related to unitarity, that is the conservation of probability and is, hence, widely applicable. In particular, this theorem describes both, elastic and inelastic scattering. The imaginary part of the scattering amplitude stands for the probability that is absorbed or taken out from the incident beam.

Remarks: ... (Blackboard)

2.4.b. Resonance approximation

➢ Partial scattering cross section:

$$\sigma_\ell \;=\; \frac{4\pi}{k}\,(2\ell+1)\,\sin^2\delta_\ell(k) \;=\; \begin{cases} 0 & \delta_\ell \;=\; 2\pi\,n, \qquad n\;\in\;\mathbb{Z} \\ \max & \delta_\ell \;=\; \left(n+\frac{1}{2}\right)\pi \;=:\; \delta_\ell(E_r) \end{cases}$$

Defines some resonance energy, where we just have $\cot[\delta_\ell(E_r)] \;=\; 0\,.$

➢ For nearby energies, $E \approx E_r$, a Taylor expansion of $\cot\delta_\ell\,|_{E_r} \;\approx\; -\,(E-E_r)\cdot\frac{\Gamma}{2}$ gives rise to the scattering amplitude and cross section near to the resonance:

$$f_\ell(\vartheta) \;\propto\; e^{i\,\delta_\ell}\,\sin\delta_\ell\,P_\ell(\cos\vartheta) \;\approx\; \frac{-\,\frac{\Gamma}{2}}{E-E_r\;+\;i\,\frac{\Gamma}{2}}\;P_\ell(\cos\vartheta)$$

$$\sigma_\ell \;\propto\; \frac{\left(\frac{\Gamma}{2}\right)^2}{(E-E_r)^2\;+\;\left(\frac{\Gamma}{2}\right)^2}$$

Breit-Wigner formula

This Breit-Wigner expression is often applied to either assign a 'widths' to some measured cross sections or, *vice versa*, to incorporate an experimental width into computed cross sections, because resonance energies and cross sections may sensitively depend upon the behaviour of certain matrix elements.

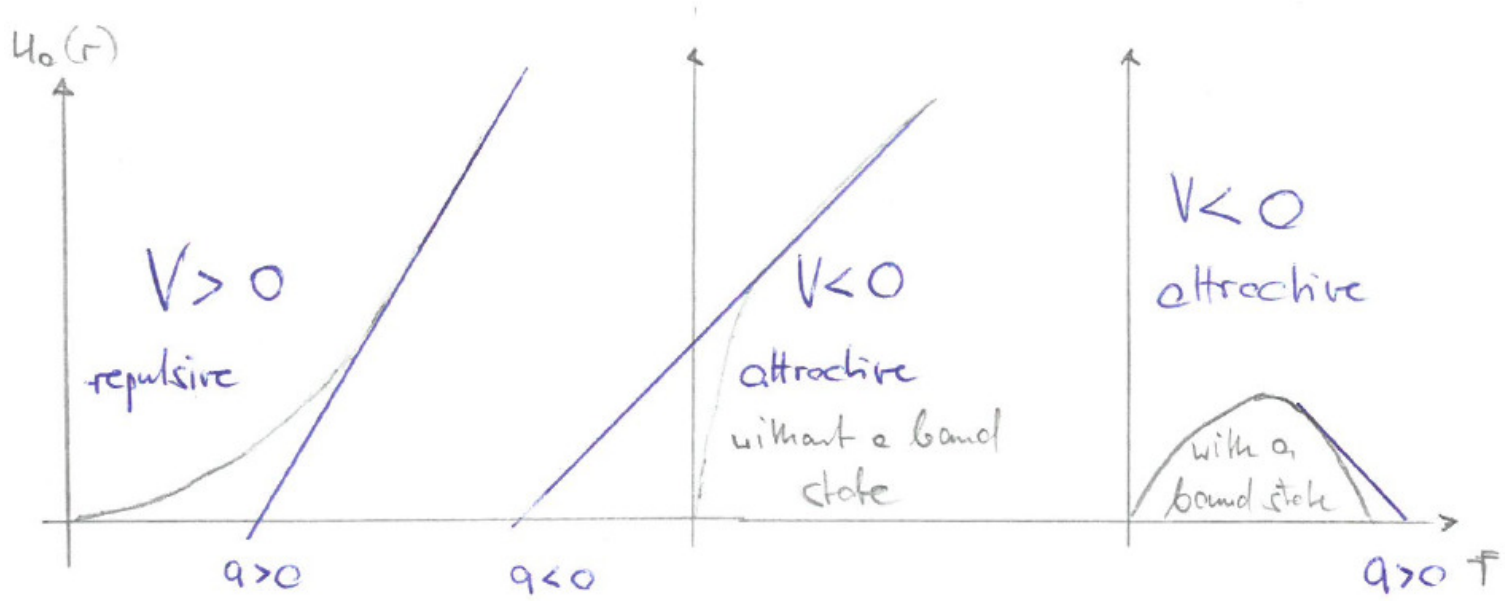


Figure 2.4.: Potential produces a first maximum near to the origin (one additional maximum).

2.4.c. Low-energy approximation

Neglecting the kinetic energy in the SE: ... (Blackboard)

2.5. Born approximation

Born's expansion: To calculate the scattering cross sections and, especially, the scattering phases for a given potential, we can expand the Lippmann-Schwinger equation by solving it iteratively:

$$\begin{aligned}\psi_{\mathbf{k}} &= \phi_{\mathbf{k}} + \int d^3\mathbf{r}' \left(-\frac{m}{2\pi\,\hbar^2}\right) \frac{e^{ik\,|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\, V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}') = \phi_{\mathbf{k}} + U\,\psi_{\mathbf{k}} \\ &= \phi_{\mathbf{k}} + U\,(\phi_{\mathbf{k}} + U\,\psi_{\mathbf{k}}) = \left(1 + U + U^2 + U^3 + \ldots + U^n\right)\phi_{\mathbf{k}} + U^{n+1}\,\psi_{\mathbf{k}} \\ &= \sum_{n=0}^{\infty} (GV)^n\,\phi_{\mathbf{k}} = \phi_{\mathbf{k}} + GV\,\phi_{\mathbf{k}} + GV\,GV\,\phi_{\mathbf{k}} + \ldots\end{aligned}$$

corresponds to an expansion in the orders of the potential $V(\mathbf{r})$

2.5.a. First-Born approximation

$$\psi_{\mathbf{k}} = \phi_{\mathbf{k}} + GV\,\phi_{\mathbf{k}} = e^{i\,\mathbf{k}\cdot\mathbf{r}} - \frac{m}{2\pi\,\hbar^2}\int d^3\mathbf{r}'\,\frac{e^{ik\,|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\,V(\mathbf{r}')\,e^{i\,\mathbf{k}\cdot\mathbf{r}'}$$

Scattering amplitude:

➢ For a sufficiently weak potential, we only consider $V(\mathbf{r})$ in first order, with $\phi_{\mathbf{k}} \to e^{i\,\mathbf{k}\cdot\mathbf{r}}$ and the asymptotic expansion $r \gg r'$:

$$f^{\,(\mathrm{Born})}(\mathbf{k},\mathbf{k}') \;=\; -\frac{m}{2\pi\hbar^2}\int d^3\mathbf{r}'\;\underbrace{e^{-i\,\mathbf{k}'\cdot\mathbf{r}'}\,V(\mathbf{r}')\,e^{i\,\mathbf{k}\cdot\mathbf{r}'}}_{V(\mathbf{r}')\,e^{i(\mathbf{k}-\mathbf{k}')\,\mathbf{r}'}} \;=\; -\frac{m}{2\pi\hbar^2}\,\tilde{V}(\mathbf{k}\,-\,\mathbf{k}')\,, \qquad\qquad \mathbf{k}\,-\,\mathbf{k}' \;=\; \mathbf{q}$$

$$\;=\; -\frac{m}{2\pi\hbar^2}\,\langle\mathbf{k}'\,|V|\,\mathbf{k}\rangle$$

first-Born scattering amplitude

➢ In first-Born approximation, the scattering amplitude is essentially the Fourier transform of the scattering potential.

➢ Since $|\mathbf{k}| \;=\; |\mathbf{k}'| \;\equiv\; k$ (for a given potential), we can express the scattering amplitude simply in terms of the deflection angle ϑ:

$$\mathbf{q}^2 \;:=\; (\mathbf{k}\,-\,\mathbf{k}')^2 \;=\; \mathbf{k}^2 + \mathbf{k}'^2 - 2\mathbf{k}\mathbf{k}'\,\cos\vartheta \;=\; 2k^2\,(1\,-\,\cos\vartheta) \;=\; \left(2k\,\sin\frac{\vartheta}{2}\right)^2$$

$$f^{\,(\mathrm{Born})}(k,\vartheta) \;=\; \int d^3\mathbf{r}'\,V(r')\,e^{-i\mathbf{q}\cdot\mathbf{r}'} \;=\; 2\pi\int_0^\infty dr'\,r'^2\,V(r')\int_{+1}^{-1} dt\,e^{-iqr'\,t} \qquad\qquad t=\cos\vartheta$$

$$\;=\; \frac{4\pi}{q}\int_0^\infty dr'\,r'\,V(r')\,\sin(qr')$$

$$\;=\; -\frac{2m}{\hbar^2}\,\frac{1}{2k\,\sin(\vartheta/2)}\int_0^\infty dr'\,r'\,V(r')\,\sin\left(|\mathbf{k}\,-\,\mathbf{k}'|\,r'\right) \;=\; -\frac{m}{2\pi\hbar^2}\,\tilde{V}\left(2k\,\sin\frac{\vartheta}{2}\right)$$

The first-Born scattering amplitude $f^{\,(\mathrm{Born})}(k,\vartheta)$ is real and, thus, violates the optical theorem.

Validity of the Born approximation: ... (Blackboard)

2.5.b. Examples of first-Born amplitudes and cross sections:

Yukawa potential: ... (Blackboard)

Coulomb potential: ... (Blackboard)

Hard-sphere potential with radius b: ... (Blackboard)

2.5.c. Scattering phases in first-Born approximation

Weak potentials:

➢ By using the partial-wave expansion of the scattering amplitude in a central-field potential, we can compare this amplitude with the first-Born amplitude

$$f(k,\vartheta) = \underbrace{\frac{1}{k}\sum_{\ell=0}^{\infty} e^{i\delta_\ell}\,\sin\delta_\ell\,(2\ell+1)\,P_\ell(\cos\vartheta)}_{\text{partial wave expansion}} \approx \underbrace{-\frac{m}{2\pi\hbar^2}\,\tilde{V}\left(\left[2k\,\sin\frac{\vartheta}{2}\right]^2\right)}_{\text{first Born}}$$

$$= -\frac{m}{\hbar^2}\,\frac{1}{k\,\sin(\vartheta/2)}\int_0^\infty dr'\,r'\,V(r')\,\sin(qr')$$

➢ Multiplication with $k\,P'_\ell(\cos\vartheta)$ and integration over $\int_{-1}^{1} dt$ with $t \equiv \cos\vartheta$ gives for suffienctly small δ_ℓ

$$\sum_{\ell=0}^{\infty} e^{i\delta_\ell}\,\sin\delta_\ell\,(2\ell+1)\,\underbrace{\int_{-1}^{1} dt\,P^*_{\ell'}(t)\,P_\ell(t)}_{\frac{2}{2\ell+1}\,\delta_{\ell\ell'}} \;=\; 2\,e^{i\delta_\ell}\,\sin\delta_\ell \qquad \text{... evaluate lhs here}$$

$$\delta_\ell \;\approx\; e^{i\,\delta_\ell}\,\sin\delta_\ell \;=\; -\frac{m\,k}{4\pi\hbar^2}\int_{-1}^{1} dt\,\tilde{V}\left(2k^2\,(1-t)\right)\;P^*_\ell(t) \qquad \delta_\ell \ll 1$$

scattering phase in first-Born approximation (for weak potentials)

Scattering phase from plane-wave expansion: ... (Blackboard)

2.5.d. Eikonal approximation

Classical action: ... (Blackboard)

Example (Small-angle scattering at high energies:):

Consider the scattering in the $x-z$ plane with

$$\begin{aligned}
\mathbf{k} &= (0,0,k) \\
\mathbf{k}' &= (k\,\sin\vartheta,\quad 0,\ k\,\cos\vartheta) \\
\mathbf{b} &= (b\cos\varphi_b,\ b\sin\varphi_b,\ 0) \\
(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}' &\simeq -\mathbf{k}'\cdot\mathbf{b} = kb\,\vartheta\,\cos\varphi_b \quad (\text{for } \vartheta \ll 1) \\
d^3\mathbf{r}' &= db\,b\,d\varphi_b\,dz \qquad \text{... Ingegration in cylinder coordinates.}
\end{aligned}$$

Integration gives rise to a Bessel function

$$\int_0^\infty db\,b\int_0^{2\pi} d\varphi_b\ e^{-ikb\,\vartheta\,\cos\varphi_b} = 2\pi\int_0^\infty db\,b\ J_0(kb\,\vartheta) \qquad J_0 \text{ ... Bessel function}$$

$$\int_{-\infty}^{\infty} dz\,V(\sqrt{b^2+z^2})\,\exp\left[-\frac{im}{\hbar^2\,k}\int_{-\infty}^{z} dz'\,V(\sqrt{b^2+z'^2})\right] = \frac{ik\,\hbar^2}{m}\left(e^{2i\,\Delta_b}-1\right)$$

$$\Delta_b := -\frac{m}{2\hbar^2\,k}\int_{-\infty}^{\infty} dz'\ V(\sqrt{b^2+z'^2})$$

eikonal ... analogue to optical diffraction

Scattering amplitude in eikonal approximation:

$$f(\mathbf{k},\mathbf{k}') \;=\; f(k,\vartheta,b) \;=\; -ik\int_0^\infty db\, b\, J_0(kb\,\vartheta)\,\left(e^{2i\,\Delta_b}\;-\;1\right)$$

Eikonal approximation also fullfills the optical theorem:

$$\sigma \;=\; \frac{4\pi}{k}\,\Im f(0) \;=\; 8\pi\int_0^\infty db\, b\,\sin^2(\Delta_b)$$

Remarks: ... (Blackboard)

2.6. Coulomb scattering

Solutions & scattering amplitude: ... (Blackboard)

Remarks: ... (Blackboard)

2.7. Formal basis-independent scattering theory

2.7.a. Troubles with the continuum

Generalized Lippmann-Schwinger equation:

➢ Time-independent SE with scattering potential V : $\quad H = H_o + V$

$$\begin{aligned} (H_o - E)\,|\psi_o\rangle &= 0 \\ (H_o - E)\,|\psi\rangle &= -V\,|\psi\rangle \\ (H_o - E)\,(|\psi\rangle - |\psi_o>\rangle) &= -V\,|\psi\rangle \end{aligned}$$

➢ We can use the same E, if H and H_o have both a contineous spectrum ; formal solution if the operator $H_o - E$ has an inverse:

$$|\psi\rangle - |\psi_o\rangle = -\left(\frac{1}{H_o - E}\right) V\,|\psi\rangle \equiv (H_o - E)^{-1}\,V\,|\psi\rangle$$

$$|\psi\rangle = |\psi_o\rangle - \frac{1}{H_o - E}\,V\,|\psi\rangle \qquad \text{WRONG, unfortunately!!}$$

➢ Correct solutions require either a proper treatment of the $\lim_{t\to-\infty}\,(\,|\psi(t)\rangle - |\psi_o(t)\rangle\,)$ or an adiabatic 'switch-on' of the potential $V(t) = e^{\eta t}\,V$.

➢ Mathematical 'trick' from the theory of complex functions:

$$|\psi_o\rangle \;=\; \frac{i0^+}{E - H_o + i0^+}\,|\psi\rangle \;\equiv\; \lim_{\eta\to 0}\,\frac{i\eta}{E - H_o + i\eta}\,|\psi\rangle$$

$$G_o^+ \;\equiv\; \frac{1}{E - H_o + i0^+} \qquad \text{... Greens operator of } \mathrm{H_o} \qquad \text{... has inverse because of } \mathrm{i0^+}$$

➢ Formal solution (again):

$$|\psi\rangle \;-\; |\psi_o\rangle \;=\; \left(\mathbb{1} \;-\; \frac{i0^+}{E - H_o + i0^+}\right)|\psi\rangle \;=\; \left[\frac{1}{E - H_o + i0^+}\,(E - H_o + i0^+) \;-\; \frac{i0^+}{E - H_o + i0^+}\right]|\psi\rangle$$

$$=\; \frac{1}{E - H_o + i0^+}\,(E - H_o)\,|\psi\rangle \;=\; \frac{1}{E - H_o + i0^+}\,(H - H_o)\,|\psi\rangle$$

$$=\; \frac{1}{E - H_o + i0^+}\,V\,|\psi\rangle$$

$$|\psi\rangle \;=\; |\psi_o\rangle \;+\; \frac{1}{E - H_o + i0^+}\,V\,|\psi\rangle \;=\; |\psi_o\rangle \;+\; G_o^+\,V\,|\psi\rangle$$

formal (basis-independent) Lippmann-Schwinger equation

Born's expansion reconsidered, $|\psi(t\to-\infty)\rangle \;=\; |\psi_o(t\to-\infty)\rangle$ **:** ... (Blackboard)

Born's expansion for $|\psi(t\to+\infty)\rangle \;=\; |\psi_o(t\to+\infty)\rangle$ **:** ... (Blackboard)

2.7.b. S-matrix and T-matrix formalism: A brief account

S-matrix:

➢ Initial preparation: Particles are prepared in the well-defined initial states

$$\left|\psi_m^+(-\infty)\right\rangle \;=\; |\psi_{o,m}(-\infty)\rangle \;=\; \lim_{t\to-\infty} e^{iH_o t}\;|\psi_{o,m}(0)\rangle\,.$$

➢ Detection for $t\to+\infty$ by projection upon the states: $\quad |\psi_{o,m}(+\infty)\rangle \;=\; \lim_{t\to+\infty} e^{iH_o t}\;|\psi_{o,m}(0)\rangle\,.$

➢ Full information about the scattering is given by (the set of) scattering amplitudes

$$\left\langle\psi_{o,m}(+\infty)\,|\,\psi_n^+(+\infty)\right\rangle \;=\; \left\langle\psi_m^-(0)\,|\,\psi_n^+(0)\right\rangle \;=\; \langle\psi_{o,m}\,|\,S\,|\,\psi_{o,n}\rangle \;=\; S_{mn}$$

Defition of the (so-called) S-matrix

➢ S-matrix can be also expressed either in terms of the Green's or the Möller operator;

$$S_{mn} \;=\; \delta(m\,-\,n)\;-\;2\pi i\,\delta(E_m\,-\,E_n)\left\langle\psi_{o,m}|\,V\,\underbrace{\Omega^+\,|\psi_{o,n}}_{\equiv\,|\psi_n^+\rangle}\right\rangle$$

fundamental formula of the S-matrix formalism

$\delta(m\,-\,n)$ describes the product of δ-functions for all quantum numbers.

➢ While the first term is the identity matrix, i.e. the unperturbed part of the incoming probability current [cf. the Lippmamn-Schwinger equation], the second terms just describes the effect due to the pertubation. Moreover, this

latter term also ensures the energy conservation for the total energy of all incoming and outgoing particles in the scattering process.

T-matrix: ... (Blackboard)

3. Many-body systems

3.1. Composite quantum systems. SE and Hilbert space

3.1.a. Reminder to postulate IV (Composite systems and entanglement):

For composite systems, as a reminder, the state space is given by the tensor product of the state space of all subsystems. Especially for N systems in state $\{|\psi_i\rangle\,,\ i = 1, ..., N\}$, the overall states is:

$$\underbrace{|\psi_1\rangle \otimes |\psi_2\rangle \otimes ... \otimes |\psi_N\rangle}_{\text{separable}} \qquad \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_N$$

... total state in the interaction free case

In general, however, such systems will not reside in such a product state due to internal interactions or interactions with some environement.

3.1.b. Hilbert spaces of composite systems

Non-relativistic many-body Hamiltonian:

➢ Time-dependent SE

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

$$H \;=\; \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} \;+\; V\underbrace{(\mathbf{r}_1,\ldots,\mathbf{r}_N)}_{\text{spatial variables}} + W\underbrace{(\mathbf{x}_1,\ldots,\mathbf{x}_N)}_{\text{spatial + spin variables + colors, flavours}} \qquad \mathbf{x} \;\equiv\; (\mathbf{r},\sigma)$$

V ... Coulomb interaction; interactions with external (electric) fields, spin-indep. nuclear forces, ...

W ... spin-dependent interactions; spin-orbit; interaction with external (magnetic) fields, ...

➢ Subsystems (of a composite system) do not always refer to individual one-particle systems: Spins, isospins, nuclei, molecular group, etc. ⇝ multi-partite systems.

➢ Behaviour ot total system arises from coupling of subsystems.

➢ Notations: $\mathcal{H}_1,\ \mathcal{H}^{(1)},\ |\Psi_1\rangle,\ \Psi^{(1)}, \Psi_\alpha^{(1)},\ \Psi_{1,\alpha}$

Tensor spaces:

➢ Tensor products:

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_N \\
|\Psi\rangle &= |\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle = |\psi_1 \ldots \psi_N\rangle \\
|n_1 \ldots n_N\rangle &\equiv |n_1\rangle \otimes \ldots \otimes |n_N\rangle \qquad \text{basis in product space} = \text{product of basis states} \\
\langle \Phi \,|\, \Psi\rangle &= \langle \Phi_1 \ldots \Phi_N \,|\, \Psi_1 \ldots \Psi_N\rangle = \langle \Phi_1 \,|\, \Psi_1\rangle \ldots \langle \Phi_N \,|\, \Psi_N\rangle \qquad \text{scalar product}
\end{aligned}$$

➢ Observables $A_1, \ldots, A_N$ of individual subsystems with $A_i : \mathcal{H}_i \to \mathcal{H}_i$ act like

$$(A_i \otimes \ldots \otimes A_N)\ (|\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle) = |A_1\,\psi_1\rangle \otimes \ldots \otimes |A_N\,\psi_N\rangle$$

A_i act upon different subsystems and cannot be 'added' to each other.

$$\begin{aligned}
A_i + \ldots + A_N &\equiv A_i \otimes \mathbb{1} \ldots \otimes \mathbb{1} + \mathbb{1} \otimes A_2 \otimes \mathbb{1} \ldots + \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes A_N \\
(A_i + \ldots + A_N)\,|\Psi\rangle &= (A_i + \ldots + A_N)\ (|\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle) \\
&= |A_1\,\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle + \ldots + |\psi_1\rangle \otimes \ldots \otimes |A_N\,\psi_N\rangle
\end{aligned}$$

Every operator always acts in its 'own' subspace.

➢ Eigenvalues and eigenstates of subsystems $A_i \; |a_i\rangle \; = \; a_i \; |a_i\rangle$

$$(A_i \; + \; \ldots \; + \; A_N) \; |a_1 \; \ldots \; a_N\rangle \; = \; \left(\sum_i \; a_i \right) \; |a_1 \; \ldots \; a_N\rangle$$

$$(A_i \otimes \; \ldots \; \otimes A_N) \; |a_1 \; \ldots \; a_N\rangle \; = \; \left(\prod_i \; a_i \right) \; |a_1 \; \ldots \; a_N\rangle$$

Classification of many-particle states: ... (Blackboard)

Example (Frequently occuring Hilbert spaces):

➢ Quantum information theory: multi-qubit systems; quantum registers, N-qudit systems

$$\mathcal{H}^{(N)} \; = \; \mathbb{C}^{2^N} \; = \; \underbrace{\mathbb{C}^2 \otimes \; \ldots \; \otimes \mathbb{C}^2}_{N \text{ times}} \qquad \text{N} - \text{qubit system}$$

$$\mathcal{H}^{(N)} \; = \; \mathbb{C}^{3^N} \; = \; \mathbb{C}^3 \otimes \; \ldots \; \otimes \mathbb{C}^3 \qquad \text{N} - \text{qutrit system}$$

➢ Atomic & molecular physics:

$$\mathcal{H}^{(N)} \; = \; \mathbb{L}^2 \left(\mathbb{R}^{3N} \right) \qquad \text{spin} - \text{less electrons; excited helium, scattering theory}$$

$$\mathcal{H}^{(N)} \; = \; \mathbb{L}^2 \left(\mathbb{R}^{3N} \right) \otimes \mathbb{C}^{2^N} \qquad \text{atomic structure; quantum chemistry}$$

➢ Nuclear & high-energy physics:

$$\mathcal{H}^{(N)} \; = \; \mathbb{L}^2 \left(\mathbb{R}^{3N} \right) \otimes \underbrace{\mathbb{C}^{2^N}}_{\text{nucleons with spin}-1/2} \otimes \underbrace{\mathcal{H}_{\text{IS}}^N}_{\text{iso}-\text{spin space}} \otimes$$

3.1.c. Interlude: Tensor products

Properties of tensor products: Suppose, we have $|v_1\rangle, |v_2\rangle \in V$ and $|w_1\rangle, |w_2\rangle \in W$ and $z \in C$, then

$$\begin{aligned} z\,(|v\rangle \otimes |w\rangle) &= (z\,|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z\,|w\rangle) \\ (|v_1\rangle + |v_2\rangle) \otimes |w\rangle &= |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle \\ |v\rangle \otimes (|w_1\rangle + |w_2\rangle) &= |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle \end{aligned}$$

Tensor product of linear operators: Suppose, we have the vectors $|v_i\rangle \in V$, $|w_i\rangle \in W$ and the operators $A : V \to V$ and $B : W \to W$, then

$$(A \otimes B)\,(|v\rangle \otimes |w\rangle) \equiv A\,|v\rangle \otimes B\,|w\rangle \qquad \forall\ |v\rangle, |w\rangle$$

defines again a linear operator $(A \otimes B) : V \otimes W \to V \otimes W$.

Generalization: If $A : V \to V'$ and $B : W \to W'$ define two maps between different vector spaces, then every linear superposition of operators also defines a linear operator $C : V \otimes W \to V' \otimes W'$ with

$$C = \sum_i c_i\, A_i \otimes B_i$$

$$\left(\sum_i c_i\, A_i \otimes B_i\right)\,(|v\rangle \otimes (|w\rangle) = \sum_i c_i\, A_i\,|v\rangle \otimes B_i\,|w\rangle$$

Scalar product in $V \otimes W$: can be naturally 'defined/reduced to' in terms of the scalar products as defined in V and W. Moreover, since $V \otimes W$ also defines a Hilbert space, all the other properties of operators, such as being adjoint, hermitian, normal, etc., can be also utilized for the operators in the product space.

$$\left\langle \sum_i a_i \, |v_i\rangle \otimes |w_i\rangle \;\middle|\; \sum_k b_i \, |v'_k\rangle \otimes |w'_k\rangle \right\rangle \;=\; \sum_{ik} a_i^* \, b_k \, \langle v_i \,|\, v'_k\rangle \, \langle w_i \,|\, w'_k\rangle$$

Kronecker product (tensor product) of matrices: Suppose, we have an $(m \times n)$ matrix A and a $(p \times q)$ matrix B, then

$$A \otimes B \;=\; \begin{pmatrix} A_{11}\,B & A_{12}\,B & \ldots & A_{1n}\,B \\ A_{21}\,B & \ldots & \ldots & \ldots \\ A_{m1}\,B & \ldots & \ldots & A_{mn}\,B \end{pmatrix}$$

is a $(mp \times nq)$ matrix and is called the Kronecker product of A and B.

Example (Tensor product of the Pauli matrices $\sigma_x = X$ and $\sigma_y = Y$):

$$X \otimes Y \;=\; \begin{pmatrix} 0 \cdot Y & 1 \cdot Y \\ 1 \cdot Y & 0 \cdot Y \end{pmatrix} \;=\; \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

3.2. Identical particles

Hamiltonian operator and wave function of N identical particles: ... with coordinates $i \equiv x_i \equiv (\mathbf{r}_i, \sigma_i)$

$H = H(1,2,\ldots,N)$, $\Psi = \Psi(1,2,\ldots,N)$, "symmetric" in coordinates $1,2,\ldots,N$.

3.2.a. Permutation group & symmetry

Permutation operators:

➢ Permutation operator P_{ij} interchanges (the coordinates of) two particles

$$P_{ij}\,\Psi(1,\ldots,i,\ldots,j,\ldots,N) = \Psi(1,\ldots,j,\ldots,i,\ldots,N), \qquad P_{ij}^2 = 1 \quad \rightsquigarrow \quad \text{eigenvalues } \pm 1\,.$$

Every permutation can also be expressed as a product of two or more two-particle interchanges.

➢ Permutation operator P_{ij} and their products form the permutation group S_N: $P\,H = H\,P \quad \forall P \in S_N\,.$

$P(e) = \mathbb{1}_{\mathcal{H}}$, $P(\pi_1)\,P(\pi_2) = P(\pi_1\pi_2)$ $P_{ii} = \mathbb{1} \quad \forall\, i$

➢ Permutation group S_N: ... we distinguish as usual between even and odd permutations and often use a phase factor $(-1)^P$.

➢ Permutations are represented by unitary operators:

$$P^+ = P^{-1} \qquad \text{since} \qquad \langle \Phi \mid P\,\Psi\rangle = \langle P^{-1}\,\Phi \mid P^{-1}\,P\,\Psi\rangle = \langle P^{-1}\,\Phi \mid \Psi\rangle = \langle P^+\,\Phi \mid \Psi\rangle\,.$$

➢ Physical processes/operators A must be symmetric

$$
\begin{aligned}
[P,\, A] \;&=\; 0 \\
\langle \Psi \,|\, A \,|\, \Psi \rangle \;&=\; \langle P\,\Psi \,|\, A \,|\, P\,\Psi \rangle \qquad\qquad \forall \quad P \in S_N \qquad \text{since} \\
\langle P\,\Psi \,|\, A \,|\, P\,\Psi \rangle \;&=\; \big\langle \Psi \,\big|\, P^+\, A\, P \,\big|\, \Psi \big\rangle \;=\; \left\langle \Psi \,\middle|\, \underbrace{P^+\, P}_{=1}\, A \,\middle|\, \Psi \right\rangle
\end{aligned}
$$

➢ Examples for symmetric operators:

$$
\mathbf{P} \;=\; \sum_i^N \mathbf{p}_i^2 \qquad\qquad \text{total momentum}
$$

$$
\mathbf{L} \;=\; \sum_i^N \mathbf{l}_i \qquad\qquad \text{total angular momentum}
$$

$$
H \;=\; \frac{1}{2m} \sum_i^N \mathbf{p}_i^2 \;+\; \sum_{i<k} V(r_{ik}) \qquad\qquad r_{ik} \;=\; |\mathbf{r}_i \;-\; \mathbf{r}_k|
$$

➢ Especially, the Hamiltonian H is symmetric under permutations

$$
[H,\, P_{ij}] \;=\; 0 \qquad \forall\, i,j \qquad\qquad \Longrightarrow \qquad\qquad H,\, \{P_{ij}\} \quad \text{are simultaneously diagonalizable}
$$

If Ψ is eigenvector of $\{P_{ij}\}$: $\quad P_{ij}\,\Psi \;=\; \pi_{ij}\,\Psi$, then all $\pi_{ij} \;=\; +1$ or $\pi_{ij} \;=\; -1\;\forall\, i,j$ since

$$
P_{ij}\,\Psi \;=\; P_{1i}\,P_{2j}\,P_{12}\,P_{1i}\,P_{2j}\,\Psi \;=\; \pi_{1i}^2\,\pi_{2j}^2\,\pi_{12}\,\Psi \;=\; \pi_{12}\,\Psi\,.
$$

➢ If Ψ is eigenvector of A, then also $P\,\Psi$ eigenvector, and with the same eigenvalue:

$$A\,\Psi \;=\; a\,\Psi \qquad \rightsquigarrow \qquad A\,P\,\Psi \;=\; P\,A\,\Psi \;=\; a\,P\,\Psi \quad \forall \quad P \in S_N .$$

➢ Therefore, Ψ and $P\,\Psi$ are equivalent and can differ only by a phase factor

$P\,\Psi \;=\; \Psi$	bosons	totally symmetric wave function
$P\,\Psi \;=\; -\,\Psi$	fermions	totally antisymmetric wave function

➢ In QFT, one can show that bosons have (always) integer spin and fermions have half-integer spin (spin-statistik theorem).

➢ Composed quantum systems: Nuclei, atoms and molecues may behave like fermions or bosons according to their overall spin.

Example (Total wave function of two hydrogenic atoms): is symmetric with regard to the exchange of the 'atomic coordinates', while it is antisymmetric w.r.t. electrons or protons alone.

$$\Psi(\mathbf{R}_1, \mathbf{r}_1;\, \mathbf{R}_2, \mathbf{r}_2) \;=\; -\,\Psi(\mathbf{R}_2, \mathbf{r}_1;\, \mathbf{R}_1, \mathbf{r}_2) \;=\; -\,\Psi(\mathbf{R}_1, \mathbf{r}_2;\, \mathbf{R}_2, \mathbf{r}_1) \;=\; \Psi(\mathbf{R}_2, \mathbf{r}_2;\, \mathbf{R}_1, \mathbf{r}_1)\,.$$

(Anti-) Symmetry of atoms: ... (Blackboard)

3.2.b. Symmetrization and antisymmetrization

(Anti-) Symmetrization: Every wave function Ψ can be symmetrized or antisymmetrized
(with P, P', $Q \in S_N$)

$$\Psi_s = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} P\,\Psi \qquad Q\,\Psi_s = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} Q\,P\,\Psi = \frac{1}{\sqrt{N!}} \sum_{P' \in S_N} P'\,\Psi = \Psi_s$$

$$\Psi_a = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P\,P\,\Psi \qquad Q\,\Psi_a = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P\,Q\,P\,\Psi = (-1)^Q \frac{1}{\sqrt{N!}} \sum_{P' \in S_N} (-1)^{P'}\,P'\,\Psi$$

$$= (-1)^Q\,\Psi_a\,,$$

Therefore, Ψ_a is totally antisymmetric.

Two identical particles $(N = 2)$

➢ Total wave function:

$$\psi_s = \frac{1}{2}\,(\psi(1,2) + \psi(2,1)) \qquad \psi_a = \frac{1}{2}\,(\psi(1,2) - \psi(2,1))\ .$$

For fermions, the antisymmetrization refers to both, the spatial and the spin part.

➢ Especially, two electrons: $\psi(1,2) = \psi(\mathbf{r}_1,\sigma_1;\mathbf{r}_2,\sigma_2) = \gamma(\mathbf{r}_1,\mathbf{r}_2)\,\chi(\sigma_1,\sigma_2)$ $\qquad \sigma_i = |\uparrow\rangle\,,\,|\downarrow\rangle$

➢ Spin-singulet $(S = 0)$:

$$\chi_{S=0}(\sigma_1, \sigma_2) = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \qquad \text{with} \qquad \chi_{S=0}(\sigma_2, \sigma_1) = -\chi_{S=0}(\sigma_1, \sigma_2) \qquad \text{antisymmetric}$$

➢ Spin-triplet $(S = 1)$:

$$\chi_{S=1}(\sigma_1, \sigma_2) = \left\{ \begin{array}{l} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right) \\ |\downarrow\downarrow\rangle \end{array} \right\} \qquad \text{with} \qquad \chi_{S=1}(\sigma_2, \sigma_1) = +\chi_{S=1}(\sigma_1, \sigma_2) \qquad \text{symmetric}$$

➢ Since total wave function must be antisymmetric, we have the constraints

$$\gamma(\mathbf{r}_2, \mathbf{r}_1) = +\gamma(\mathbf{r}_1, \mathbf{r}_2) \qquad \text{for spin} - \text{singulet}$$

$$\gamma(\mathbf{r}_2, \mathbf{r}_1) = -\gamma(\mathbf{r}_1, \mathbf{r}_2) \qquad \text{for spin} - \text{triplet}$$

➢ Especially, $\psi(\mathbf{r}, \sigma; \mathbf{r}, \sigma) = 0$

Pauli's exclusion principle: Two fermions can neither occupy the same single-particle state nor can they be found with the same spin projection at the same position.

3.2.c. Wave functions of non-interacting indistinguishable particles

Symmetry properties of wave functions:

➢ Hamiltonian:

$$H \;=\; \sum_{i=1}^{N} h_i, \qquad\qquad h_i \;=\; \frac{\mathbf{p}_i^2}{2m} \;+\; V(\mathbf{r}_i)$$

➢ Total Hilbert space: $\mathcal{H}_{\rm tot} \;=\; \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_N$

➢ Consider stationary single-particle solutions: $\phi_\alpha(\mathbf{r}_i,\sigma_i) \;\in\; \mathcal{H}_i, \qquad h_i\,\phi_\alpha(\mathbf{r}_i,\sigma_i) \;=\; \epsilon_\alpha\,\phi_\alpha$

➢ Obviously, product wave functions are eigenfunction of H :

$$\Psi(1,...,N) \;=\; \phi_{\alpha_1}(\mathbf{r}_1,\sigma_1)\,\cdots\,\phi_{\alpha_N}(\mathbf{r}_N,\sigma_N) \qquad \Longrightarrow \qquad H\,\Psi \;=\; \left(\sum_i^N \varepsilon_{\alpha_i}\right)\,\Psi \;=\; \left(\sum_\alpha \varepsilon_\alpha\right)\,\Psi$$

but without proper symmetry under particle exchange

➢ (Anti-) Symmetrization:

$$\Psi_s(1,...,N) = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} \phi_{\alpha_1}(\mathbf{r}_{P(1)}, \sigma_{P(1)}) \cdots \phi_{\alpha_N}(\mathbf{r}_{P(N)}, \sigma_{P(N)}) \qquad \text{bosons}$$

$$\Psi_a(1,...,N) = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P \, \phi_{\alpha_1}(\mathbf{r}_{P(1)}, \sigma_{P(1)}) \cdots \phi_{\alpha_N}(\mathbf{r}_{P(N)}, \sigma_{P(N)}) \qquad \text{fermions}$$

$$= \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \phi_{\alpha_1}(1) & \dots & \phi_{\alpha_1}(N) \\ \phi_{\alpha_2}(1) & \dots & \phi_{\alpha_2}(N) \\ : & & : \\ \phi_{\alpha_N}(1) & \dots & \phi_{\alpha_N}(N) \end{vmatrix}$$

$$\Psi_a = 0 \quad \Longleftarrow \quad \phi_{\alpha_i} = \phi_{\alpha_k} \quad \text{for} \quad i \neq k$$

Pauli principle ensured by Slater determinant

➢ Normalization: if $\{\phi_\alpha(i)\}$ orthonormal, i.e. for $||\phi_\alpha|| = 1$

$\langle \Psi_s \,|\, \Psi_s \rangle = n_{\alpha_1}! \cdots n_{\alpha_r}!$ bosons $\quad n_\alpha$ ... number of particles in state ϕ_α

$\langle \Psi_a \,|\, \Psi_a \rangle = 1$ fermions

➢ Ground state & ground state energy:

$$E_s\,(\text{ground state}) \;=\; N\,\varepsilon_0, \qquad \Psi_s(\text{ground}) \;=\; \phi_0(1)\;\ldots\;\phi_0(N) \qquad \text{bosons}$$

$$E_a\,(\text{ground state}) \;=\; \sum_i^N \varepsilon_i, \qquad \Psi_a(\text{ground}) \;=\; \frac{1}{\sqrt{N!}}\,\text{Det}\,|\ldots| \qquad \text{fermions}$$

For (the ground state of) fermions, we have a successive filling of the one-electron states.

Example (Neon in its ground state):

$$1s^2 2s^2 2p^6$$

$n=1,\ \ell=0,\ m=0,\ m_s=\pm 1/2, \qquad n=2,\ \ldots, \qquad n=2,\ \ell=1,\ m=0,\pm 1,\ m_s=\pm 1/2$

3.2.d. Pauli's (exclusion) principle

For identical fermions, we have

$$h\,\phi_\alpha(\mathbf{x}) \;=\; \varepsilon_\alpha\,\phi_\alpha(\mathbf{x}), \qquad E \;=\; \sum_i \varepsilon_{\alpha_i}, \qquad \alpha_i \;=\; (n_i,\ell_i,m_i,m_{s_i}) \quad \ldots \text{ in atoms}$$

$1s$ ground state of hydrogen: $\alpha_{1s} \;=\; (1,0,0,\pm 1/2)$ ... degenerate

Pauli's exclusion principle: (Wolfgang Pauli, 1925)

Every one-particle state ϕ_α can be occupied by just **no** or (maximally) **one** electron. or

The wave functions of (a system of) identical fermions is totally antisymmetric.

Spin-statistic relation: There is a remarkable relation between the spin and statistics that particle follow

$$\text{bosons} \longleftrightarrow \text{integer spin}$$

$$\text{fermions} \longleftrightarrow \text{half} - \text{integer spin} \qquad \text{proof in relativistic QFT} \quad \text{(Pauli, 1940)}$$

3.2.e. Scattering of two indentical particles

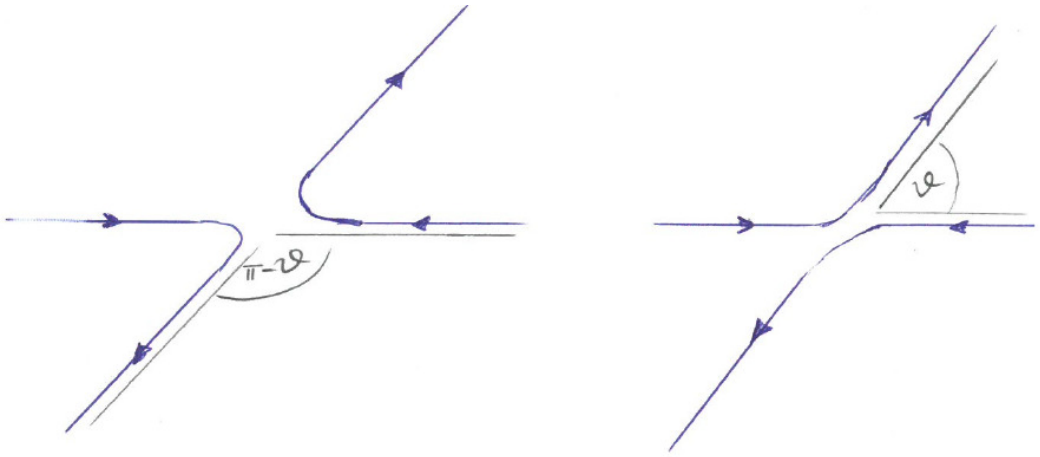


Figure 3.1.: Same outcome for the scattering of two identical particles for the two shown 'trajectories', and which cannot be distinguished experimentally.

Identical bosons without spin

➢ Wave functions of the bosons in the center-of-mass system (CM)

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) \;=\; e^{i\,\mathbf{P}\cdot\mathbf{R}/\hbar}\,\psi(\mathbf{r}) \qquad \begin{aligned}\mathbf{R} &= \mathbf{r}_1 + \mathbf{r}_2, \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2\\ \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2\end{aligned}$$

➢ Total wave function must be symmetric:

$$\psi(\mathbf{r}) \;=\; +\psi(-\mathbf{r})$$

$$\psi^{\,(out)}(r\to\infty) \;=\; \underbrace{e^{i\,\mathbf{k}\cdot\mathbf{r}} + e^{-i\,\mathbf{k}\cdot\mathbf{r}}}_{\text{symmetric}} + \frac{e^{i\,kr}}{r}\,\underbrace{[f_k(\vartheta)+f_k(\pi-\vartheta)]}_{f_k^{\text{symmetric}}(\vartheta)}$$

$$f(\mathbf{k},\mathbf{k}' \;=\; f(k,\vartheta) \;\equiv\; f_k(\vartheta) \;\ldots \text{ because of symmetry}$$

➢ Differential cross section for observing a particle under the angle ϑ :

$$\frac{d\sigma}{d\Omega}^{(\text{bosons})}(\vartheta) \;=\; |f_k(\vartheta)+f_k(\pi-\vartheta)|^2 \;=\; |f_k(\vartheta)|^2 + |f_k(\pi-\vartheta)|^2 \;+\; 2\Re\,[f_k^*(\vartheta)\,f_k(\pi-\vartheta)]$$

qm interference of the two 'trajectories'

➢ Especially $\vartheta = \pi/2$:

$$\frac{d\sigma}{d\Omega}^{(\text{bosons})}\Big|_{\vartheta=\pi/2} = 4\,|f_k(\vartheta)|^2$$

➢ Partial-wave expansion:

$$f_k^{(\text{bosons})}(\vartheta) = \sum_{\ell=0}^{\infty} i^\ell\,(2\ell+1)\,P_\ell(\cos\vartheta)\cdot f_\ell \qquad\qquad f_\ell \text{ ...const.}$$

$$f_k^{\text{bosons}}(\vartheta) = f_k(\vartheta) + f_k(\pi-\vartheta) = 2\sum_{\ell=\text{even}} i^\ell\,(2\ell+1)\,P_\ell(\cos\vartheta)\cdot f_\ell$$

Identical spin-1/2 fermions

General assumption: The scattering (i.e. interaction potential) is spin-independent !!

i) Fermions in well-defined spin-states, $S = 0, 1$:

➢ Wave functions of two fermions in the center-of-mass system (CM)

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \underbrace{e^{i\,\mathbf{P}\cdot\mathbf{R}/\hbar}}_{\text{symmetric}}\;\underbrace{\psi(\mathbf{r})\,\chi(\sigma_1,\sigma_2)}_{\text{antisymmetric}}$$

$\chi_{S=0}(\sigma_1,\sigma_2)$ antisymmetric, singulet

$\chi_{S=1}(\sigma_1,\sigma_2)$ symmetric, triplet

➢ Two fermions in the singulet state, $\chi_{S=0}$: $\psi(\mathbf{r})$ ... symmetric

. Scattering amplitude (and behaviour) like for spin-less bosons.

➢ Two fermions in the triplet state, $\chi_{S=1}$: $\psi(\mathbf{r}) = -\psi(-\mathbf{r})$ ... antisymmetric

$$\psi^{(out)}(r \to \infty) = e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{e^{i\,kr}}{r} \underbrace{[f_k(\vartheta) - f_k(\pi - \vartheta)]}_{f_k^{\text{fermions,S=1}}(\vartheta)}$$

$$\frac{d\sigma}{d\Omega}^{\text{(fermions,S=1)}} = |f_k^{\text{(fermions,S=1)}}(\vartheta) + f_k(\pi - \vartheta)|^2 = |f_k(\vartheta)|^2 + |f_k(\pi - \vartheta)|^2 - 2\Re\,[f_k^*(\vartheta)\, f_k(\pi - \vartheta)]$$

$$\frac{d\sigma}{d\Omega}^{\text{(fermions,S=1)}}\Big|_{\vartheta = \pi/2} = 0 \qquad \text{... zero scattering cross section for ident. fermions (S = 1) under } 90^{\text{o}}$$

$$f_k^{\text{(fermions, S=1)}}(\vartheta) = 2 \sum_{\ell=\text{odd}} i^\ell\, (2\ell + 1)\, P_\ell(\cos\vartheta) \cdot f_\ell$$

... just contributions from the odd Legendre polynomials.

ii) Unpolarized spin-1/2 fermions: ... (Blackboard)

iii) Two $s = 1/2$ fermions with well-defined spin-projection: ... (Blackboard)

3.3. Helium atom

➢ If we neglect the motion of the nucleus , we have

$$H = \underbrace{\frac{\mathbf{p}_1^2}{2m} - \frac{Z\,e^2}{4\pi\epsilon_o\,r_1}}_{h_1} + \underbrace{\frac{\mathbf{p}_2^2}{2m} - \frac{Z\,e^2}{4\pi\epsilon_o\,r_2}}_{h_2} + \underbrace{\frac{e^2}{4\pi\epsilon_o\,|\mathbf{r}_1 - \mathbf{r}_2|}}_{V}, \qquad \Psi(\mathbf{r}_1,\sigma_1,\,\mathbf{r}_2,\sigma_2)$$

$$\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2 = \frac{\hbar}{2}\,(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\,, \qquad \boldsymbol{\sigma} = (\sigma_x,\sigma_y,\sigma_z)\,, \qquad \sigma_i \quad \text{... Pauli matrices}$$

$$S_z = \frac{\hbar}{2}\,(\sigma_{1,z} + \sigma_{2,z}) = \frac{\hbar}{2}\,\underbrace{(\sigma_{1,z}\otimes I_{2x2} + I_{2x2}\otimes\sigma_{2,z})}_{\text{tensor product space}}$$

➢ Since H is spin-independent , we look for eigenfunctions

$$\left\{H,\,\mathbf{S}^2,\,S_z\right\}, \qquad \Psi(\mathbf{r}_1,\sigma_1,\,\mathbf{r}_2,\sigma_2) = \gamma(\mathbf{r}_1,\mathbf{r}_2)\;\chi_{S=0,1}(\sigma_1,\sigma_2)$$

$S = 0$ ... singulet, antisymmetric, parahelium

$S = 1$ ... triplet, symmetric, orthohelium

3.3.a. Perturbation approach

➢ Decomposition of the Hamiltonian

$$H \;=\; H_o \,+\, V \;=\; \underbrace{h_1 \,+\, h_2}_{H_o} + V, \qquad h_i\,\phi_{\alpha_i} \;=\; h_i\,\phi_{n_i\ell_i m_i} \;=\; \varepsilon_{n_i}\,\phi_{n_i\ell_i m_i}, \qquad \varepsilon_n \;=\; -\,\frac{Z^2\,R}{n^2}$$

$R \simeq 13.6$ eV ... Rydberg unit (Rydberg constant)

➢ Energies of unperturbed system

$$E^{(0)}_{n_1,n_2} \;=\; \varepsilon_{n_1} \,+\, \varepsilon_{n_2} \;=\; -\,Z^2\,R\,\left(\frac{1}{n_1^2} \,+\, \frac{1}{n_1^2}\right)$$

➢ Ground state: $n_1 \,=\, n_2 \,=\, 1$

$$E^{(0)}_{11} \;=\; -\,2\,Z^2\,R \;=\; -\,8\,R \;=\; -\,108,8\,\mathrm{eV}, \qquad \gamma(\mathbf{r}_1,\mathbf{r}_2) \;=\; \phi_{100}(\mathbf{r}_1)\,\phi_{100}(\mathbf{r}_2) \quad \rightsquigarrow \quad \text{parahelium}$$

➢ Ground state for orthohelium:

$$\gamma(\mathbf{r}_1,\mathbf{r}_2) \;=\; \frac{1}{\sqrt{2}}\,(\phi_\alpha(\mathbf{r}_1)\phi_\beta(\mathbf{r}_2) \;-\; \phi_\beta(\mathbf{r}_1)\phi_\alpha(\mathbf{r}_2)) \;=\; \frac{1}{\sqrt{2}}\,(\phi_\alpha\phi_b \;-\; \phi_\beta\phi_\alpha) \qquad\qquad \alpha \;=\; (n,\ell,m)$$

$$\Longrightarrow \quad \alpha \;\neq\; \beta \quad \rightsquigarrow \quad n_1 = 1,\; n_2 = 2$$

$$\gamma \;=\; \frac{1}{\sqrt{2}}\,(\phi_{100}\phi_{2\ell m} \;-\; \phi_{2\ell m}\phi_{100})$$

$$E_{12}^{(0)} \;=\; -\,\frac{5}{4}\,Z^2\,R \;=\; -\,5\,R \;=\; -\,68\,\text{eV}.$$

➢ First-order perturbation correction: $\quad E_{1n}^{(1)} \;\equiv\; \Delta\,E_{1n}\,,$

especially parahelium $(S = 0)$

$$\Delta\,E_{11}^{(1)} \;=\; \langle 100,\; 100\,|\,V\,|\,100,\; 100\rangle \;=\; \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2\,|\phi_{100}(\mathbf{r}_1)|^2\,|\phi_{100}(\mathbf{r}_2)|^2\,\frac{e^2}{4\pi\,\epsilon_o\,|\mathbf{r}_1 \;-\; \mathbf{r}_1|}$$

$$\phi_{100}(\mathbf{r}) \;=\; \frac{1}{\sqrt{2}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-\frac{Zr}{a_o}}$$

$$\Delta\,E_{11}^{(1)} \;=\; \frac{5}{4}\,\frac{Ze^2}{2a_o\,(4\pi\,\epsilon_o)} \;=\; \frac{5}{4}\,Z\,R \;=\; 34\,\text{eV}$$

$$E_{11}^{(1)} \;=\; -\,108,8\,\text{eV} \;+\; 34\,\text{eV} \;=\; -\,74,8\,\text{eV} \qquad \longleftrightarrow \qquad E_{11}^{(\text{exp})} \;=\; -\,78,975\,\text{eV}$$

Perturbation calculation does not result in a high accuracy but provides good qualitative understanding of the binding (energies) for helium.

➢ For orthohelium and for all excited states, we need the integrals

$$\Delta E_{\alpha\beta} = \frac{1}{2}\frac{Ze^2}{4\pi\,\epsilon_o}\int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2\; |\phi_\alpha(\mathbf{r}_1)\,\phi_\beta(\mathbf{r}_2) \pm \phi_\beta(\mathbf{r}_1)\,\phi_\alpha(\mathbf{r}_2)|^2 \cdot \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$= \frac{1}{2}\frac{Ze^2}{4\pi\,\epsilon_o}\left\{\iint d^3\mathbf{r}_1\, d^3\mathbf{r}_2\, |\phi_\alpha(\mathbf{r}_1)\,\phi_\beta(\mathbf{r}_2)|^2 \cdot \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \iint d^3\mathbf{r}_1\, d^3\mathbf{r}_2\, [\phi^*_\alpha\,\phi^*_\beta]_{\mathbf{r}_1}\,[\phi_\alpha\,\phi_\beta]_{\mathbf{r}_2} \cdot \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right\}$$

$$= J_{\alpha\beta} \pm K_{\alpha\beta} = \text{Coulomb term} + \text{exchange term} \qquad J_{\alpha\beta} = J_{n_\alpha\ell_\alpha, n_\beta\ell_\beta},\ \ldots$$

Exchange integrals (terms) arise from the antisymmetry of the total wave function (Pauli principle) and is a purely qm effect.

➢ Total energies of the $1s2s\ ^3S$ and $1s2s\ ^3P$ terms of orthohelium

$$J_{1s,2p} = Z\,R\cdot\tfrac{118}{243} = 13,2\,\text{eV} \qquad J_{1s,2s} = Z\,R = \ldots$$
$$K_{1s,2p} = Z\,R\cdot\tfrac{7}{12} = 15,8\,\text{eV} \qquad K_{1s,2s} = Z\,R\cdot\tfrac{32}{729} = 0.6\,\text{eV}$$

$$E_{12} = E^{(0)}_{12} + J_{1s,2\ell} \pm K_{1s,2\ell} = \begin{cases} + & \text{parahelium} \quad 1s2s\ ^1S_0,\ 1s2p\ ^1P \\ - & \text{orthohelium} \quad 1s2s\ ^3S_1,\ 1s2p\ ^3P \end{cases}$$

Remarks

- The lowest $1s2s\ ^3S$ term of orthohelium is metastable; it decays via a spin-flip (intercombination) transition into the $1s^2\ ^1S_0$ ground state.
- $1s2s\ ^3S$ has an extremely long lifetime $\tau \approx 8000/s$.
- First-order perturbation theory is typically not very accurate on the atomic/spectroscopic scale.
- Helium has been the 'testbed' for very many – analytical, numerical and field-theoretical – methods in atomic physics, quantum chemistry and elsewhere.
- The most accurate (variational) methods give rise to 20 and more digits of numerical accuracy.

3.3.b. Variational approach

Ritz's principle

- If H is bounded from below with lowest eigenvalue E_o , we have

$$\langle\Psi\,|\,H\,|\,\Psi\rangle \;\geq\; E_o\,||\Psi||^2 \qquad \longleftrightarrow \qquad \langle\Psi\,|\,H\,|\,\Psi\rangle \;=\; \sum_n \langle\Psi|\left\{\begin{array}{c} H \\ E_n \end{array}\right\}|n\rangle\,\langle n\,|\,\Psi\rangle \;\geq\; E_o\,\langle\Psi\,|\,\Psi\rangle \;=\; E_o\,||\Psi||^2$$

$$E_o \;=\; \min_{\{\Psi\}} \frac{\langle\Psi\,|\,H\,|\,\Psi\rangle}{\langle\Psi\,|\,\Psi\rangle}$$

➢ Choice of proper test function $\Psi(\alpha_1, \ldots, \alpha_p)$ with parameters $\alpha_1, \ldots, \alpha_p$:

$$E(\alpha_1, \ldots, \alpha_p) \;=\; \frac{\langle \Psi(\alpha_1, \ldots, \alpha_p) \,|\, H \,|\, \Psi(\alpha_1, \ldots, \alpha_p) \rangle}{\langle \Psi(\alpha_1, \ldots, \alpha_p) \,|\, \Psi(...) \rangle}$$

and computation of the minimum value

$$E_o \;\leq\; \min_{\{\alpha_k\}} E(\alpha_1, \ldots, \alpha_p) \;=\; E_v$$

Ritz's variation for the helium ground state ... (Blackboard)

3.4. Elementary atomic structure; 'aufbau' principle

3.4.a. Central-field model

➢ Static nucleus: Since the nucleus is much heavier that the electrons, we need just to consider the motion of the N electrons in a central-field potential $V(r) = -\frac{Ze^2}{4\pi\,\epsilon_o\,r}$.

➢ Many-electron Hamiltonian is (to a good approximation) spin-independent; $r_{ik} \equiv |\mathbf{r}_i - \mathbf{r}_k|$

$$H = \sum_i^N h_i + V(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \sum_i^N \underbrace{\left(\frac{\mathbf{p}_i^2}{2m} - \frac{Ze^2}{4\pi\,\epsilon_o\,r_i}\right)}_{h_i} + \frac{1}{2}\sum_{i\neq k}\frac{Ze^2}{4\pi\,\epsilon_o\,r_{ij}}, \qquad \Psi(\mathbf{r}_1,\sigma_1,\ldots,\mathbf{r}_N,\sigma_N)$$

➢ Central-field approximation:

$$H = \sum_i^N (h_i + w(\mathbf{r}_i)) = \sum_i^N \left(\frac{\mathbf{p}_i^2}{2m} - \frac{Ze^2}{4\pi\,\epsilon_o\,r_i} + w(\mathbf{r}_i)\right)$$

$w(r)$ ... mean-field potential as approximately caused by the $N-1$ other electrons.

Hamiltonian = (symmetric) sum of one-electron Hamiltonians

➢ Determine solutions:

$$H\,\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \sum_i^N (h_i + w(\mathbf{r}_i))\;(\phi_1(\mathbf{r}_1)\otimes\phi_2(\mathbf{r}_2)\otimes\ldots\otimes\phi_N(\mathbf{r}_N)) = E\,(..) \qquad \phi_k \to \phi_{\alpha_k}$$

$$\phi = \frac{u_{n\ell}(r)}{r}\,Y_{\ell m}(\vartheta,\varphi)\,\chi_{m_s}$$

➢ Like for hydrogen, each electron is characterized by four QN $\alpha_i = (n_i, \ell_i, m_i, m_{si})$ as well as the single-electron energy $\varepsilon_i = \varepsilon_{n_i,\ell_i}, \quad n_i > \ell_i$:

$$E = \sum_i \varepsilon_{n_i,\ell_i} \qquad \varepsilon_{n\ell} \quad \text{... an eigenenergy of one} - \text{electron Hamiltonian} \quad \tilde{h} = h + w(r)$$

3.4.b. Atomic 'aufbau' principle

➢ Successive filling of the atomic subshells with account of the Pauli principle;

Subshell $n\ell$ with eigen energy $\varepsilon_{n\ell}$: max. occupation $2(2\ell+1)$

$n=1$	$\ell=0$	$1s$	$2e^-$	K-shell	K	He $(N=2)$
$n=2$	$\ell=0$	$2s$	$2e^-$	L-shell	L_1	
	$\ell=1$	$2p$	$6e^-$		L_{23}	Ne $(N=10)$
$n=3$	$\ell=0$	$3s$	$2e^-$	M-shell	M_1	
	$\ell=1$	$3p$	$6e^-$		M_{23}	Ar $(N=18)$
	$\ell=2$	$3d$	$10e^-$		M_{45}	Ni $(N=28)$
$n=4$	$\ell=0$	$4s$	$2e^-$	N-shell	N_1	
	$\ell=1$	$4p$	$6e^-$		N_{23}	Kr $(N=36)$

➢ Beyond $Z = N = 18$ (argon), the filling of subshells is not always regular; atoms with full shells are particularly stable (noble gases).

➢ Electron configurations, terms, etc.

$$\text{Cl} \quad (\text{chlorium},\ Z = 17): \qquad \underbrace{1s^2 2s^2 2p^6 3s^2 3p^5}_{\text{configuration}} \ \underbrace{{}^2P}_{\text{term}} \underbrace{{}_{1/2,3/2}}_{\text{level}} \ \underbrace{M_J = \pm 1/2,\ \pm 3/2}_{\text{atomic state}}$$

Atomic states are often also called magnetic substates.

Example (Low-lying levels of selected atoms):

He: $1s^2\ {}^1S_0$ ... ground state = ground level of atomic helium.

He: $1s2p\ {}^3P$ ... triplet term of helium with three ${}^3P_{0,1,2}$ fine-structure levels and $1\,({}^3P_0,\ M = 0) + 3\,({}^3P_1,\ M = 0, \pm 1) + 5\,({}^3P_2,\ M = 0, \pm 1, \pm 2) = 9$ magnetic substates.

O: $1s^2 2s^2 2p^4$ ... ground configuration of atomic oxygen with ${}^3P$, ${}^1D$, ${}^1S$ terms and with the five ${}^3P_{0,1,2}$, ${}^1D_2$, ${}^1S_0$ fine-structure levels.

3.4.c. Hartree approximation

➢ Single-particle Schrödinger-like equations:

$$(h \,+\, w(\mathbf{r}))\;\phi_\alpha \;=\; \left(\; -\;\frac{Ze^2}{4\pi\,\epsilon_o\,r} \,+\, \frac{e^2}{4\pi\,\epsilon_o}\int d^3\mathbf{r}'\,\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right)\phi_\alpha \;=\; \varepsilon_\alpha\,\phi_\alpha(\mathbf{r})$$

$$\rho(\mathbf{r}) \;=\; \sum_{k\neq i}\,|\phi_k(\mathbf{r})|^2 \qquad\qquad i \;=\; \alpha_i \;=\; (n_i,\ell_i)$$

➢ Spherical symmetric potential

$$\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \qquad\longrightarrow\qquad \left\langle\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right\rangle_{\Omega_\mathbf{r}} \;=\; \int\frac{d\Omega_\mathbf{r}}{4\pi}\,\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$w_{n\ell} \;=\; \int d^3\mathbf{r}'\,\frac{R^2_{n\ell}(r')\;|Y_{\ell m}|^2}{|\mathbf{r}-\mathbf{r}'|} \qquad\longrightarrow\qquad \frac{e^2}{4\pi\,\epsilon_o}\,\frac{1}{2\ell+1}\sum_m\int d\Omega'\,dr'\,r'^2\,R^2_{n\ell}(r')\;|Y_{\ell m}|^2\cdot\frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

$$\;=\; \frac{e^2}{4\pi\,\epsilon_o}\int d\Omega'\,dr'\,r'^2\,\frac{R^2_{n\ell}(r')}{4\pi}\;\cdot\frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

$$w_{n\ell} \qquad = \qquad \frac{e^2}{4\pi\,\epsilon_o\,r}\int_0^r dt\,u_{n\ell}(t) \;+\; \frac{e^2}{4\pi\,\epsilon_o}\int_r^\infty dt\,\frac{u_{n\ell}(t)}{t^2}$$

➢ Hartree equation(s) in atomic units $(\hbar = m_e = \frac{e^2}{4\pi\,\epsilon_o} = 1)$:

$$-\frac{1}{2}\,\frac{d^2\,u_\alpha(r)}{dr^2} + \left(\frac{\ell_\alpha(\ell_\alpha+1)}{2r^2} - \frac{Z}{r}\right)\,u_\alpha + \left(\sum_{\beta\neq\alpha} q_\beta\,w_\beta(r) + (q_\alpha-1)\,w_\alpha(r)\right)\,u_\alpha = \varepsilon_\alpha\,u_\alpha(r)$$

q_α ... occupation number of shell $\alpha = (n_\alpha, \ell_a lpha)$, see electron configuration.

Remarks: ... (Blackboard)

3.5. Free-electron gas & Thomas-Fermi approximation

3.5.a. Free-electron gas

➢ Gas of identical electrons (fermions) in a box of length L and volume $V = L^3$.

➢ Ideal (cold) Fermi gas: Even in the ground-state, Pauli principle forbids that all particles are in the lowest (one-electron) state ϕ_o .

➢ Fermi energy ε_F : highest one-particle energy in an ultra-cold gas $(T = 0)$.

➢ Eigenfunction of free one-particle Hamiltonian $H = \frac{\mathbf{p}^2}{2m}$:

$$\phi_k(\mathbf{r},\sigma) = \frac{1}{\sqrt{V}}\,e^{i\,\mathbf{k}\cdot\mathbf{r}}\,|s\sigma\rangle \qquad \varepsilon(\mathbf{k}) = \frac{\hbar^2}{2m}\,\mathbf{k}^2 \qquad \mathbf{k} \in \frac{2\pi}{L}\,\mathbf{v}$$

$$\sigma \in \{-s,\,-s+1,\,\ldots,\,s\} \qquad \sigma = \pm\frac{1}{2} \qquad \text{... electrons, protons}$$

wave vector $\mathbf{k}$ is quantized because of finite box

➢ Density of states in $\mathbf{k}$-space:

$$dN \;=\; (2s+1)\,\frac{V}{(2\pi)^3}\,d^3\mathbf{k}$$

➢ Spectral density and Fermi energy:

$$d\varepsilon(k) \;=\; \frac{\hbar^2}{m}\,k\,dk \qquad \Longrightarrow \qquad d^3\mathbf{k} \;=\; k^2\,dk\,d\Omega_k \;=\; d\varepsilon\,\frac{m}{\hbar^2}\,k\,d\Omega_k \;=\; \frac{1}{2}\,d\Omega_k\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}\,d\varepsilon$$

$$dN \;=\; V\,D(\varepsilon)\,d\varepsilon \qquad\qquad D(\varepsilon) \;=\; \frac{2s+1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}$$

spectral density of a Fermi gas in a box

➢ Number density:

$$n \;\equiv\; \frac{N}{V} \;=\; \int_0^{\varepsilon_F} d\varepsilon\,D(\varepsilon) \;=\; \left(\frac{\varepsilon_F}{\eta}\right)^{3/2} \qquad\qquad \eta \;=\; \left(\frac{6\pi^2}{2s\,n}\right)\frac{\hbar^2}{2m} \;\approx\; 5.84\ \mathrm{J\,m^2} \;\approx\; 0.365\ \mathrm{eV\,nm^2}$$

$$\varepsilon_F \;=\; \frac{p_F^2}{2m} \;=\; \eta\,n^{2/3}$$

number density $\propto\; p_F^3$

➢ Energy density of free-electron gas:

$$\frac{E}{V} = \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon\, D(\varepsilon) = \frac{3}{5}\,\eta\, n^{5/3} \qquad \text{internal energy density at } T = 0$$

$$E\,(T=0) = \frac{3}{5}\,N\,\eta\, n^{2/3} = \frac{3}{5}\,N\,\varepsilon_F \qquad \text{internal energy of the electron gas at } T = 0$$

➢ A Fermi gas typically strongly resist to compression since this requires to increase the Fermi number density and, hence, the mean energy of the particles in the gas.

Example (Fermi energies of characteristic Systems): L ... characteristic length of cube/particle = mean particle distance.

$$\varepsilon_F = \eta \left(\frac{N}{V}\right)^{2/3} = \begin{cases} 5 \text{ eV} & L = 10^{-8} \text{ cm} & \text{atoms, metals, liquids } (m = m_e) \\ 0.5 \text{ MeV} & L = 10^{-11} \text{ cm} & \text{white dwarfs } (m = m_e) \\ 5 \text{ MeV} & L = 10^{-13} \text{ cm} & \text{atomic nucleus } (m = m_N) \end{cases}$$

These systems are in equilibrium due to their (repulsive) kinetic energies $\bar{\varepsilon} = \frac{\bar{p}}{2m}$ and their attractive interaction between the particles, i.e. the Coulomb interaction with the nuclues for atoms and metals, the gravitational force in white dwards and the strong interaction in atomic nuclei, respectively.

Example (Incompressibility of TF gas):

Mean energy of matter: $\bar{\varepsilon} \propto V^{-2/3} \propto \bar{p}^2$.

Decrease of Volume by 30 %: $V \to 0.7\,V \quad \Longrightarrow \quad p_F \to 1.1\,p_F \quad \Longrightarrow \quad \varepsilon_F \to 1.2\,\varepsilon_F$.

Therefore, the internal energy must increase by a few eV/electron $\gg$ energy of any chemical reaction/ explosion.

Indeed, the incompressibility of the solid-state is therefore based on Pauli's principle.

3.5.b. Thomas-Fermi approximation

Density $n(\mathbf{r})$ of the electron gas:

➢ We assume a sufficiently large No. of electrons in each volume of (nearly) constant potential; i.e. $E(n) \sim n^{5/3}$

➢ Electron density in the nuclear potential of charge Z ; energy functional:

$$E[n(\mathbf{r})] = \underbrace{\frac{3\eta}{5}\int d^3\mathbf{r}\, n^{5/3}(\mathbf{r})}_{\text{free-electron gas}} - \underbrace{Ze^2\int d^3\mathbf{r}\,\frac{n(\mathbf{r})}{|\mathbf{r}|}}_{\text{Coulomb energy; nuclear potential}} + \underbrace{\frac{e^2}{2}\int d^3\mathbf{r}\, d^3\mathbf{r}'\,\frac{n(\mathbf{r})\, n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}}_{\text{electron-electron interaction energy}}$$

➢ Minimize energy under the constraint: $\int d^3\mathbf{r}\, n(\mathbf{r}) = N$

$$E[n] - \lambda\left(\int d^3\mathbf{r}\, n(\mathbf{r}) - N\right) \qquad \Longrightarrow \qquad \delta\left(E[n] - \lambda\int \ldots\right) = 0$$

$$\delta E[n] = \int d^3\mathbf{r}\, \delta n(\mathbf{r})\left(\eta\, n^{2/3}(\mathbf{r}) - \frac{Z\,e^2}{|\mathbf{r}|} + e^2\int d^3\mathbf{r}'\,\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right)$$

$$\lambda = \eta\, n^{2/3}(\mathbf{r}) - \frac{Ze^2}{|\mathbf{r}|} + e^2\int d^3\mathbf{r}'\,\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \equiv -e\,\Phi_o = \text{const.} \qquad \Phi_o > 0$$

$$\lambda = \text{const. ... total energy of electron} < 0 \quad \text{since; electrons are bound}$$

Thomas-Fermi equation

First term describe the position-dependent Fermi energy of the electron, the second the Coulomb energy in the nuclear field and the third term the Coulomb interaction with the mean-field of the remaining electrons.

➢ Thomas -Fermi equation describes the total energy of the N -electron (TF) atom in terms of the electron density.

➢ Thomas-Fermi potential:

$$\Phi(\mathbf{r}) = \frac{Ze}{|\mathbf{r}|} - e\int d^3\mathbf{r}'\,\frac{n(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|} \qquad \Longrightarrow \qquad \eta\, n^{2/3}(\mathbf{r}) = \varepsilon_F(\mathbf{r}) = e\,[\Phi(\mathbf{r}) - \Phi_o]$$

Modified Thomas-Fermi equation: which describes the spatially-dependent kinetic energy ε_F in order to keep the total energy, including the Coulomb energy, per volume element constant.

➢ In addition, the Thomas-Fermi potential must fulfill the Poisson equation

$$\Delta\,\Phi \;=\; -\,4\pi\,\rho \;=\; -\,4\pi\,\left[Ze\,\delta(\mathbf{r}) \;-\; en(\mathbf{r})\right] \;=\; 4\pi\,e\,n(\mathbf{r}) \qquad\qquad r \neq 0$$

$$\Delta\,\Phi \;=\; 4\pi\,e\,\left(\frac{e}{\eta}\right)^{3/2}\,(\Phi \;-\; \Phi_o)^{3/2}$$

➢ Electron density:

$$n(\mathbf{r}) \;=\; \begin{cases} 0 & \Phi(\mathbf{r}) \;=\; \Phi_{\mathrm{o}} \text{ at surface} \qquad \Phi(\mathbf{r}) \;<\; \Phi_{\mathrm{o}} \\ & \text{no negative kinetic energy} \end{cases}$$

➢ Neutral atom: $\Phi_o \;=\; 0$ potential vanished at the surface of the atom.

➢ Radial symmetric solution of the TF equation with $\Phi_o \;=\; 0$

$$\Phi(\mathbf{r}) \;=\; \frac{Ze}{r}\,\chi(r) \qquad\qquad \chi(r) \quad \text{... screening function of nuclear potential due to electron gas}$$

➢ Substitution into the $\Delta\,\Phi$ equation:

$$\frac{Ze}{r}\,\chi''(r) \;=\; 4\pi\,e\,\left(\frac{Ze^2}{\eta\,r}\,\chi\right)^{3/2} \qquad r \;=\; \frac{1}{2}\,\left(\frac{3\pi}{4}\right)^{2/3}\,Z^{-1/3}\,a_o\,s \qquad a_o \;=\; \frac{\hbar^2}{me^2}$$

$$\chi''(s) \;=\; \frac{\chi^{3/2}}{\sqrt{s}} \qquad\qquad \begin{aligned} \chi(s \to \infty) \;&=\; 0 \qquad \text{... electron gas is bound to nucleus} \\ \chi(s \to 0) \;&=\; 1 \qquad \text{... no screening near to the nucleus} \end{aligned}$$

➢ Non-linear equation which need to solved numerically; asymptotic solution:

$$\begin{aligned} \chi(s\to\infty) &\approx \tfrac{144}{s^3} && \Longrightarrow && n(s\to\infty) &\simeq s^{-6} \\ \chi(s\to 0) &\approx 1 - 1.59\,s + \tfrac{4}{3}\cdot s^{3/2} + \ldots && && n(s\to 0) &\simeq s^{-3/2} \end{aligned}$$

Remarks: ... (Blackboard)

3.5.c. Thomas-Fermi atoms

➢ System of non-interacting particles which move in the TF central field:

$$H_o = \sum_{i=1}^{N}\left(\frac{\mathbf{p}_i^2}{2m} + v_{\rm TF}(r_i)\right) \qquad\qquad v_{\rm TF}(r) = \frac{Ze^2}{r}\,\chi(r)$$

➢ Orbital functions in the TF central field:

$$|nlm\,m_s\rangle = \frac{u_{n\ell}}{r}\,Y_{lm}(\vartheta,\varphi)\,\chi_{m_s}$$

$$h_{\rm TF}\,|nlm\,m_s\rangle = \left(\frac{\mathbf{p}^2}{2m} + v_{\rm TF}(r)\right)|nlm\,m_s\rangle = \varepsilon_{n\ell}\,|nlm\,m_s\rangle \qquad \ldots\, 2\,(2\ell+1)\text{fold degenerate}$$

➢ Numerical solution of the one-electron SE:

$$\varepsilon_{1s} < \varepsilon_{2s} < \varepsilon_{2p} < \varepsilon_{3s} < \ldots. \qquad \text{proper order in many}-\text{electron atoms}$$

3.5.d. Interlude: Nuclear shell model

Hamiltonian and nuclear potential:

➢ A nucleus consists out of N neutrons (mass m_n) and Z protons (mass m_p) with:

$$m_n \approx m_p; \approx m_N \qquad \Longrightarrow \qquad A \quad \text{nucleons (mass } m_N)$$

➢ Hamiltonian:

$$H = \sum_{i=1}^{A} \left(-\frac{\mathbf{p}^2}{2m_N} + v_{\text{nuc}}(\mathbf{x}) \right) = \sum_{i=1}^{A} h_i \qquad \mathbf{x} = (\mathbf{x}, \sigma, \tau)$$

➢ Isospin:

$$|\tau = +1/2\rangle = |p\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\tau = -1/2\rangle = |n\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{basis in isospin space}$$

Small differences in the mass can be accounted for by an iso-spin dependent central-field potential.

➢ Nuclear potential:

$$V^{\,(\text{Hartree})} = \int d^3\mathbf{r}\, v((r) - (r)')\, \rho((r)') \qquad \begin{cases} v(|\mathbf{r}_i - \mathbf{r}_k|) & \text{... interaction between nucleons} \\ \rho(\mathbf{r}) & \text{... nuclear density} \end{cases}$$

approximate potential of a nucleon in the field of the $N-1$ other nucleons

➢ Nuclear potential is not well known (until today) and must usually be derived from empirical and observed (nuclear) data.

There are various simple potentials which help understand the central properties of nuclei, such as nculear size, charge radii, etc. We may then use the occupied one-particle states (below the Fermi energy) to define the density distribution of nucleons.

➢ Magic numbers: No. of protons and/or neutrons for which nuclei/isotopes are particular stable (shell closure).

2, 8, 20, 28, 50, 82, ...

Simple nuclear potentials: ... (Blackboard)

Remarks:

➢ Every realistic nuclear model must account for in addition the Coulomb interaction among the protons as well as spin-orbit, spin-spin interactions, etc.

➢ In an improved model, the Coulomb interaction can be approximated by the potential of a homogenously charged sphere.

➢ To understand the neutron excess in heavy nuclei, an isospin-dependent potential must be applied.

➢ The nuclear shell model was first suggested by Maria Goeppert-Mayer and Hans Jensen for which they received the Noble price in 1963.

➢ A more fundamental approach applies QFT and, especially, the quantem chromodynamics (QCD) and lattice gauge theory.

3.6. Hartree-Fock (HF) approximation

3.6.a. HF ansatz

$$H = \sum h_i + \sum_{i<j} v_{ij}, \qquad H\,\Psi_g = E_g\,\Psi_g, \qquad \Psi_g \text{ ... ground state function}$$

$$E_g = \min_{\langle\Psi|\,\Psi\rangle=1} \langle\Psi \,|\, H \,|\, \Psi\rangle \qquad \text{... Ritz}' \text{ variational principle}$$

$$E_g^{(\mathrm{HF})} = \min_{\Psi\in\mathrm{SD}} \langle\Psi \,|\, H \,|\, \Psi\rangle \qquad \Psi(1,\ldots,N) = \frac{1}{\sqrt{N}} \begin{vmatrix} \phi_1(1) & \ldots & \phi_1(N) \\ \vdots & & \vdots \\ \phi_N(1) & \ldots & \phi_N(N) \end{vmatrix}$$

$$\phi_{\alpha_i}(\mathbf{x}_k) \equiv \phi_i(k) = \phi_i(\mathbf{r}_k, \sigma_k)$$

$$\langle\phi_i \,|\, \phi_k\rangle = \delta_{ik}$$

Remarks:

- ➢ Orthogonality: Use of a linear combination $\phi_\alpha \longrightarrow \phi_\alpha + \sum_\beta c_\beta\,\phi_\beta$ does not change the determinant. $\rightsquigarrow$ (One-electron) Orbitals can be chosen orthogonal.
- ➢ Normalization: $\langle\Psi \,|\, \Psi\rangle = \prod_{i=1}^{N} \langle\phi_i \,|\, \phi_i\rangle = 1$

  A scaling $\phi_{\alpha_i} \longrightarrow \lambda_i\,\phi_{\alpha_i}$ with $\prod_i \lambda_i = 1$ does not change the determinant. $\rightsquigarrow$ Orbitals can be normalized individually.

3.6.b. HF equations

➢ Expectation value for single Slater determinant:

$$\langle \Psi \,|\, H \,|\, \Psi \rangle \;=\; \sum_{i=1}^{N} \langle \phi_i \,|\, h_i \,|\, \phi_i \rangle \;+\; \sum_{i<k}^{N} \left(\langle \phi_i\, \phi_k \,|\, v_{ik} \,|\, \phi_i\, \phi_k \rangle \;-\; \langle \phi_i\, \phi_k \,|\, v_{ik} \,|\, \phi_k\, \phi_i \rangle \right)$$

$$\langle \phi_i \,|\, h_i \,|\, \phi_i \rangle \;=\; \int d^3\mathbf{r}_i \; \phi_i^*(\mathbf{r}_i)\; h_i\; \phi_i(\mathbf{r}_i) \qquad\qquad \text{usually independent of index } i \text{ but not of } \alpha, \beta$$

$$\langle \phi_i\, \phi_k \,|\, v_{ik} \,|\, \phi_i\, \phi_k \rangle \;=\; \iint d^3\mathbf{r}\; d^3\mathbf{r}'\; \phi_i^*(\mathbf{r})\; \phi_k^*(\mathbf{r}')\; \frac{1}{4\pi\epsilon_o\, |\mathbf{r}-\mathbf{r}'|}\; \phi_i(\mathbf{r})\; \phi_k(\mathbf{r}')$$

$$\langle \phi_i\, \phi_k \,|\, v_{ik} \,|\, \phi_k\, \phi_i \rangle \;=\; \iint d^3\mathbf{r}\; d^3\mathbf{r}'\; \phi_i^*(\mathbf{r})\; \phi_k^*(\mathbf{r}')\; \frac{1}{4\pi\epsilon_o\, |\mathbf{r}-\mathbf{r}'|}\; \phi_k(\mathbf{r})\; \phi_i(\mathbf{r}')$$

➢ Search for the minimum under the constraint $\{\langle \phi_i \,|\, \phi_k \rangle \;=\; \delta_{ik} \;\; \forall\; i,k \;=\; 1,\, \ldots,\, N\}$, i.e. by using Lagrange multipliers $\lambda_{ik} \;=\; \lambda_{ki}^*$

$$\delta \left[\langle \Psi \,|\, H \,|\, \Psi \rangle \;-\; \sum_{ik} \lambda_{ik}\; \left(\langle \phi_i \,|\, \phi_k \rangle \;-\; \delta_{ik} \right) \right] \;=\; 0$$

$$\delta\, [\ldots] \;-\; \delta\, [\ldots]^* \;=\; -\sum_{ik} \left(\lambda_{ik} \;-\; \lambda_{ki}^* \right)\; \delta\, \langle \phi_i \,|\, \phi_k \rangle \;=\; 0 \qquad\qquad \Longrightarrow \quad \lambda_{ik} \;=\; \lambda_{ki}^*$$

➢ Variation of one-electron orbital functions: $\phi_i \longrightarrow \phi_i + \delta\phi_i$.

$$\delta \langle\phi_i | h_i | \phi_i\rangle = \langle\delta\phi_i | h_i | \phi_i\rangle + \langle\phi_i | h_i | \delta\phi_i\rangle = \int d^3\mathbf{r}\ \{\delta\phi_i^* h_i \phi_i + \phi_i^* h_i \delta\phi_i\}$$

$$\delta [\ldots] = \sum_i \underbrace{\left\{ \langle\delta\phi_i | M | \phi_i\rangle - \sum_{k=1}^{N} \lambda_{ik} \langle\delta\phi_i | \phi_k\rangle \right\}}_{\text{for all variations } \delta\phi_i} + \text{conj. complex} = 0$$

$$M\,\phi_{\alpha_i}(\mathrm{r}) = h\,\phi_{\alpha_i}(\mathrm{r}) + \left\{ \sum_{k\neq i}^{N} \int d^3\mathbf{r}'\ |\phi_k(\mathbf{r}')|^2\ \frac{1}{4\pi\epsilon_o\,|\mathbf{r} - \mathbf{r}'|} \right\} \phi_{\alpha_i}(\mathbf{r})$$

$$- \sum_{k\neq i}^{N} \left[\int d^3\mathbf{r}'\ \phi_k^*(\mathbf{r}') \frac{1}{4\pi\epsilon_o\,|\mathbf{r} - \mathbf{r}'|}\ \phi_i^*(\mathbf{r}')\ \delta_{m_{s_i},m_{s_k}} \right] \phi_{\beta_k}(\mathrm{r})$$

$$=: (h_i + v_{\mathrm{HF}})\,\phi_{\alpha_i}(\mathbf{r}) = (h_i + J_i - K_i)\,\phi_{\alpha_i}(\mathbf{r})$$

v_{HF}	... HF operator
J_i	... direct operator
K_i	... exchange operator

➢ Hermitian matrix of Lagrange multipliers $\boldsymbol{\lambda} = (\lambda_{ik})$ can be diagonalized and gives rise to the one-particle energies

$$\boldsymbol{\lambda} \equiv (\lambda_{ik}) = \mathbf{v}\,\boldsymbol{\varepsilon}\,\mathbf{v}^{+} \qquad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_1 & & \\ & \ddots & \\ & & \varepsilon_N \end{pmatrix} \qquad \phi_k = \sum_i v_{ki}\,\phi_i$$

unitary transformation does not change the determinant

➢ Hartree-Fock equations:

$$(h + v_{\mathrm{HF}})\,\phi_i(\mathbf{r}) = (h + J - K)\,\phi_i(\mathbf{r}) = \varepsilon_i\,\phi_i(\mathbf{r}) \qquad \equiv \varepsilon_\alpha\,\phi_\alpha(\mathbf{r}) \qquad \langle \phi_i \,|\, \phi_k \rangle = \delta_{ik}$$

HF equations provide approximative wave function for the ground state.

➢ Hartree-Fock energy:

$$E_g^{(\mathrm{HF})} = \langle \Psi \,|\, H \,|\, \Psi \rangle = \sum_{i=1}^{N} \varepsilon_i - \frac{1}{2} \sum_{ik}^{N} \left[\langle \phi_i\,\phi_k \,|\, v \,|\, \phi_i\,\phi_k \rangle - \langle \phi_i\,\phi_k \,|\, v \,|\, \phi_k\,\phi_i \rangle \right] \qquad v = \frac{1}{4\pi\epsilon_o\,|\mathbf{r} - \mathbf{r}'|}$$

$$\equiv \sum_{i=1}^{N} \varepsilon_i - \frac{1}{2} \sum_{ik}^{N} \left[\langle ik \,|\, v \,|\, ik \rangle - \langle ik \,|\, v \,|\, ki \rangle \right] = \sum_{i=1}^{N} \varepsilon_i - \frac{1}{2} \sum_{ik}^{N} \langle ik | \,|\, ik \rangle$$

Remarks:

➢ Use of a product function $\Psi = \prod_{i=1}^{N} \phi_i$ instead of a Slater determinant leads to the (so-called)

Hartree equation

$$(h + J)\,\phi_i(\mathrm{r}) = \varepsilon_i\,\phi_i(\mathrm{r})\,.$$

These (product function) solution also coincides with the solution of central-field approximation.

➢ The HF equations can be easily understood: Each electron i moves in the (mean-) field of the nucleus and the $(N-1)$ other electrons.

➢ Self-consistent field: Since the Hartree-Fock potential (operator) $v_{\mathrm{HF}} = J - K$ depends on the function ϕ_i, the HF equations must be solved iteratively.

➢ The Hartree-Fock (ground-state) energy is typically accurate within 5–10 % and is frequently applied in nuclear and atomic structure theory as well as in quantum chemistry.

➢ Koopman theorem: For frozen HF orbitals $\varepsilon_\alpha = I_b^{(\alpha)} = E_{\mathrm{HF}}(N) - E_{\mathrm{HF}}(N-1,\alpha)$

3.6.c. Beyond Hartree-Fock

➢ Further improvements beyond the HF approximation are possible and frequently applied in nuclear, atomic, molecular, condensed-matter physics and elsewhere: configuration interaction approach; multi-configuration Hartree-Fock (MCHF); many-body perturbation theory; coupled-cluster theory, all-order methods.

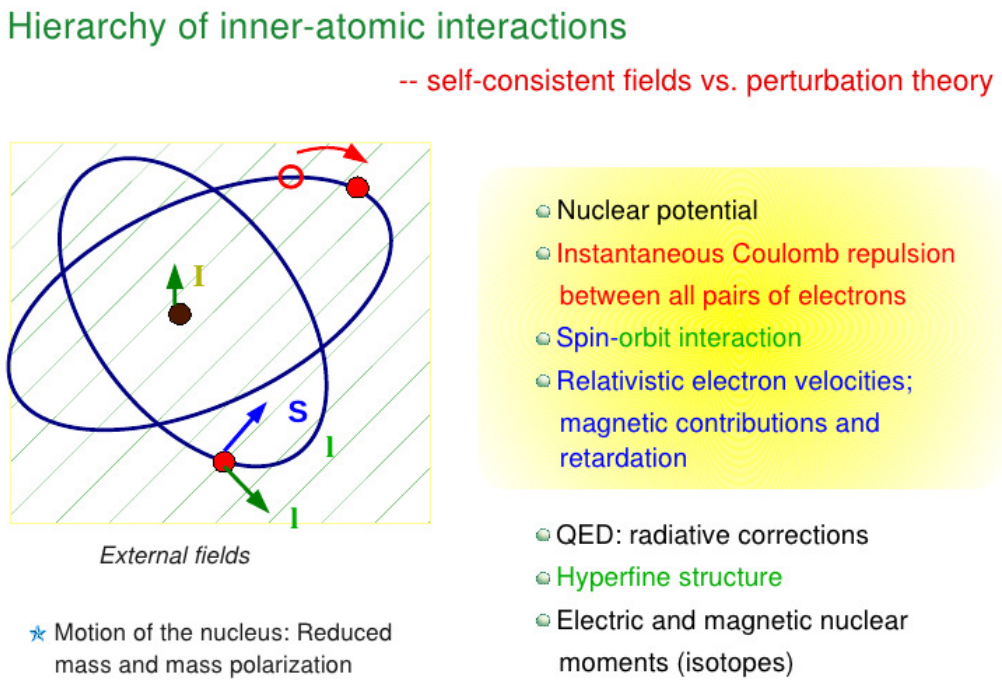


Figure 3.2.: Atomic interactions that need to be considered for a quantitative description/prediction of atoms.

3.7. Second quantization

3.7.a. Creation and annihilation operators

Spin-less bosons, $s = 0$

Application upon single-particle states:

➢ Consider a system of identical, non-interacting and spin-less bosons with single-particle states: $\{\phi_\alpha\}$.

➢ Creation and annihilation operators:

symmetrized product state :	$\|n_\alpha\rangle$					
annihilation operator :	$a_\alpha \, \|n_\alpha\rangle$	$=$	$\sqrt{n_\alpha} \, \|n_\alpha - 1\rangle$	$\langle n_\alpha \| \, a_\alpha^+$	$=$	$\sqrt{n_\alpha} \, \langle n_\alpha - 1\|$
creation operator :	$a_\alpha^+ \, \|n_\alpha\rangle$	$=$	$\sqrt{n_\alpha + 1} \, \|n_\alpha + 1\rangle$	$\langle n_\alpha \| \, a_\alpha$	$=$	$\sqrt{n_\alpha + 1} \, \langle n_\alpha + 1\|$
vacuum state :	$a_\alpha \, \|0\rangle$	$=$	0	$\langle 0 \| \, a_\alpha^+$	$=$	0

➢ Commutator relations:

$$[a_\alpha, \, a_\alpha] \;=\; [a_\alpha^+, \, a_\alpha^+] \;=\; 0 \qquad \text{... obvious}$$

$$[a_\alpha, \, a_\alpha^+] \;=\; 1 \qquad \text{... since}$$

$$[a_\alpha, \, a_\alpha^+] \, |n_\alpha\rangle \;=\; a_\alpha \, a_\alpha^+ \, |n_\alpha\rangle \;-\; a_\alpha^+ \, a_\alpha \, |n_\alpha\rangle$$

$$= \sqrt{n_\alpha + 1} \, a_\alpha \, |n_\alpha + 1\rangle \;-\; \sqrt{n_\alpha} \, a_\alpha^+ \, |n_\alpha - 1\rangle \;=\; [(n_\alpha + 1) \;-\; n_\alpha] \, |n_\alpha\rangle \;=\; |n_\alpha\rangle$$

$$|n_\alpha\rangle \;=\; \frac{(a_\alpha^+)^{n_\alpha}}{\sqrt{n_\alpha!}} \, |0\rangle$$

➢ Number operators:

$\hat{n}_\alpha$	$= \; a_\alpha^+ \, a_\alpha$	$\hat{n}_\alpha \, \|n_\alpha\rangle$	$= \; n_\alpha \, \|n_\alpha\rangle$
$[\hat{n}_\alpha, \, a_\alpha]$	$= \; - \, a_\alpha$	$[\hat{n}_\alpha, \, a_\alpha^+]$	$= \; a_\alpha^+$

Application upon general boson states: ... (Blackboard)

Spin-1/2 fermions

Application upon single-particle states:

➢ Creation and annihilation operators:

$$a_\alpha\,|1\rangle \;=\; |0\rangle\,, \qquad a_\alpha\,|0\rangle \;=\; 0, \qquad a_\alpha^+\,|1\rangle \;=\; 0, \qquad a_\alpha^+\,|0\rangle \;=\; |1\rangle$$

➢ Anticommutation relations:

$$\{a_\alpha,\, a_\alpha\} \;=\; 0 \qquad\qquad \text{since} \qquad a_\alpha\, a_\alpha \;=\; 0$$

$$\{a_\alpha^+,\, a_\alpha^+\} \;=\; 0 \qquad\qquad a_\alpha^+\, a_\alpha^+ \;=\; 0$$

$$\{a_\alpha,\, a_\alpha^+\} \;=\; 1 \qquad\qquad \begin{cases} \{a_\alpha,\, a_\alpha^+\}\,|0\rangle \;=\; a_\alpha\, a_\alpha^+\,|0\rangle \;=\; |0\rangle \\ \{a_\alpha,\, a_\alpha^+\}\,|1\rangle \;=\; a_\alpha^+\, a_\alpha\,|1\rangle \;=\; |0\rangle \end{cases}$$

➢ Number operator: $\hat{n}_\alpha \;=\; a_\alpha^+\, a_\alpha$

Application upon general fermion states:

... (Blackboard)

3.7.b. Field operators

Field operators for boson and fermions:

➢ We assume a complete one-particle basis in position space: $\{\phi_\alpha = \phi_\alpha(\mathbf{r})\}$.

$$f(\mathbf{r}) = \sum_\alpha c_\alpha \, \phi_\alpha(\mathbf{r}) = \sum_\alpha \phi_\alpha(\mathbf{r}) \int d^3\mathbf{r}' \, \phi^*_\alpha(\mathbf{r}') \, f(\mathbf{r}')$$

$$\sum_\alpha \phi^*_\alpha(\mathbf{r}') \, \phi_\alpha(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}') \qquad \text{completentess relation}$$

➢ Operator-valued functions:

$$\Psi_\sigma(\mathbf{r}) = \sum_\alpha \phi_\alpha(\mathbf{r}) \, a_{\alpha,\sigma}, \qquad \Psi^+_\sigma(\mathbf{r}) = \sum_\alpha \phi^*_\alpha(\mathbf{r}) \, a^+_{\alpha,\sigma}$$

field operators that create/annihilate a particles in the spin-state σ and at the position $\mathbf{r}$

➢ (Anti-) commutator relations:

$$[\Psi_{\sigma_\alpha}(\mathbf{r}), \, \Psi_{\sigma_\beta}(\mathbf{r}')]_\pm = [\Psi^+_{\sigma_\alpha}(\mathbf{r}), \, \Psi^+_{\sigma_\beta}(\mathbf{r}')]_\pm = 0$$

$$[\Psi_{\sigma_\alpha}(\mathbf{r}), \, \Psi^+_{\sigma_\beta}(\mathbf{r}')]_\pm = \delta_{\sigma_\alpha,\sigma_\beta} \, \delta(\mathbf{r} - \mathbf{r}')$$

$$\text{... since} = \sum_{\alpha\beta} \phi_\alpha(\mathbf{r}) \, \phi_\beta(\mathbf{r}') \, [a_{\alpha\sigma_\alpha}, \, a^+_{\beta\sigma_\beta}]_\pm = \delta_{\sigma_\alpha,\sigma_\beta} \sum_{\alpha\beta} \phi_\alpha(\mathbf{r}) \, \phi_\beta(\mathbf{r}') \, \delta_{\alpha\beta} = \delta_{\sigma_\alpha,\sigma_\beta} \, \delta(\mathbf{r} - \mathbf{r}')$$

➢ Generation of many-particle states: ... in position and spin-space

$$|\mathbf{r}_1\sigma_1, \ldots, \mathbf{r}_n\sigma_n\rangle = \frac{1}{\sqrt{n!}} \, \Psi^+_{\sigma_n}(\mathbf{r}_n) \cdots \Psi^+_{\sigma_1}(\mathbf{r}_1) \, |0\rangle$$

$$|\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_n\sigma_n\rangle = \pm \, |\mathbf{r}_2\sigma_2, \mathbf{r}_1\sigma_1, \ldots, \mathbf{r}_n\sigma_n\rangle$$

➢ Action of the field operators:

$$\begin{aligned}
\Psi_\sigma^+(\mathbf{r})\ |\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_n\sigma_n\rangle &= \sqrt{n+1}\ |\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_n\sigma_n,\mathbf{r}\sigma\rangle \\
\Psi_\sigma(\mathbf{r})\ |\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_n\sigma_n\rangle &= \Psi_\sigma(\mathbf{r})\,\frac{1}{\sqrt{n!}}\,\Psi_{\sigma_n}^+(\mathbf{r}_n)\cdots\Psi_{\sigma_1}^+(\mathbf{r}_1)\ |0\rangle \\
&= \frac{1}{\sqrt{n!}}\,\left[\delta(\mathbf{r}-\mathbf{r}_n)\,\delta_{\sigma\sigma_n}\ \pm\ \Psi_{\sigma_n}^+(\mathbf{r}_n\,\Psi_\sigma^+(\mathbf{r})\right]\,\Psi_{\sigma_{n-1}}^+(\mathbf{r}_{n-1})\cdots\Psi_{\sigma_1}^+(\mathbf{r}_1)\ |0\rangle \\
&= \frac{1}{\sqrt{n}}\,\left[\delta(\mathbf{r}-\mathbf{r}_n)\,\delta_{\sigma\sigma_n}\ |\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_{n-1}\sigma_{n-1}\rangle\ \pm\ \delta(\mathbf{r}-\mathbf{r}_{n-1})\,\delta_{\sigma\sigma_{n-1}}\ |\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_{n-2}\sigma_{n-2},\mathbf{r}_n\sigma_n\rangle\right. \\
&\quad \left.+\,(\pm1)^{n-1}\,\delta(\mathbf{r}-\mathbf{r}_1)\,\delta_{\sigma\sigma_1}\ |\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_n\sigma_n\rangle\right]
\end{aligned}$$

➢ The field operators can be used to defined scalar products, expectation values, operators of observables, matrix elements, etc. — This is frequently applied in quantum field theory.

➢ In many-particle physics, where the total number of particles is fixed, one typically makes use of the creation and annihilation operators to express the matrix elements in an convinient manner.

Fock space: ... (Blackboard)

4. Angular momentum (AM) in quantum physics

4.1. Angular momentum operators

Commutation relation & eigenfunctions:

$$
\begin{aligned}
[l_i,\, l_j] &= i\hbar\, \epsilon_{ijk}\, l_k \\
\mathbf{l}^2\, Y_{lm} &= \hbar^2\, \ell(\ell+1)\, Y_{lm} \qquad\qquad \ell = 0, 1, 2, ... \qquad\qquad \text{orbital angular momentum QN} \\
l_z\, Y_{lm} &= m\, \hbar\, Y_{lm} \qquad\qquad m = -\ell, -\ell+1, ..., \ell \qquad\qquad \text{magnetic QN}
\end{aligned}
$$

4.1.a. Algebraic definition of angular momentum

Definition of AM operators by their commutator:

➢ In the algebraic method of AM theory, one defines the commutators of the cartesian components by:

$$[j_i,\, j_j] = i\hbar\, \epsilon_{ijk}\, j_k\ , \qquad \ldots \text{ defines an algebra for all (half}-\text{)integer values } j \geq 0$$

with the consequence that the eigenvalues include all (non-negative) integer and half-integer values.

➢ One then finds with $\mathbf{j}^2 = j_x^2 + j_y^2 + j_z^2$ and the ladder operators $j_\pm = j_x \pm i\, j_y$:

$$[j_i,\, \mathbf{j}^2] = 0 \qquad (i = 1,2,3)$$

$$[j_+,\, j_-] = 2\,\hbar\, j_z \qquad [j_z,\, j_\pm] = \pm\hbar\, j_\pm \qquad [j_\pm,\, \mathbf{j}^2] = 0$$

➢ The operators $j_\pm$ are non-hermitian and related to each other by: $j_+ = j_-^\dagger$

$$j_\pm\, |jm\rangle = N_\pm\, |j, m \pm 1\rangle\,, \qquad N_\pm(j,m) = \hbar\sqrt{j(j+1) - m(m\pm 1)}$$

Algebraic method ... (Blackboard)

4.1.b. Matrix representation of angular momentum operators

Let us construct a matrix representation of $\mathbf{j}^2$ and the cartesian components j_x, j_y and j_z.

$$\langle u_{jm} \,|\, \mathbf{j}^2\, u_{jm'}\rangle = \hbar^2\, j(j+1)\, \delta_{mm'} \qquad \langle u_{jm} \,|\, j_z\, u_{jm'}\rangle = \hbar\, \delta_{mm'}$$

$$\langle u_{jm} \,|\, j_\pm\, u_{jm'}\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\, \delta_{m,m'\pm 1}$$

and

$$\langle u_{jm} \,|\, j_x\, u_{jm'}\rangle = \frac{\hbar}{2}\left[\sqrt{j(j+1) - m(m-1)}\, \delta_{m,m'+1} + \sqrt{j(j+1) - m(m+1)}\, \delta_{m,m'-1}\right]$$

$$\langle u_{jm} \,|\, j_y\, u_{jm'}\rangle = \frac{\hbar}{2i}\left[\sqrt{j(j+1) - m(m-1)}\, \delta_{m,m'+1} - \sqrt{j(j+1) - m(m+1)}\, \delta_{m,m'-1}\right] .$$

Example (Spin-1/2 systems): We have $m = (+1/2, -1/2)$ and, thus, the matrix representations

$$(j_{x;mm'}) \equiv j_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad j_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad j_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$j_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad j_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \mathbf{j}^2 = \hbar^2\frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Blackboard example (Spin-1 systems):

4.1.c. Algebra of Pauli matrices

➢

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_o = I_{2x2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

➢ These Pauli matrices obey several important relations:

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \sigma_o\,, \qquad [\sigma_i, \sigma_j] = 2i\,\epsilon_{ijk}\,\sigma_k$$

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}\,\sigma_o\,, \qquad \sigma_i\sigma_j = \delta_{ij}\,\sigma_o + i\,\epsilon_{ijk}\,\sigma_k$$

➢ Linear independence of the Pauli matrices: ... only holds iff $a_o = a_1 = a_2 = a_3 = 0$.

$$a_o\,\sigma_o + a_1\,\sigma_1 + a_2\,\sigma_2 + a_3\,\sigma_3 = 0$$

➢ Therefore, the Pauli matrices form a basis for arbitrary 2×2 matrices:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_o\,\sigma_o + a_1\,\sigma_1 + a_2\,\sigma_2 + a_3\,\sigma_3 = \sum_i a_i\,\sigma_i$$

$$a_0 = \frac{1}{2}\,(a_{11} + a_{22})\,, \qquad a_1 = \frac{1}{2}\,\mathrm{Tr}\,(\sigma_x\,A)\,, \qquad a_2 = \frac{1}{2}\,\mathrm{Tr}\,(\sigma_y\,A)\,, \qquad a_3 = \frac{1}{2}\,\mathrm{Tr}\,(\sigma_z\,A)$$

$$a_i = \frac{1}{2}\,\mathrm{Tr}\,(\sigma_i\,A)\,, \qquad (\mathbf{a}\cdot\boldsymbol{\sigma})\,(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b} + i\,\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})\,, \qquad (\mathbf{a}\cdot\boldsymbol{\sigma})^2 = a^2\,.$$

4.2. Coupling of angular momenta

4.2.a. AM of spin-1/2 particles. Electrons, ...

Electrons, protons, etc.

➢ Hilbert space: Product of the position space and spin space

$$|\mathbf{r},\pm\rangle \;=\; |\mathbf{r}\rangle \otimes |\uparrow,\downarrow\rangle\,; \qquad\qquad \mathcal{H} \;=\; \{|\mathbf{r},\pm\rangle\} \;=\; \mathcal{H}_p \otimes \mathcal{H}_2$$

➢ AM operators:

$$\mathbf{j} \;=\; \mathbf{l}\otimes\mathbf{1} \;+\; \mathbf{1}\otimes\mathbf{s} \;=\; \mathbf{l} \;+\; \mathbf{s}\,, \qquad [l_i,\, l_j] \;=\; i\hbar\,\epsilon_{ijk}\,l_k\,, \qquad [s_i,\, s_j] \;=\; i\hbar\,\epsilon_{ijk}\,s_k\,, \qquad [l_i,\, s_j] \;=\; 0\,,$$

➢ Rotation operator in product space: If $\mathbf{n}$ is a unit vector along the rotation axis

$$U_R(\mathbf{n},\vartheta) \;=\; \exp\left(\frac{-i\,\mathbf{j}\cdot\mathbf{n}\,\vartheta}{\hbar}\right) \;=\; \exp\left(\frac{-i\,\mathbf{l}\cdot\mathbf{n}\,\vartheta}{\hbar}\right)\,\exp\left(\frac{-i\,\mathbf{s}\cdot\mathbf{n}\,\vartheta}{\hbar}\right)\,.$$

➢ Wave functions in product space: Superposition of two spin components

$$\psi(\mathbf{r},\sigma) \;=\; \begin{pmatrix}\psi_\uparrow(\mathbf{r})\\ \psi_\downarrow(\mathbf{r})\end{pmatrix} \;=\; \psi_\uparrow(\mathbf{r})\,|\uparrow\rangle \;+\; \psi_\downarrow(\mathbf{r})\,|\downarrow\rangle \;=\; \underbrace{\psi_0\,|0\rangle \;+\; \psi_1\,|1\rangle}_{\text{QIP}} \;=\; \underbrace{\psi_\alpha\,|\alpha\rangle \;+\; \psi_beta\,|beta\rangle}_{\text{quantum chemistry}}\,.$$

➢ Operators and product states of composite system, if diagonal in $\{\mathbf{l}^2, l_z, \mathbf{s}^2, s_z\}$

$$|\ell, s, m_\ell, m_s\rangle \;=\; |\ell, m_\ell\rangle\,|s, m_s\rangle \;=\; |\ell s m_\ell m_s\rangle$$

$$\mathbf{l}^2\;|\ell m_\ell\rangle \;=\; \ell(\ell+1)\,\hbar^2\;|\ell m_\ell\rangle\,, \qquad\qquad l_z\;|\ell m_\ell\rangle \;=\; m_\ell\,\hbar\;|\ell m_\ell\rangle$$

$$\mathbf{s}^2\;|s m_s\rangle \;=\; s(s+1)\,\hbar^2\;|s m_s\rangle\,, \qquad\qquad s_z\;|s m_s\rangle \;=\; m_s\,\hbar\;|s m_s\rangle$$

(so-called) product or uncoupled basis

➢ Spin-orbital motion of electrons can be described by different sets of commuting operators $\{\mathbf{l}^2, l_z, \mathbf{s}^2, s_z\}$ or $\{\mathbf{l}^2, \mathbf{s}^2, \mathbf{j}^2, j_z\}$ and with the well-known commutators from above.

➢ Coupled basis: $|\ell s j m_j\rangle$ with eigenvalue equations from above.

$$\mathbf{l}^2\ |\ell s j m_j\rangle = l(l+1)\,\hbar^2\ |\ell s j m_j\rangle\ , \qquad \mathbf{j}^2\ |\ell s j m_j\rangle = j(j+1)\,\hbar\ |\ell s j m_j\rangle$$

$$\mathbf{s}^2\ |\ell s j m_j\rangle = \frac{3}{4}\,\hbar^2\ |\ell s j m_j\rangle\ , \qquad j_z\ |\ell s j m_j\rangle = m_j\,\hbar\ |\ell s j m_j\rangle$$

coupled basis

4.2.b. Coupling of two angular momenta (AM)

Uncoupled *vs.* coupled basis states: ... (Blackboard)

Clebsch-Gordan expansion:

➢ The functions of the uncoupled and coupled bases can be easily transformed into each other:

$$|j_1 j_2 j m_j\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 m_1 j_2 m_2\rangle\ \langle j_1 m_1, j_2 m_2\,|\,j_1 j_2 j m_j\rangle$$

$$|j_1 m_1 j_2 m_2\rangle = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m_j=-j}^{j} |j_1 j_2 j m_j\rangle\ \langle j_1 j_2 j m_j\,|\,j_1 m_1, j_2 m_2\rangle$$

Clebsch-Gordan coefficients $\equiv \langle j_1 m_1, j_2 m_2\,|\,j m_j\rangle = C^{jm}_{j_1 m_1, j_2 m_2} = C(j_1 j_2 j; m_1 m_2 m)$

➢ The Clebsch-Gordan coefficients are the Fourier coefficients in a basis change between two orthonormal basis.

➢ The Clebsch-Gordan coefficients freqently appear in the description of multi-qubit and quantum many-particle systems. elsewhere.

➢ Group theory: Tensor product of two representations $\mathfrak{h}_{j_1}$ and $\mathfrak{h}_{j_2}$ of the individually AM gives generally rise to a 'sum' of irreducible representations of the total AM

$$\mathfrak{h}_{j_1} \otimes \mathfrak{h}_{j_2} \;=\; \mathfrak{h}_{j_1+j_2} \oplus \mathfrak{h}_{j_1+j_2-1} \oplus \ldots \oplus \mathfrak{h}_{|j_1-j_2|}.$$

Example (Irreducible representations of coupled angular momenta):

1) $\ell_1 = 1,\ \ell_2 = 2; \quad L = 1,2,3: \qquad \mathbf{3} \otimes \mathbf{5} \;=\; \mathbf{3} \oplus \mathbf{5} \oplus \mathbf{7}; \qquad\qquad$ "$p + d$" $\;=\; P + D + F$

2) $L_1 = 2,\ L_2 = 3; \quad L = 1,2,3,4,5: \qquad \mathbf{5} \otimes \mathbf{7} \;=\; \mathbf{3} \oplus \mathbf{5} \oplus \mathbf{7} \oplus \mathbf{9} \oplus \mathbf{11}$

3) $\ell = 2,\ s = 1/2; \quad J = 3/2, 5/2: \qquad \mathbf{5} \otimes \mathbf{2} \;=\; \mathbf{4} \oplus \mathbf{6}; \qquad\qquad$ "$d + 1/2$" $\;=\; d_{3/2} + d_{5/2}$

4) $j_1 = 1/2,\ j_2 = 3/2,\ j_3 = 1/2; \quad J = 1/2, 3/2, 3/2, 5/2: \qquad \mathbf{2} \otimes \mathbf{4} \otimes \mathbf{2} \;=\; \mathbf{2} \oplus \mathbf{4} \oplus \mathbf{4} \oplus \mathbf{6};$ indep. coupling seq.

Successive coupling; can be generalized to arbitrarely large No. of angular momenta.

4.2.c. Properties of Clebsch-Gordan (CG) coefficients

Although the Clebsch-Gordan coefficients need to be calculated explicitly in several cases, one often wishes to just use their properties in order to understand the behaviour of physical systems, at least qualitatively.

➢ The CG coefficients: $\langle j_1 m_1, j_2 m_2 \,|\, j, m_j \rangle \;=\; 0\ , \qquad$ unless $\; m_j \;=\; m_1 \,+\, m_2\,.$

➢ CG coefficients are taken to be real: $\underbrace{\langle j_1 m_1, j_2 m_2 \,|\, jm\rangle}_{standard\ form} = \langle jm \,|\, j_1 m_1, j_2 m_2\rangle$.

➢ Triangular rule: CG coefficients vanish unless $|j_1 - j_2| \le j \le j_1 + j_2$

Indeed, one can show for all integer and half-integer values of $j_1,\ j_2$: $\sum_{j=|j_1-j_2|}^{j_1+j_2} = (2j_1+1)(2j_2+1)$.

➢ For each j, the values of m_j are: $-j \le m_j \le j$.

➢ Orthogonality and sum rules: There are a large number of such 'sum rules', for example:

$$\sum_{m_1,m_2} \langle j_1 m_1, j_2 m_2 \,|\, jm\rangle^2 = 1 \qquad \Longleftrightarrow \qquad \sum_{j,m} \langle j_1 m_1, j_2 m_2 \,|\, jm\rangle^2 = 1$$

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

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

➢ CG coefficients are closely related to the (so-called) Wigner 3–j symbols which obey higher symmetries:

$$\langle j_1 m_1, j_2 m_2 \,|\, jm\rangle = (-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} .$$

	$m_2 = \frac{1}{2}$	$m_2 = -\frac{1}{2}$
$J = j_1 + 1/2$	$\left(\frac{j_1+M+1/2}{2j_1+1}\right)^{1/2}$	$\left(\frac{j_1-M+1/2}{2j_1+1}\right)^{1/2}$
$J = j_1 - 1/2$	$-\left(\frac{j_1-M+1/2}{2j_1+1}\right)^{1/2}$	$\left(\frac{j_1+M+1/2}{2j_1+1}\right)^{1/2}$

Figure 4.1.: Clebsch-Gordan coefficients for the case $j_2 = 1/2$; taken from H. Machmer, Einführung in die Kern- und Elementarteilchenphysik (VCH-Verlag, 2005).

4.2.d. Calculation of Clebsch-Gordan coefficients

➢ Recursion relations: From $\langle j_1 j_1,\, j_2 j_2 \,|\, j(j_1+j_2)\rangle = 1$ with $j = j_1 + j_2$ and the properties of the $j_\pm$ operators:

$$j_\pm \,|j_1 j_2, jm_j\rangle = (j_{1,\pm} + j_{2,\pm})\,|j_1 j_2, jm_j\rangle = \sum_{m_1', m_2'} (j_{1,\pm} + j_{2,\pm})\,|j_1 m_1', j_2, m_2'\rangle\,\langle j_1 m_1' j_2, m_2' \,|\, j_1 j_2, jm_j\rangle$$

one find the (recursion) relations

$$\sqrt{(j-m)(j+m+1)}\;\langle j_1 m_1, j_2 m_2 \,|\, j, m+1\rangle$$
$$= \sqrt{(j_1 - m_1 + 1)(j_1 + m_1)}\;\langle j_1, m_1 - 1, j_2 m_2 \,|\, jm\rangle + \sqrt{(j_2 - m_2 + 1)(j_2 + m_2)}\;\langle j_1 m_1, j_2, m_2 - 1 \,|\, jm\rangle$$

$$\sqrt{(j+m)(j-m+1)}\;\langle j_1 m_1, j_2 m_2 \,|\, j, m-1\rangle$$
$$= \sqrt{(j_1 + m_1 + 1)(j_1 - m_1)}\;\langle j_1, m_1 + 1, j_2 m_2 \,|\, jm\rangle + \sqrt{(j_2 + m_2 + 1)(j_2 - m_2)}\;\langle j_1 m_1, j_2, m_2 + 1 \,|\, jm\rangle\ .$$

➢ Use of Racah's formula.

	$m_2 = 1$	$m_2 = 0$	$m_2 = -1$
$J = j_1 + 1$	$\left(\frac{(j_1+M)(j_1+M+1)}{(2j_1+1)(2j_1+2)}\right)^{1/2}$	$\left(\frac{(j_1-M+1)(j_1+M+1)}{(2j_1+1)(2j_1+2)}\right)^{1/2}$	$\left(\frac{(j_1-M)(j_1-M+1)}{(2j_1+1)(2j_1+2)}\right)^{1/2}$
$J = j_1$	$\left(\frac{(j_1+M)(j_1-M+1)}{2j_1(j_1+2)}\right)^{1/2}$	$\left(\frac{M(j_1-M+1)}{j_1(2j_1+1)}\right)^{1/2}$	$\left(\frac{(j_1-M)(j_1-M+1)}{2j_1(2j_1+1)}\right)^{1/2}$
$J = j_1 - 1$	$\left(\frac{(j_1-M)(j_1-M+1)}{2j_1(j_1+2)}\right)^{1/2}$	$\left(\frac{(j_1-M)(j_1+M)}{j_1(2j_1+2)}\right)^{1/2}$	$\left(\frac{(j_1+M+1)(j_1+M)}{2j_1(2j_1+2)}\right)^{1/2}$

Figure 4.2.: Clebsch-Gordan coefficients for the case $j_2 = 1$; taken from H. Machmer, Einführung in die Kern- und Elementarteilchenphysik (VCH-Verlag, 2005).

➢ Use computer-algebra or program libraries.

➢ Look up tables and books; there are extensive tabulations available from the past.

4.2.e. Coupling of three and more angular momenta; re-coupling coefficients

Coupling of three angular momenta:

➢ Three particles with AM operators $\mathbf{j}_1,\ \mathbf{j}_2,\ \mathbf{j}_3$ and eigenfunctions: $\{|j_1 m_1\rangle\ ,\ |j_2 m_2\rangle\ ,\ |j_3 m_3\rangle\}$

➢ One coupling sequence: i) $\mathbf{j}_1 + \mathbf{j}_2 = \mathbf{J}_{12}$ and $\mathbf{J}_{12} + \mathbf{j}_3 = \mathbf{J}$

$$|(j_1, j_2)\, J_{12}\, j_3 :\ JM\rangle \ = \sum_{m_1,m_2,m_3} \sum_{M_{12}} |j_1 m_1,\ j_2 m_2,\ j_3 m_3\rangle\ \langle j_1 m_1,\ j_2 m_2\,|\,J_{12} M_{12}\rangle\ \langle J_{12} M_{12},\ j_3 m_3\,|\,JM\rangle$$

uncoupled basis $|j_1 m_1,\ j_2 m_2,\ j_3 m_3\rangle \ = \ |j_1 m_1\rangle\,|j_2 m_2\rangle\,|j_3 m_3\rangle$

➢ Another coupling sequence: ii) $\mathbf{j}_2 + \mathbf{j}_3 = \mathbf{J}_{23}$ and $\mathbf{j}_1 + \mathbf{J}_{23} = \mathbf{J}$

$$|j_1\,(j_2, j_3)\,J_{23}:\,JM\rangle = \sum_{m_1,m_2,m_3}\sum_{M_{23}} |j_1 m_1,\, j_2 m_2,\, j_3 m_3\rangle\,\langle j_2 m_2,\, j_3 m_3\,|\,J_{23} M_{23}\rangle\,\langle j_1 m_1,\, J_{23} M_{23},\,|\,JM\rangle$$

➢ Both set of states $\{|(j_1, j_2)\,J_{12}\,j_3:\,JM\rangle\}$ and $\{|j_1\,(j_2, j_3)\,J_{23}:\,JM\rangle\}$ each form an orthonormal basis in the product space $\mathfrak{h}_{j_1} \otimes \mathfrak{h}_{j_2} \otimes \mathfrak{h}_{j_3}$ ... and are related to each other by a unitary transformation.

$$|j_1\,(j_2, j_3)\,J_{23}:\,JM\rangle = \sum_{J_{12}} |(j_1, j_2)\,J_{12}\,j_3:\,JM\rangle\,\langle (j_1, j_2)\,J_{12} j_3:\,JM\,|\,j_1\,(j_2, j_3))\,J_{23}:\,JM\rangle$$

re-coupling coefficient ... form a unitary matrix

Calculation of recoupling coefficients: ... (Blackboard)

Wigner 6–j symbols: ... (Blackboard)

Coupling of four angular momenta: ... (Blackboard)

Example (LS vs. jj-coupling:): The 9–j symbols appears frequently in atomic structure in going from LS- to jj-coupled functions

$$|(\ell_1, s_1)\,j_1\,(\ell_2, s_2)\,j_2:\,JM\rangle = \sum_{LS} [j_1,\, j_2,\, L,\, S]^{1/2} \begin{Bmatrix} \ell_1 & s_1 & j_1 \\ \ell_2 & s_2 & j_2 \\ L & S & J \end{Bmatrix} |(\ell_1, \ell_2)\,L\,(s_1, s_2)\,S:\,JM\rangle$$

4.3. Rotations of states and operators

Since the AM operators are the generators of rotations and to make use of the symmetry, it is often necessary to transform states and operators from an unrotated coordinate frame $\Sigma\,(x, y, z)$ to a rotated frame $\Sigma'\,(x', y', z')$

$$R_{\mathbf{n}}(\beta) \;=\; \exp\left(-i\beta\,\mathbf{n}\cdot\mathbf{J}\right), \qquad\qquad |jm\rangle' \;=\; R_{\mathbf{n}}(\beta)\;|jm\rangle \;=\; R(\varphi,\vartheta,\chi),$$

where the rotation can be specified by just three angles: i) the rotation angle and ii) two angles to specify the rotation axis.

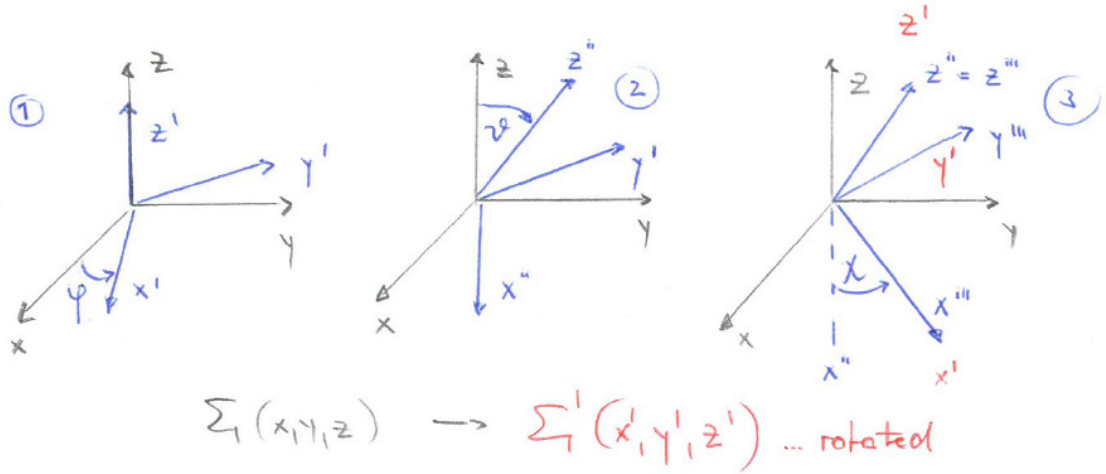


Figure 4.3.: Definition of the Euler angles

Different views of rotations:

➢ Active view: Rotation of the qm. system.

➢ Passive view: Rotation of the coordinates in counter-direction.

4.3.a. Definition of Euler angles

1. Rotate counterclockwise by angle φ around z-axis
2. Rotate (counterclockwise) by angle ϑ around new y'-axis
3. Rotate (counterclockwise) by angle χ around new z''-axis

These rotations can be expressed mathematically as:

$$\begin{aligned} R(\varphi,\vartheta,\chi) &= \exp\left(-i\chi\,\mathbf{n}_\chi\cdot\mathbf{J}\right)\cdot\exp\left(-i\vartheta\,\mathbf{n}_\vartheta\cdot\mathbf{J}\right)\cdot\exp\left(-i\varphi\,\mathbf{n}_\varphi\cdot\mathbf{J}\right) \\ &= \exp\left(-i\chi\,J_{z''}\right)\cdot\exp\left(-i\vartheta\,J_{y'}\right)\cdot\exp\left(-i\varphi\,J_z\right) \end{aligned}$$

H'm, this formula contains operators that are defined in different coordinate systems and, thus, is tediuos to apply.

Transformation of operators : ... (Blackboard)

4.3.b. Wigner's rotation matrix

➢ Rotation of eigenfunctions:

$$\underbrace{|jm\rangle'}_{\text{rotated coord.}} = R(\varphi,\vartheta,\chi) \quad \underbrace{|jm\rangle}_{\text{unrotated coord.}} = \sum_{m'} |jm'\rangle \, \langle jm'|R(\varphi,\vartheta,\chi)|\, jm\rangle = \sum_{m'} D^{j}_{m'm}(\varphi,\vartheta,\chi) \; |jm'\rangle$$

$$D^{j}_{m'm}(\varphi,\vartheta,\chi) \equiv \langle jm'|R(\varphi,\vartheta,\chi)|\, jm\rangle = \langle jm'|\exp(-i\varphi\, J_z)\cdot\exp(-i\vartheta\, J_y)\cdot\exp(-i\chi\, J_z)|\, jm\rangle$$

$$= e^{-i\varphi m'}\cdot d^{j}_{m'm}(\vartheta)\cdot e^{-i\chi m}$$

Wigner's rotation matrix ... matrix elements of rotation operator

➢ Wigner's small d-matrices:

$$d^{j}_{m'm}(\vartheta) = \langle jm'|\exp(-i\vartheta\, J_y)|\, jm\rangle$$

Example (Wigner's small $d^{1/2}_{m'm}(\vartheta)$ matrix): $\exp\left(-i\vartheta\, J_y\right) \;\to\; \exp\left(-i\vartheta\, \frac{\sigma_y}{2}\right)$

$$\begin{aligned}
\exp\left(-i\vartheta\,\frac{\sigma_y}{2}\right) &= \exp\left[-i\frac{\vartheta}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\right] = I + \frac{\vartheta}{2}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} + \frac{1}{2!}\left(\frac{\vartheta}{2}\right)^2\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}^2 + \ldots \\
&= \left[1 - \frac{1}{2!}\left(\frac{\vartheta}{2}\right)^2 + \ldots\right]\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \left[\frac{\vartheta}{2} - \frac{1}{3!}\left(\frac{\vartheta}{2}\right)^3 + \ldots\right]\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \\
&= \cos\frac{\vartheta}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \sin\frac{\vartheta}{2}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \\
&= \begin{pmatrix}\cos\frac{\vartheta}{2} & -\sin\frac{\vartheta}{2}\\ \sin\frac{\vartheta}{2} & \cos\frac{\vartheta}{2}\end{pmatrix} \qquad \text{w.r.t. eigenvectors} \quad |1/2,\,1/2\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}
\end{aligned}$$

$$\rightsquigarrow \qquad d^{1/2}_{1/2,1/2} = d^{1/2}_{-1/2,-1/2} = \cos\frac{\vartheta}{2}$$

Properties of the rotation matrices: ... (Blackboard)

Example (Classical interpretation of the D-matrix): In the classical vector model, the angular momentum describes a vector with length $\sqrt{j(j+1)}$ and projection m that precesses around the quantization axis.

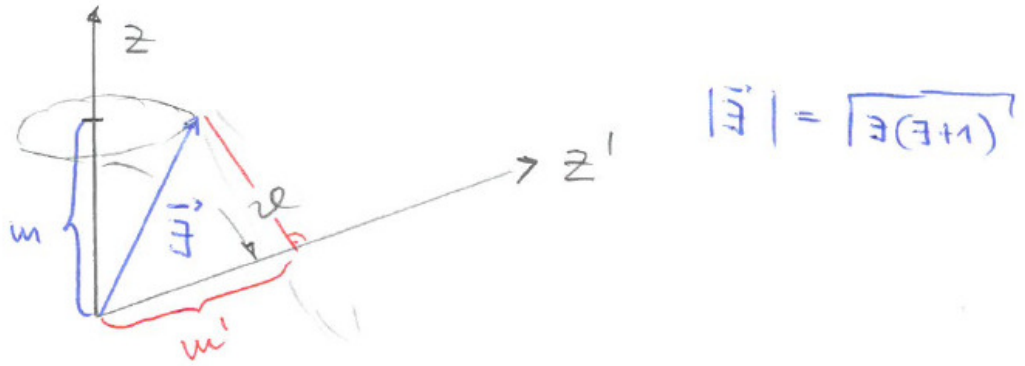


Figure 4.4.: Rotation of angular momentum in the classical vector model.

If we rotate the coordinates, the probability to find this vector with projection m' w.r.t. to the z'-axis is:

$$P \;=\; |\,\langle (jm')'\,|\,jm\rangle\,|^2 \;=\; |\,\langle jm'\,|R^+|\,jm\rangle\,|^2 \;=\; |D^j_{mm'}(\varphi,\vartheta,\chi)|^2 \;=\; |d^j_{mm'}(\vartheta)|^2$$

4.4. Wigner n–j symbols, etc.

4.4.a. Wigner 3–j symbols

➢ Wigner n–j symbols obey a high symmetry.

➢ Racah's expression (1942):

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta_{m_1+m_2+m_3,0}\,(-1)^{j_1-j_2-m_3}\;\Delta(j_1,j_2,j_3)$$
$$\times\,[(j_1-m_1)!\,(j_1+m_1)!\,(j_2-m_2)!\,(j_2+m_2)!\,(j_3-m_3)!\,(j_3+m_3)!]^{1/2}$$
$$\times\sum_l\left[\frac{(-1)^l}{l!\,(j_1+j_2-j_3-l)!\,(j_1-m_1-l)!\,(j_2+m_2-l)!\,(j_3-j_2+m_1+l)!\,(j_3-j_1-m_2+l)!}\right]$$

$$\Delta(a,b,c) = \left[\frac{(a+b-c)!\,(a-b+c)!\,(-a+b+c)!}{(a+b+c+1)!}\right]^{1/2}$$

This expression has a non-zero value only if the arguments of all factorials are non-negative integers.

➢ Symmetry of the Wigner 3–j symbols: under the exchange of two (columns of) angular momenta

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}$$
$$= (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix}$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

In total, there are known 12 classical and 60 additional symmetries with changes of the quantum numbers by $\pm 1/2$ due to Regge. Or, in other words, a Wigner 3–j symbol can be written and might have to be recognized properly in 72 different forms.

➢ Recursion relations for the Wigner3–j symbols: are listed by Rotenberg *et al.* (1959), eqs. (1.45)–(1.48). If we here assume $J = j_1 + j_2 + j_3$, one finds for instance:

[halfstep]-recursion: decreases two j-values by 1/2:

$$[(J+1)(J-2j_1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

$$= [(j_2+m_2)(j_3-m_3)]^{1/2} \begin{pmatrix} j_1 & j_2-1/2 & j_3-1/2 \\ m_1 & m_2-1/2 & m_3+1/2 \end{pmatrix} - [(j_2-m_2)(j_3+m_3)]^{1/2} \begin{pmatrix} j_1 & j_2-1/2 & j_3-1/2 \\ m_1 & m_2+1/2 & m_3-1/2 \end{pmatrix}.$$

[Louck]-recursion (1958): provides another 1/2-step recursion relation

$$(j_2+m_2)^{1/2}\,(2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_2-m_3 & -m_2 & m_3 \end{pmatrix}$$

$$= - [(J-2j_1)(J+1)(j_3+m_3)]^{1/2} \begin{pmatrix} j_1 & j_2-1/2 & j_3-1/2 \\ m_2-m_3 & -m_2+1/2 & m_3-1/2 \end{pmatrix}$$

$$- [(J-2j_3)(J-2j_2+1)(J+1)(j_3-m_3+1)]^{1/2} \begin{pmatrix} j_1 & j_2-1/2 & j_3+1/2 \\ m_2-m_3 & -m_2+1/2 & m_3-1/2 \end{pmatrix}.$$

4.4.b. Wigner 6–j and 9–j symbols

Apart from the Wigner 3–j symbols, one can define Wigner 6–j, 9–j or further $3n$–j symbols, which also obey high symmetries. For example:

$$\begin{Bmatrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{Bmatrix} = \sum_j (-1)^{2j} \begin{Bmatrix} j_{11} & j_{21} & j_{31} \\ j_{32} & j_{33} & j \end{Bmatrix} \begin{Bmatrix} j_{12} & j_{22} & j_{32} \\ j_{21} & j & j_{23} \end{Bmatrix} \begin{Bmatrix} j_{13} & j_{23} & j_{33} \\ j & j_{11} & j_{12} \end{Bmatrix}.$$

From the symmetry properties of the Wigner 6–j symbols (not shown here), one would see that the 9–j symbol is zero unless the arguments in each row and column satisfy the triangular relation.

4.4.c. Sum rules of the Wigner n–j symbols

The Wigner n–j symbols obey a very large number of sum rules which can be utilized to simplify the spin-angular integration in evaluating quantum many-particle matrix elements for systems with some rotational symmetry. An extensive list of such sum rules are given in the monograph by Varshalovich *et al.* (1988).

➢ Sum rules for one 3–j symbol: ... see, for instance, Varshalovich *et al.* (1988), eq. (12.1.2)

$$\sum_m (-1)^{j-m} \begin{pmatrix} j & j & j' \\ m & -m & m' \end{pmatrix} = [j]^{1/2}\ \delta_{m'0}\, \delta_{j'0}$$

and with $[a, b, ...] = (2a+1)(2b+1)...$.

➢ Sum rules for one 6–j symbol: ... for these and further rules, see Rotenberg *et al.* (1959), eqs. (2.9–10) and Varshalovich *et al.* (1988), eqs. (12.2.3–4).

$$\sum_X [X] \begin{Bmatrix} a & b & X \\ a & b & c \end{Bmatrix} = (-1)^{2c}\, \delta(a, b, c)$$

$$\sum_X (-1)^{a+b+X}\ [X] \begin{Bmatrix} a & b & X \\ b & a & c \end{Bmatrix} = [a, b]^{1/2}\ \delta_{c0}$$

➢ Sum rules for two 3–j symbols: ... see Rotenberg *et al.* (1959), eqs. (1.13–14).

$$\sum_{j_3,m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta(m_1, m_1')\, \delta(m_2, m_2')$$

$$\sum_{m_1,m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{\delta(j_3, j_3')\, \delta(m_3, m_3')}{(2j_3+1)}\ \delta(j_1, j_2, j_3)$$

➢ Sum rules for two 3–j symbols and one 6–j symbol: ... see Varshalovich *et al.* (1988), eq. (12.1.5).

$$\sum_{l_3,n_3} (-1)^{j_3+l_3+m_1+n_1}\ [l_3] \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ n_1 & m_2 & n_3 \end{pmatrix} \begin{pmatrix} j_1 & l_2 & l_3 \\ m_1 & n_2 & -n_3 \end{pmatrix}$$

$$= \sum_{m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & j_3 \\ n_1 & n_2 & -m_3 \end{pmatrix}$$

➢ Sum rules for three 6–j symbols: ... from Biedenharn and Elliot [see Rotenberg *et al.* (1959), eq. (2.8)].

$$\sum_X (-1)^{R+X}\ [X] \begin{Bmatrix} a & b & X \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & X \\ e & f & q \end{Bmatrix} \begin{Bmatrix} e & f & X \\ b & a & r \end{Bmatrix} = \begin{Bmatrix} p & q & r \\ e & a & d \end{Bmatrix} \begin{Bmatrix} p & q & r \\ f & b & c \end{Bmatrix}$$

with $R = a+b+c+d+e+f+p+q+r$.

➢ Sum rules for one 6–j symbol and three 9–j symbols: ... see Varshalovich *et al.* (1988), eq. (12.2.44)

$$\sum_{XYZ} [X,Y,Z] \begin{Bmatrix} a & b & X \\ c & d & Y \\ t & s & r \end{Bmatrix} \begin{Bmatrix} a & b & X \\ h & j & q \\ e & f & Z \end{Bmatrix} \begin{Bmatrix} k & l & p \\ c & d & Y \\ e & f & Z \end{Bmatrix} \begin{Bmatrix} p & q & r \\ X & Y & Z \end{Bmatrix}$$

$$= \begin{Bmatrix} k & l & p \\ h & j & q \\ t & s & r \end{Bmatrix} \begin{Bmatrix} k & h & t \\ a & c & e \end{Bmatrix} \begin{Bmatrix} l & j & s \\ b & d & f \end{Bmatrix}$$

4.5. The RACAH program in Maple

In atomic and nuclear structure theory, the evaluation and spin-angular integration of many-particle matrix elements is typically based on standard quantities like the matrix elements of the unit tensor, the (reduced) coefficients of fractional parentage as well as a number of other reduced matrix elements. These quantities occur very frequently in both, configuration interaction approaches and in many-body perturbation theory.

In the framework of the RACAH program (Fritzsche 1997; Fritzsche *et al.* 1998), we provide a set of MAPLE procedures for the manipulation and computation of such standard quantities in atomic theory. These (so-called) RACAH tools are designed for interactive work and appropriate for almost any complexity of expressions from Racah algebra; cf. Figure 4.5.

4.5.a. Selected symbols and functions in the RACAH program

The following (and several more) symbols and quantities from the theories of angular momentum and irreducible tensor operators are known to the RACAH program.

Figure 4.5.: Structure of a Racah expression, i.e. typical expressions which appear in Racah's algebra.

$$\text{Racahexpr} \;:=\; \sum_{j_1,\,j_2,\,l_1,\,\ldots} (-1)^{2j_1-j_2+\ldots}\; j_1^{3/2}\; [j_2]\ldots \begin{pmatrix} \cdot & \cdot & j_1 \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} j_1 & j_2 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{Bmatrix} \cdot & j_3 & \cdot \\ j_1 & \cdot & \cdot \\ J & \cdot & j_2 \end{Bmatrix} \ldots$$

$$\times \int d\Omega_1\, Y_{l_1 m_1}(\Omega_1)\, Y_{l_2 m_2}(\Omega_2) \int d\beta\; d^{j_3}_{p_3 q_3}(\beta)\; d^{j_4}_{p_4 q_4}(\beta')\; \ldots$$

Symbol	Designation	RACAH program
$\begin{pmatrix} a & b & c \\ m_a & m_b & m_c \end{pmatrix}$	Wigner 3–j symbol	Racah_w3j()
$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix}$	Wigner 6–j symbol	Racah_w6j()
$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}$	Wigner 9–j symbol	Racah_w9j()
$\langle a\ m_a,\ b\ m_b \,\vert\, c\ m_c\rangle$	Clebsch–Gordan coefficient	Racah_ClebschGordan()
$W(abcd;ef)$	Racah's W coefficient	Racah_Wcoefficient()
$d^j_{mm'}(\beta)$	Wigner $d^j_{mm'}(\beta)$ rotation matrix	Racah_dmatrix()
$D^j_{mm'}(\alpha,\beta,\gamma)$	Wigner's $D-$function	Racah_Dmatrix()
$U^j_{mm'}(\omega;\Theta,\Phi)$	Rotation matrix $U(\omega)$	Racah_Umatrix()
$Y_{lm}(\vartheta,\varphi)$	Spherical harmonic	Racah_Ylm()
$\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\cdot\cdot\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\}_{LM}$	Bipolar spherical harmonic	Racah_bipolarY()
$\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\cdot\cdot\{\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\cdot\cdot\mathbf{Y}_{l_3}(\vartheta_3,\varphi_3)\}_{l_{23}}\}_{LM}$	Tripolar spherical harmonic	Racah_tripolarY()
$\mathbf{Y}^{l}_{l_1 l_2}(\vartheta,\varphi)$	Vector spherical harmonic	Racah_vectorY()

Further remarks on the quantities above:

➢ Spherical harmonics: The $Y_{lm}(\theta,\phi)$ functions form a complete and orthonormal set on the unit sphere, and are therefore widely used in classical and quantum physics; the spherical harmonics frequently appear in the representation of wave functions for a wide range of physical systems, in the evaluation of the corresponding (quantum) matrix elements, and at many places elsewhere.

➢ Bipolar and tripolar spherical harmonics: When defined as *irreducible tensors*, linear combinations of products of p spherical harmonics often form a convenient basis to represent (distribution) functions in physics which depend on p vector directions. For this purpose, for instance, the *bipolar spherical harmonics* are defined as the irreducible tensor product of two spherical harmonics with different arguments (Varshalovich *et al.*, 1988)

$$\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\otimes\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\}_{LM} \;=\; \sum_{m_1 m_2}\langle l_1 m_1,\, l_2 m_2 \,|\, LM\rangle\; Y_{l_1 m_1}(\vartheta_1,\varphi_1)\, Y_{l_2 m_2}(\vartheta_2,\varphi_2)\;.$$

For different l_1, l_2, L, and M, the bipolar harmonics form a complete and orthonormal set

$$\int\int d\Omega_1 d\Omega_2\;\{\mathbf{Y}_{l_1}(\Omega_1)\otimes\mathbf{Y}_{l_2}(\Omega_2)\}^*_{LM}\;\left\{\mathbf{Y}_{l_1'}(\Omega_1)\cdot\cdot\mathbf{Y}_{l_2'}(\Omega_2)\right\}_{L'M'} \;=\; \delta_{l_1 l_1'}\,\delta_{l_2 l_2'}\,\delta_{LL'}\,\delta_{MM'}$$

of functions which depend on two unit vectors, say, $\mathbf{n_1}$ and $\mathbf{n_2}$, respectively. A similar definition also applies for the *tripolar spherical harmonic*

$$\left\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\otimes\left\{\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\otimes\mathbf{Y}_{l_3}(\vartheta_3,\varphi_3)\right\}_{l_{23}}\right\}_{LM}$$

$$= \sum_{m_1,m_2,m_3,m_{23}}\langle l_1 m_1,\, l_{23} m_{23}\,|\,LM\rangle\;\langle l_2 m_2,\, l_3 m_3\,|\,l_{23} m_{23}\rangle\; Y_{l_1 m_1}(\vartheta_1,\varphi_1)\, Y_{l_2 m_2}(\vartheta_2,\varphi_2)\, Y_{l_2 m_2}(\vartheta_3,\varphi_3)\;,$$

where, however, different coupling sequences are possible and have to be taken into account in applications.

➢ Tensor spherical harmonics: Following the standard coupling of two angular momenta, the tensor spherical harmonics are constructed as the product of the spherical harmonics $Y_{lm}(\vartheta,\varphi)$ (eigenfunctions of $\mathbf{l}^2$ and l_z) and the spin function χ_{sm} (eigenfunctions of $\mathbf{s}^2$ and s_z)

$$Y^{ls}_{jm}(\vartheta,\varphi) \;\equiv\; \{\mathbf{Y}_l\otimes\chi_s\}_{jm} \;=\; \sum_{m_l,m_s} Y_{lm_l}(\vartheta,\varphi)\,\chi_{sm_s}\;\langle lm_l,\; sm_s\,|\,jm\rangle$$

so that a irreducible tensor of rank j is obtained. While the l quantum number always occurs as a (nonnegative) integer, the indices j and s are both either integers or half-integers. For given j and s, the (orbital) angular momentum l can take the values $|j-s|,\;|j-s|+1,\;\ldots,\;j+s$;

the allowed values of m are $-j,\ -j+1,\ ...,\ j$. Similar to the spherical harmonics, which form a complete set of functions on the unit sphere, the tensor spherical harmonics $Y^{ls}_{jm}(\vartheta,\varphi)$ form a complete and orthonormal set of functions for the expansion of rank s spinors with the domain of arguments $0 \leq \vartheta \leq \pi$, $0 \leq \varphi \leq 2\pi$.

According to different definitions of the spin functions such as in a cartesian, spherical, or helicity basis representation, different components of the tensor spherical harmonics need to be distinguished.

➢ Spinor spherical harmonics: For the case $s = 1/2$, the tensor harmonics are also called spinor spherical harmonics

$$\Omega^{l}_{jm}(\vartheta,\varphi) \equiv Y^{l\frac{1}{2}}_{jm}(\vartheta,\varphi)$$

which are eigenfunctions of the operators $\mathbf{j}^2$, j_z, $\mathbf{l}^2$ and $\mathbf{s}^2$, where $\mathbf{s}$ is assumed to be the spin operator for $s = 1/2$. As for the tensor spherical harmonics, a number of different components need to be distinguished, including contravariant and covariant tensor components.

➢ Vector spherical harmonics: The other *special* case of tensor spherical harmonics are those for spin $s = 1$, i.e. the vector spherical harmonics

$$\mathbf{Y}^{l}_{jm}(\vartheta,\varphi) \equiv Y^{l1}_{jm}(\vartheta,\varphi)\ .$$

A large deal of representations, integrals, and algebraic relations are known for the vector sphercial harmonics which play an crucial role, for instance, in the quantum theory of light and in the current (hop) topic of laser-matter interactions.

4.6. Irreducible tensor operators. Wigner-Eckardt theorem

4.6.a. Irreducible tensor operators

Remember & definition:

$$|jm\rangle' = \sum_{m'} D^{j}_{m',m}(\varphi,\vartheta,\chi)\ |jm'\rangle \qquad \text{rotation of eigenstate}$$

$$T' = R_{\mathbf{n}}(\beta)\, T\, R^{-1}_{\mathbf{n}}(\beta) \qquad \text{rotation of general operator}$$

$$T^{'}_{kq} := \sum_{q'} D^{k}_{q',q}(\varphi,\vartheta,\chi)\, T_{kq'}$$

transformation of irreducible tensor operator (components)

An irreducible tensor operator is a set of $2k+1$ functions (tensor components) that transform like above, i.e. like the spherical harmonics.

Example ([Spherical] Scalar operators, T_{00}): ... just single component, invariant under rotations.

$$T^{'}_{00} = \underbrace{D^{0}_{00}(\varphi,\vartheta,\chi)}_{1}\, T_{00} = T_{00}$$

Example ([Spherical] Vector operators, $T_{1q},\ q = 0, \pm 1$): ... three vector components.

$$T'_{1q} \;=\; \sum_{q'} D^{1}_{q',q}(\varphi,\vartheta,\chi)\, T_{1q'}$$

Every cartesian vector $\mathbf{A} = (A_x, A_y, A_z)$ can be also considered as spherical tensor of rank one with the irreducible tensor components

$$T_{11} \;=\; -\frac{A_x + iA_y}{\sqrt{2}}, \qquad T_{10} \;=\; A_z, \qquad T_{1,-1} \;=\; \frac{A_x - iA_y}{\sqrt{2}} \qquad \text{since}$$

$$T_{1q} \;=\; |\mathbf{A}| \sqrt{\frac{4\pi}{3}} \cdot Y_{1q}(\vartheta,\varphi), \qquad \big(Y_{\ell m}(\bar{\vartheta},\bar{\varphi})\big)' \;=\; \sum_{m'} D^{\ell}_{m',m}(\varphi,\vartheta,\chi)\, Y_{\ell m}(\bar{\vartheta},\bar{\varphi})$$

4.6.b. Wigner-Eckart theorem

ME of irreducible tensor operators: ... (Blackboard)

Wigner-Eckart theorem & reduced ME:

➢ Definition of reduced ME:

$$\langle \alpha J \,\|\, T_K \,\|\, \alpha' J' \rangle \;:=\; \frac{1}{\sqrt{2J+1}} \sum_{mm'q} \langle J'm', Kq \,|\, Jm \rangle \; \langle \alpha Jm \,|\, T_{Kq} \,|\, \alpha' J'm' \rangle$$

$$\langle \alpha JM \,|\, T_{KQ} \,|\, \alpha' J'M' \rangle \;=\; \frac{1}{\sqrt{2J+1}} \; \langle J'M', KQ \,|\, JM \rangle \; \langle \alpha J \,\|\, T_K \,\|\, \alpha' J' \rangle$$

Wigner-Eckart theorem

This theorem shows that the matrix element $\langle \alpha JM \,|\, T_{KQ} \,|\, \alpha' J'M' \rangle$ can always be factorized into a Clebsch-Gordan coefficient (the geometrical part) and a reduced matrix element $\langle \alpha J \,\|\, T_K \,\|\, \alpha' J' \rangle$ which does not depend on the magnetic QN M, M', Q

➢ In short: Wigner-Eckart decomposition of ME = radial × effective interaction part.

Blackboard example (Eletric-dipole ME:):

5. Quantum measurements & correlations. Density operators

Reminder to axiomatic QM: ... (Blackboard)

5.1. Measurements in quantum mechanics

5.1.a. Indistinguisable quantum states

In QM, nonorthogonal states cannot be distinguished with 'certainty'.

Blackboard example (Determination of nonorthogonal states):

5.1.b. Projective measurements (von Neumann measurements)

➢ Measurement of some observable M with hermitian operator and the spectral decomposition

$$M = \sum_m m\, P_m, \qquad P_m \quad \text{... projectors upon the eigenspace with eigenvalue } m$$

➢ Probability to find this result and the state after the measurement are:

$$p(m) \;=\; \langle\psi\,|P_m|\,\psi\rangle \qquad\qquad \frac{P_m\,|\psi\rangle}{\sqrt{p(m)}}$$

Blackboard example (Action of $P_0 \otimes I$ and $I \otimes P_1$ upon two-qubit state):

Blackboard example (Y -gate operation and single-qubit measurement):

Properties of projective measurements: ... (Blackboard)

Example (Measurement of $Z \equiv \sigma_z$): Suppose we have $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \equiv |+\rangle$, then

- eigenvalue $+1$: $\langle\psi\,|\,0\rangle\,\langle 0\,|\,\psi\rangle = 1/2$
- eigenvalue -1 : $\langle\psi\,|\,1\rangle\,\langle 1\,|\,\psi\rangle = 1/2$

Blackboard example (Average value of a two-qubit operator):

5.1.c. POVM measurements

... positive operator-valued measure; non-negative eigenvalues or positive operator norm

POVM formalism:

➢ The POVM formalism provides a proper tool for analysing a measurement if the state (just) after the measurement is not important.

➢ Since the probability $p(m) = \langle\psi|M_m^+ M_m|\psi\rangle$ for the outcome m is positive, the operator

$$E_m = M_m^+ M_m \quad \Longrightarrow \quad \text{positive operator} \quad \Longrightarrow \quad \sum_m E_m = I, \qquad p(m) = \langle\psi|E_m|\psi\rangle .$$

➢ Therefore, any set of positive operators $\{E_m\}$ is sufficient to characterize a quantum measurement uniquely ... set of probabilities for possible outcomes of an experiment;

E_m ... POVM elements $\quad\Longrightarrow\quad$ $\{E_m\}$ ... POVM

➢ Especially, projective measurements also form a POVM $\{P_m\}$

$$E_m = P_m^+ P_m = P_m \quad \Longrightarrow \quad \sum_m P_m = I, \qquad P_m P'_m = \delta_{mm'} P_m$$

➢ Moreover, any set of positive operators $\{E_m\}$ with $\sum_m E_m = I$ also also form a POVM since:

$$M_m = \sqrt{E_m} \qquad \Longrightarrow \qquad \sum_m M_m^+ M_m = \sum_m E_m = I\,.$$

➢ Alternative definition: A POVM is a set of operators $\{E_m\}$ that are

(i) positive
(ii) fulfill the completeness relation $\sum_m E_m = I$

$\Longrightarrow$ $p(m) = \langle\psi\,|E_m|\,\psi\rangle$ probability for measuring outcome m

Example (POVM for a single qubit):

Let's consider the state $|\psi\rangle = \frac{2}{\sqrt{5}}|0\rangle + \frac{1}{\sqrt{5}}|1\rangle$. Instead of the projectors P_0 and P_1, we can apply the POVM formalism to determine the probabilities to find the outcomes 0 and 1. In fact, we can use

$$E_0 = P_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad E_1 = P_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

which fulfill $E_0 + E_1 = I$ and which have both the two eigenvalues 0 and 1 (i.e. they are positive semi-definite. The probabilities in the POVM formalism are then

$$\Pr(0) = \langle\psi\,|E_0|\,\psi\rangle = \frac{4}{5}, \qquad \Pr(1) = \langle\psi\,|E_1|\,\psi\rangle = \frac{1}{5}\,.$$

Example (Transmission of non-orthogonal states):

Alice sends to Bob either the state $|\psi_1\rangle = |0\rangle$ or $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$.

Question: Is it possible for Bob to distinguish which state he got send ?

Consider POVM elements

$$E_a = \frac{\sqrt{2}}{1+\sqrt{2}} |1\rangle\langle 1|, \qquad E_b = \frac{\sqrt{2}}{1+\sqrt{2}} \frac{(|0\rangle + |1\rangle)(\langle 0| + \langle 1|)}{2}, \qquad E_c = I - E_a - E_b$$

- If $|\psi_1\rangle = |0\rangle$, then $\langle\psi_1 |E_a| \psi_1\rangle = 0 \quad \Longrightarrow \quad$ if one measures outcome $E_a \quad \Longrightarrow \quad |\psi\rangle = |\psi_2\rangle$.
- Analogue: Outcome of $E_b \quad \Longrightarrow \quad |\psi\rangle = |\psi_1\rangle$.
- If outcome E_c is found, then no distinction is possible.

Remarks: ... (Blackboard)

Weak measurements: ... (Blackboard)

5.1.d. Mach-Zehnder interferometer

Mach-Zehnder: ... (Blackboard)

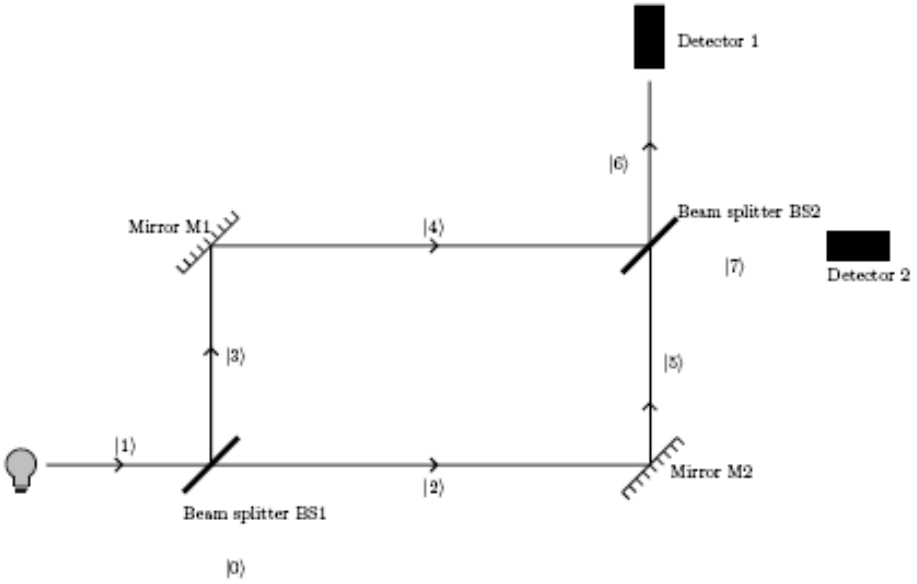


Figure 5.1.: The Mach-Zehnder interferometer. A photon is sent through a beam splitter and bounced off at two mirrors into another beam splitter. Mysteriously, only one of the detectors registers a photon.

5.2. Density matrices and operators

5.2.a. Ensemble of quantum systems

➢ Ensemble of pure states & density operator: The density operator formalism provides a suitable language if the state of a system is not completely known, for example

$$\{p_i,\ |\psi_i\rangle\} \quad \Longleftrightarrow \quad \begin{cases} p_i - \text{th part of ensemble in state } |\psi_i\rangle \\ \text{system in one of the states } \{|\psi_i\rangle\} \text{with probability } p_i. \\ p_i \text{ ... classical probability distribution;} \quad \sum_i p_i = 1 \end{cases}$$

The density operator is then given by:

$$\rho \;=\; \sum_i p_i \;|\psi_i\rangle\,\langle\psi_i| \;.$$

➢ Time evolution of a closed quantum system:

$$|\psi_i\rangle \;\longrightarrow\; U\,|\psi_i\rangle$$

$$\rho \;=\; \sum_i p_i \;|\psi_i\rangle\,\langle\psi_i| \;\longrightarrow\; \sum_i p_i\, U\;|\psi_i\rangle\,\langle\psi_i|\;U^+ \;=\; U\rho\,U^+$$

➢ Measurement with operator M_m on state $|\psi_i\rangle$:

$$p(m|i) \;=\; \big\langle\psi_i\,\big|\,M_m^+M_m\big|\,\psi_i\big\rangle \;=\; \mathrm{Tr}\,(M_m^+M_m\;|\psi_i\rangle\,\langle\psi_i|)$$

$$p(m) \;=\; \sum_i p(m|i)\,p_i \;=\; \sum_i p_i\,\mathrm{Tr}\,(M_m^+M_m\;|\psi_i\rangle\,\langle\psi_i|) \;=\; \mathrm{Tr}\,(M_m^+M_m\,\rho)$$

➢ State after the measurement:

$$|\psi_i^m\rangle \;=\; \frac{M_m\,|\psi_i\rangle}{\sqrt{p(m|i)}} \qquad\Longrightarrow\qquad \rho_m \;=\; \sum_i p(i|m)\;|\psi_i^m\rangle\,\langle\psi_i^m| \;=\; \sum_i p(i|m)\,\frac{M_m\,|\psi_i\rangle\,\langle\psi_i|\,M_m^+}{\langle\psi_i\,|\,M_m^+M_m\,|\,\psi_i\rangle} \;=\; \frac{M_m\,\rho\,M_m^+}{\mathrm{Tr}\,(M_m^+\,M_m\,\rho)}$$

➢ Notations: pure states vs. mixed states

$$\rho \;=\; |\psi\rangle\,\langle\psi| \qquad\qquad \rho \;=\; \sum_i p_i\;|\psi_i\rangle\,\langle\psi_i|$$

$$\mathrm{Tr}(\rho^2) \;=\; 1 \qquad\qquad \mathrm{Tr}(\rho^2) \;<\; 1$$

➢ Mixture of density operators: Any mixture is again a valid density operator ... since with

$$\rho_i \;=\; \sum_k q_k \,|\psi_{ik}\rangle\,\langle\psi_{ik}| \qquad\qquad \Longrightarrow \qquad\qquad \sum_i p_i\,\rho_i \;=\; \sum_k p_i q_k \,|\psi_{ik}\rangle\,\langle\psi_{ik}| \;=\; \sum_r p_r \,|\psi_r\rangle\,\langle\psi_r|$$

➢ In QI, the density matrix occurs especially in the description of composed systems and of decoherence processes that result from the (not controllable) interaction of some systems with its environment.

Formal definition of density operators:

➢ Beside of the ensemble interpretation of the density matrix, there is an independent definition that does not rely on the term of the state vector.

➢ An operator ρ is a valid density operator, i.e. the density operator for ensemble $\{p_i,\ |\psi_i\rangle\}$, if

- $\mathrm{Tr}(\rho) \;=\; 1$ (trace condition, normalization)
- ρ is a positive (and hermitian) operator

➢ Proof: If $\rho \;=\; \sum_i p_i \,|\psi_i\rangle\,\langle\psi_i|$, then

$$\mathrm{Tr}(\rho) \;=\; \sum_i p_i\,\mathrm{Tr}(|\psi_i\rangle\,\langle\psi_i|) \;=\; \sum_i p_i \;=\; 1$$

$$\langle\phi\,|\rho|\,\phi\rangle \;=\; \sum_i p_i\,\langle\phi\,|\,\psi_i\rangle\,\langle\psi_i\,|\,\phi\rangle \;=\; \sum_i p_i\,|\,\langle\phi\,|\,\psi_i\rangle\,|^2 \;\geq\; 0 \qquad\qquad \text{... positive}$$

$$\text{positive ...} \qquad \rho \;=\; \sum_j \lambda_j \,|j\rangle\,\langle j|\,, \qquad \begin{matrix}\{|j\rangle\}\ \text{... orthon.l}\\ \lambda_j \;\geq\; 0\ \text{... real}\end{matrix} \qquad \Longrightarrow \qquad \mathrm{Tr}\,(\rho) \;=\; \sum_j \lambda_j\,\mathrm{Tr}(|j\rangle\,\langle j|) \;=\; \sum_j \lambda_j \;=\; 1$$

ensembles $\{p_i,\ |\psi_i\rangle\}$ and $\lambda_j,\ |j\rangle$ have both density operator ρ

Example (Density matrix of a pure state):

Consider the state $|\psi\rangle = \frac{1}{2}|u_1\rangle + \frac{1}{\sqrt{2}}|u_2\rangle + \frac{1}{2}|u_3\rangle$. What is the corresponding density operator ?? And what is the trace of this operator ??

$$\begin{aligned}\rho = |\psi\rangle\langle\psi| &= \left(\frac{1}{2}|u_1\rangle + \frac{1}{\sqrt{2}}|u_2\rangle + \frac{1}{2}|u_3\rangle\right)\left(\frac{1}{2}\langle u_1| + \frac{1}{\sqrt{2}}\langle u_2| + \frac{1}{2}\langle u_3|\right) \\ &= \frac{1}{4}\left(|u_1\rangle\langle u_1| + 2\,|u_2\rangle\langle u_2| + |u_3\rangle\langle u_3|\right) \\ &\quad + \frac{1}{2\sqrt{2}}\left(|u_1\rangle\langle u_2| + |u_2\rangle\langle u_1| + |u_3\rangle\langle u_2| + |u_2\rangle\langle u_3|\right) + \frac{1}{4}\left(|u_1\rangle\langle u_3| + |u_3\rangle\langle u_1|\right) .\end{aligned}$$

As expected, we find $\mathrm{Tr}(\rho) = 1$.

Example (Test for being a valid density operator):

Does the matrix $\rho = \begin{pmatrix} \frac{1}{4} & \frac{1-i}{4} \\ \frac{1-i}{4} & \frac{1}{4} \end{pmatrix}$ represent a valid density operator ?? — Well, we find $\mathrm{Tr}(\rho) = 1$ ... but $\rho^+ = \begin{pmatrix} \frac{1}{4} & \frac{1+i}{4} \\ \frac{1+i}{4} & \frac{1}{4} \end{pmatrix} \neq \rho$. Since ρ is not hermitian, it does not represent a valid density operator.

Blackboard example (Expectation value of an operator):

Example (Probability for finding the $|-\rangle$ state):

Consider the $|\pm\rangle$ basis: What is (i) the projector upon the $|-\rangle$ in the computational basis ?? ..... And what is (ii) the probability to find the state $|-\rangle$ after an measurement of the state $|\psi\rangle = \frac{1}{\sqrt{5}}|0\rangle + \frac{2}{\sqrt{5}}|1\rangle$ in the diagonal basis ??

$$P_- = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \qquad \rho = |\psi\rangle\langle\psi| = \frac{1}{5}\begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}, \qquad p(-) = \mathrm{Tr}(P_-\,\rho) = \frac{1}{10}.$$

Completely mixed state ... (Blackboard)

5.2.b. Postulates of quantum mechanics for density operators

Postulate I (State space & density operators):

A scalar product space (Hilbert space) is associated with each quantum-mechanical systems. Every positive (and hermitian) operator ρ with $\mathrm{Tr}\,(\rho) = 1$, that acts in the state space, defines a possible state of the system. Especially, if the system is in state ρ_i with probablility p_i, then $\rho = \sum_i p_i\,\rho_i$.

Postulate II (Time evolution of closed systems):

Every (discrete) time evolution of a closed system can be described by a unitary transformation

$$\rho' = U\,\rho\,U^+ = U(t_2,t_1)\,\rho(t_1)\,U^+(t_2,t_1)$$

Postulate III (Quantum measurements and measurement operators):

Quantum measurements are described by a set of measurement operators $\{M_m\}$, that act in the state space and where m denotes the possible outcomes.

If, before the measurement, the system is in state ρ, then

- Probability for outcome m: $p(m) = \mathrm{Tr}(M_m^+ M_m \rho)$
- State after the measurement: $\frac{M_m \rho M_m^+}{\mathrm{Tr}\,(M_m \rho M_m^+)}$
- Completeness: $\sum_m M_m^+ M_m = I$

Postulate IV (Composite systems and entanglement):

The state space of a composed system is the product space of the state spaces of the subsystems; if the n subsystems are in the state $\{\rho_i,\ i = 1, .., n\}$, then the total state is:

$\rho_{\mathrm{tot}} = \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_n$ but, generally, ... $\rho_{\mathrm{tot}} \neq \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_n$

... for interacting systems

Advantages of the density-matrix concept:

➢ Incomplete knowledge about the system.

➢ Description of subsystems that should be considered independent of some total system.

Example (Post-measurement state): Let's consider again the state $\rho = \frac{3}{4}|+\rangle\langle+| + \frac{1}{4}|-\rangle\langle-|$, and a measurement in the computational basis $\{|0\rangle, |1\rangle\}$ which detects the state $|0\rangle$. How can we 'write' this within the density operator formalism ??

In the density operator formalism, the post-measurement state is given by $\rho \longrightarrow \frac{P_n \rho P_n}{\mathrm{Tr}(P_n \rho)}$; if expressed in the computational basis, we obtain

$$\rho = \frac{3}{4}\cdot\frac{1}{2}(|0\rangle+|1\rangle)(\langle 0|+\langle 1|) + \ldots = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{4}|0\rangle\langle 1| + \frac{1}{4}|1\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{4}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},$$

$$\rho^2 = \frac{1}{16}\begin{pmatrix} 5 & 4 \\ 4 & 5 \end{pmatrix}, \qquad \mathrm{tr}(\rho^2) = \frac{5}{8}$$

while the projector upon $|0\rangle$ is $P_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Therefore

$$\rho P_0 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 0| \quad\Longrightarrow\quad \mathrm{Tr}(\rho P_0) = \frac{1}{2}, \quad P_0\rho P_0 = \frac{1}{2}|0\rangle\langle 0| \quad\Longrightarrow\quad \rho \longrightarrow \frac{P_0\rho P_0}{\mathrm{Tr}(\rho P_0)} = |0\rangle\langle 0|\,.$$

Expectation value for measuring X

➢ Let's assume a measurement is made with respect to the observable X on the state $|\psi\rangle = \frac{1}{\sqrt{6}}|0\rangle + \sqrt{\frac{5}{6}}|1\rangle$.

➢ This means that a measurement is made with regard to the eigenstates of X: $|\pm\rangle$ with eigenvalues ± 1. The corresponding projectors and probabilities are

$$|+\rangle\langle +| = \frac{1}{2}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) \quad \Longrightarrow \quad \Pr(+1) = \langle\psi|P_+|\psi\rangle = \frac{6+2\sqrt{5}}{12}$$

$$|-\rangle\langle -| = \frac{1}{2}(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|) \quad \Longrightarrow \quad \Pr(-1) = \langle\psi|P_+|\psi\rangle = \frac{6-2\sqrt{5}}{12}$$

➢ Total probability & expectation value: $\Pr(+1) + \Pr(-1) = 1$, while $\langle X\rangle = (+1)\Pr(+1) + (-1)\Pr(-1) \approx 0.75$.

➢ For a single-qubit system, more generally, orthogonal projection operators are given by

$$P_\pm = \frac{I \pm \mathbf{n}\cdot\sigma}{2} \quad \Longrightarrow \quad \mathbf{n} = \mathbf{e}_x : \quad P_\pm = \frac{I \pm X}{2} = \frac{1}{2}(|0\rangle\langle 0| \pm |0\rangle\langle 1| \pm |1\rangle\langle 0| + |1\rangle\langle 1|) ,$$

again, the projectors upon the $|\pm\rangle$ states

5.2.c. Uniqueness of the density operator

Unitary freedom: ... (Blackboard)

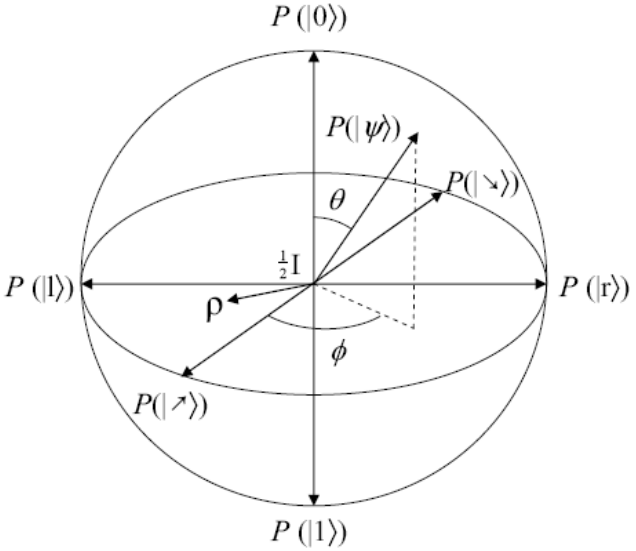


Figure 5.2.: Statistical operators represented in the unit Bloch ball, a real-valued representation of the space of qubit states via the expectation values, S_i, of the Pauli operators σ_i, $i = 1, 2, 3$. $P(|x\rangle) = |x\rangle\langle x|$. Orthogonal quantum states are antipodal in this representation; the 'conjugate bases' correspond to orthogonal axes. The pure qubit states $|\psi(\theta, \phi)\rangle$ lie on the periphery, known as the (Poincare-) Bloch sphere. The mixed qubit states, $\rho(r, \theta, \phi)$, lie in the interior and are weighted convex combinations of pure states. The maximally mixed state, $\frac{1}{2}I$, lies at the center of the ball, being an evenly weighted linear combination of any two orthogonal pure states. In the Poincare presentation that is often used in polarization optics, the sphere is rotated counterclockwise about the diagonal-basis axis by 90^o with respect to the one here; taken from ...

5.2.d. Bloch-sphere representation of qubits

Frequently applied qubit bases: ... (Blackboard)

Blackboard example (Stern-Gerlach filter):

5.2.e. Stokes parameters

Stokes parameters ... (Blackboard)

Blackboard example (Stoke's parameters of a single-qubit state):

Example (Pauli representation for two qubits):

$$\rho \;=\; \frac{1}{4}\sum_{ij} c_{ij}\,\sigma_i \otimes \sigma_j \qquad\qquad c_{ij} \;=\; \mathrm{Tr}(\rho(\sigma_i \otimes \sigma_j)); \qquad\qquad \rho \text{ is separable, iff } \quad |c_{11}| + |c_{22}| + |c_{33}| \;\leq\; 1.$$

5.2.f. Reduced density operators and partial trace

➢ Reduced density operator of subsystem A: ρ^{AB} ... density operator of two subsystems A and B; then

$$\rho^A \;=\; \mathrm{Tr}_B(\rho^{AB}) \qquad\qquad \text{partial trace over system } \; B$$

➢ Partial trace: density matrix ρ^{AB} of a composed systemwith respect to two orthonormal bases $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$,

$$\rho^{AB} \;=\; \sum_{ik}^{n_A}\sum_{jl}^{n_B} \rho_{ij,kl}\;|i_A\rangle\,|j_B\rangle\,\langle k_A|\,\langle l_B| \qquad\Longrightarrow\qquad \mathrm{Tr}_B\left(\rho^{AB}\right) \;=\; \sum_{ik}^{n_A}\left(\sum_{m}^{n_B}\rho_{im,km}\right)|i_A\rangle\,\langle k_A|\;.$$

The partial trace is independent of the basis $\{|j_B\rangle\}$ and, thus, suitable to describe observations and measurements for subsystem A.

➢ Reduced density matrix of a Bell state: Consider $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$; then

$$\rho = \frac{|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|}{2}$$

$$\rho_1 = \mathrm{Tr}_2(\rho) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{I}{2} = \rho_2 \qquad \Longrightarrow \qquad \mathrm{Tr}(\rho_1^2) = \mathrm{Tr}(\rho_2^2) = \frac{1}{2} \leq 1\,.$$

➢ Although the total system is in a pure state, the reduced density matrix of any subsystem represents in general a mixed state.

Example (Reduced density matrix of a product state): For $\rho^{AB} = \sigma \otimes \tau = \rho^A \otimes \rho^B$, we find

$$\rho^A = \mathrm{Tr}_B(\sigma \otimes \tau) = \sigma\,\mathrm{Tr}(\tau) = \sigma \qquad \text{... since} \quad \mathrm{Tr}(\tau) = 1\,.$$

5.2.g. Schmidt decomposition of pure states

➢ Schmidt decomposition: Suppose $|\psi\rangle = |\psi^{AB}\rangle$ is a pure state of a bipartite system AB. Then, there always exist orthonormal states $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$ so that

$$|\psi\rangle = \sum_i \lambda_i\, |i_A\rangle\, |i_B\rangle\,, \qquad \lambda_i \geq 0,\ \text{real}, \qquad \sum_i \lambda_i = 1$$

Schmidt coefficients λ_i

➢ Reduced density operators for subsystems A and B

$$\rho^A = \sum \lambda_i^2 \, |i_A\rangle \langle i_A| \,, \qquad \rho^B = \sum \lambda_i^2 \, |i_B\rangle \langle i_B| \,, \qquad \rho^A, \, \rho^B \quad \text{... with same eigenvalues } \{\lambda_i^2\}$$

(so-called) Schmidt bases $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$

➢ Schmidt number: Number of non-zero eigenvalues $\lambda_i > 0$ ... measure for entanglement between A and B.

➢ For composed systems:

$$|\psi^{AB}\rangle \text{ is product state; separable} \iff \mathrm{Tr}(\rho^{A^2}) = \mathrm{Tr}(\rho^{B^2}) = 1; \quad \text{Schmidt} - \text{No. is 1;} \quad \rho^A, \, \rho^B \text{... pure}$$

5.2.h. Purification of reduced density operators

➢ Given: ρ^A of a quantum system A.

➢ Look for pure state $|AR\rangle$ with: $\rho^A = \mathrm{Tr}_R(|AR\rangle \langle AR|)$.

This pure state is to be obtained from the 'composed' system A together with some chosen reference system R.

➢ Suppose,

$$\rho^A = \sum p_i \, |i_A\rangle \langle i_A| \qquad \text{and} \qquad \text{reference system R in same state space with basis } \{|i_R\rangle\}$$

$$|AR\rangle = \sum_i \sqrt{p_i} \, |i_A\rangle \, |i_R\rangle \; .$$

➢ Obviously,

$$\mathrm{Tr}_R(|AR\rangle\langle AR|) \;=\; \sum_{ik} \sqrt{p_i p_k}\; |i_A\rangle\langle k_A|\, |i_R\rangle\, \mathrm{Tr}(|i_R\rangle\langle k_R|) \;=\; \sum_i p_i\; |i_A\rangle\langle i_A| \;=\; \rho^A\,.$$

Apparently, there is a close relation between the Schmidt decomposition and the purification of states.
Schmidt basis of A is the same basis in which ρ^A diagonal is.

➢ However, pure state $|AR\rangle$ is not unique but pairs of such states are related to each other by some unitary transformation

$$|AR_1\rangle \;=\; (I_A \otimes U_R)\, |AR_2\rangle\;.$$

5.3. The EPR paradoxon and Bell's inequality

(Einstein, Podolsky und Rosen, 1935)

5.3.a. Bohr–Einstein debate (1926–35)

The Bohr-Einstein debate refers to a series of public disputes about quantum mechanics between Albert Einstein and Niels Bohr, and it was later summarized by Bohr in an article titled *Discussions with Einstein on Epistemological Problems in Atomic Physics.*

Historical remarks: ... (Blackboard)

5.3.b. EPR 'gedanken' experiment

➢ The idea of the EPR paper was to show that quantum mechanics is not a 'complete theory' in the sense that it provides only an imcomplete description of Nature.

➢ 'Elements of reality' (local realism):

- every complete theory must be able to predict the physical properties of an object with certainty.
- Physical events and measurements must be independent if they are causal unrelated to each other.

➢ Core value of EPR: Prior to a measurement, a property of the system does not have a definite or sharply defined value in QM.

➢ EPR experiment:

Alice		Charlie		Bob
$P_Q:\ Q=\pm 1$	$\longleftarrow$	source	$\longrightarrow$	$P_S:\ S=\pm 1$
$P_R:\ R=\pm 1$		produces equivalent pairs of particles		$P_T:\ T=\pm 1$

with P_X property and X the outcome of a measurement.

➢ How to interprete and understand such an experiment classically and quantum mechanically ??

Correlations of–entangled–Bell states: ... (Blackboard)

5.3.c. Classical vs. quantum mechancical 'anticorrelations' in the EPR experiment. Bell' inequalities

➢ Classical expectation value (average): Consider classical treatment of the outcomes Q, R, S, T as random variables with $p(q,r,s,t)$ as classical (discrete) probability distribution; this gives rise to the equation:

$$QS + RS + RT - QT = (Q+R)S - (Q-R)T = \pm 2\,.$$

$$E(QS+RS+RT-QT) = \sum_{qrst} p(q,r,s,t)\,(qs+rs+rt-qt) \leq 2\sum_{qrst} p(q,r,s,t) = 2$$

$$E(QS) + E(RS) + E(RT) - E(QT) \leq 2$$

Bell's inequality: Classical expectation for any experiment has an 'upper limit'.

➢ QM experiment:

Alice $\quad |\psi\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}} \quad$ Bob

$P_Q:\ Z_1 \quad \longleftarrow \quad$ source $\quad \longrightarrow \quad P_S:\ \dfrac{-Z_2 - X_2}{\sqrt{2}}, \qquad \langle QS\rangle = \left\langle \psi \middle| Z \otimes \left(\dfrac{-Z-X}{\sqrt{2}}\right) \middle| \psi \right\rangle$

$P_R:\ X_1 \qquad\qquad\qquad\quad P_T:\ \dfrac{Z_2 - X_2}{\sqrt{2}}, \qquad \langle RS\rangle = \left\langle \psi \middle| X \otimes \left(\dfrac{-Z-X}{\sqrt{2}}\right) \middle| \psi \right\rangle$

➢ expectation values: ... after some computation

$$\langle QS\rangle + \langle RS\rangle + \langle RT\rangle - \langle QT\rangle = 2\sqrt{2} \geq 2$$

Bell's inequality can be violated by an quantum mechanical experiment.

➢ Nature: Suitable chosen experiments confirm QM and are in clear conflict with the classical expectations.

Consequences of the violation of Bell's inequalities : ... (Blackboard)

5.3.d. Bipartite systems and the Bell basis

➢ Bipartite system ... two subsystems of Alice and Bob each have one member of an entangled pair of particles. The Hilbert space of the composite system is $H_A \otimes H_B$, and a basis for this systems is found by taking the tensor products $|a_i\rangle \otimes |b_j\rangle \equiv |a_i b_j\rangle$. Moreover, if the basis for Alice and Bob are both orthonormal, we have

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B, \qquad |a_i\rangle \otimes |b_j\rangle \equiv |a_i b_j\rangle \quad \text{... basis in } \mathcal{H}, \qquad \langle a_i b_j \,|\, a_k b_l\rangle = \delta_{ik}\,\delta_{jl}$$

$$\Pr(a_i b_j) = |\,\langle a_i b_j \,|\, \psi\rangle\,|^2, \qquad A = \sum_{ijkl} |a_i b_j\rangle\, \langle a_i b_j\,|A|\, a_k b_l\rangle\, \langle a_k b_l| = \sum_{ijkl} |a_i b_j\rangle\, \langle a_k b_l|\, A_{ijkl}$$

for the scalar product, probability and representation of an operator in this product basis.

➢ Bell basis for two-qubit systems:

$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \qquad |\beta_{01}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \qquad |\beta_{10}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}} \quad \text{(triplet state; can be symmetrized)}$$

$$|\beta_{11}\rangle = \frac{|10\rangle - |01\rangle}{\sqrt{2}} \quad \text{(singulet state; anti} - \text{symmetric)}$$

$$|\beta_{xy}\rangle = \frac{|0y\rangle + (-1)^x |1\bar{y}\rangle}{\sqrt{2}}, \qquad \bar{y} \text{ "not" } y \quad \begin{cases} x \text{ ... phase bit} \\ y \text{ ... parity bit} \end{cases} \qquad \text{... compact form}$$

Blackboard example ($Z \otimes Z \; |\beta_{xy}\rangle$):

Example (Is the state $H \otimes H \, |00\rangle$ entangled ??): No, since

$$H \otimes H \, |00\rangle = (H \; |0\rangle) \otimes (H \; |0\rangle) = |{+}{+}\rangle$$

However, this is much harder to 'see' if we would use the matrix representation; check it !

$$H \otimes H \, |00\rangle = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

5.3.e. Bell state representation of a two-qubit density operator

A two-qubit density operator that is diagonal with respect to the Bell states can be written in the form

$$\rho \;=\; \sum_{i,j=1,2} c_{ij}\; |\beta_{ij}\rangle\langle\beta_{ij}| \;=\; c_{00}\; |\beta_{00}\rangle\langle\beta_{00}| \;+\; c_{01}\; |\beta_{01}\rangle\langle\beta_{01}| \;+\; c_{10}\; |\beta_{10}\rangle\langle\beta_{10}| \;+\; c_{11}\; |\beta_{11}\rangle\langle\beta_{11}| \;.$$

The outer products in this expansion can be expressed also in terms of the Pauli matrices

$$|\beta_{00}\rangle\langle\beta_{00}| \;=\; \frac{1}{4}\,(I\otimes I \,+\, X\otimes X \,-\, Y\otimes Y \,+\, Z\otimes Z), \qquad |\beta_{01}\rangle\langle\beta_{01}| \;=\; \frac{1}{4}\,(I\otimes I \,+\, X\otimes X \,+\, Y\otimes Y \,-\, Z\otimes Z)$$

$$|\beta_{10}\rangle\langle\beta_{10}| \;=\; \frac{1}{4}\,(I\otimes I \,-\, X\otimes X \,+\, Y\otimes Y \,+\, Z\otimes Z), \qquad |\beta_{11}\rangle\langle\beta_{11}| \;=\; \frac{1}{4}\,(I\otimes I \,-\, X\otimes X \,-\, Y\otimes Y \,-\, Z\otimes Z)\,.$$

When expressible in this form, a density operator ρ is separable if and only if: $\quad c_{00} \;\leq\; \frac{1}{2}\;.$

5.4. Di'Vincenzo's criteria on physical requirements for quantum computing

In an important article in 2000, Di'Vincenzo proposed five criteria that any physical system should satisify in order to represent a viable quantum computer; cf. Salomaa and Nakahara, conference contribution, World Scientific Publishing, 2005).

Five (+ two) criteria for a successful realization of a quantum computer:

- ➢ A scalable physical system with well characterized qubits.
- ➢ Initializiation to a simple fiducial (and usually) pure state.

- ➢ Long decoherence times, much longer than the gate operation time.
- ➢ Universal set of quantum gates.
- ➢ A qubit-specific measurement capability.
- ➢ Ability to interconvert stationary and flying qubits.
- ➢ Ability to faithfully transmitting qubits between specified locations.

Details on the five (+ two) criteria for a realization of a quantum computer: ... (Blackboard)

There are numerous physical systems proposed as possible candidates for a viable quantum computer; they include

Physical realizations:

- ➢ Liquid-state/solid-state NMR
- ➢ Trapped ions
- ➢ Neutral atoms in optical lattice
- ➢ Cavity QED with atoms
- ➢ Linear optics
- ➢ Solid state (spin-based, charge-based)
- ➢ Josephson junctions (charge, flux, phase)
- ➢ Electrons on liquid helium surface
- ➢ Other "unique" realizations

Further reading (ARDA QIST roadmap:):

➢ This roadmap evaluates each of these realizations; see "A Quantum Information Science and Technology (QIST) Roadmap, Part 1: Quantum Computation" compiled by Advanced Research and Development Activity (ARDA), Los Alamos, USA. This article is updated annually.

5.5. Different models for quantum computing: A short overview

Promising models for quantum computing

➢ Quantum circuit model.

➢ "One-way" or measurement-based quantum computations (MBQC).

➢ Adiabatic quantum computations (AQC).

➢ Topological quantum computations (TQC).

➢ Quantum Programming Language.

Details on promising models for quantum computing ... (Blackboard)

6. Relativistic wave equations

Maxwell's equation in covariant form: ... (Blackboard)

6.1. Klein-Gordon (KG) equation

6.1.a. Heuristic approach

➢ Non-relativistic SE reflects the non-relativistic energy-momentum relation:

$$i\hbar\,\frac{\partial}{\partial t}\,\psi(\mathbf{r},t) \;=\; H_o\,\psi(\mathbf{r},t) \qquad \Longleftrightarrow \qquad H_o \;=\; \frac{\mathbf{p}^2}{2m}, \qquad \mathbf{p} \;=\; -i\hbar\,\boldsymbol{\nabla}, \qquad E \;=\; i\hbar\,\frac{\partial}{\partial t}$$

➢ Lorentz-covariant form:

- quadratic in p^μ , i.e. $E,\ \mathbf{p}$ $\rightsquigarrow$ Klein-Gordan equation
- linear in p^μ , i.e. $E,\ \mathbf{p}$ $\rightsquigarrow$ Dirac equation

➢ Relativistic momentum & energy-momentum relation:

$$p^\mu \;=\; \left(\frac{E}{c},\, \mathbf{p}\right)^T, \qquad p_\mu \;=\; \left(\frac{E}{c},\, -\mathbf{p}\right)^T, \qquad p_\mu\, p^\mu \;=\; \frac{E^2}{c^2} \;-\; \mathbf{p}^2 \;=\; m^2\, c^2$$

$$E_\pm \;=\; \pm\, E_{\mathbf{p}}, \qquad E_{\mathbf{p}} \;\equiv\; +c\,\sqrt{p^2 \;+\; m^2\, c^2} \;>\; 0, \qquad \mathbf{p} \quad \ldots\, 3-\text{momentum}$$

... solutions for positive energy $E_+ \;=\; E_{\mathbf{p}} > 0$ as well as for negative energy $E_- \;=\; -E_{\mathbf{p}} < 0$

➢ Physical interpretation: ... prediction of anti particles.

➢ Relativistic 4-momentum operator:

$$p^\mu \;\equiv\; \left(\frac{E}{c},\, \mathbf{p}\right)^T \;=\; \left(i\hbar\,\frac{\partial}{\partial(ct)},\, -i\hbar\,\boldsymbol{\nabla}\right)^T \;\equiv\; i\hbar\,\partial^\mu$$

$$\partial^\mu \;\equiv\; \frac{\partial}{\partial x_\mu} \;=\; \left(\frac{\partial}{\partial x_0},\, \frac{\partial}{\partial x_1},\, \frac{\partial}{\partial x_2},\, \frac{\partial}{\partial x_3}\right)^T \;\equiv\; \left(\frac{\partial}{\partial x^0},\, -\frac{\partial}{\partial x^1},\, -\frac{\partial}{\partial x^2},\, -\frac{\partial}{\partial x^3}\right)^T \;\equiv\; \left(\frac{\partial}{\partial(ct)},\, -\boldsymbol{\nabla}\right)^T$$

$$\partial_\mu \;\equiv\; \left(\frac{\partial}{\partial(ct)},\, \boldsymbol{\nabla}\right)^T \qquad \ldots \text{ nabla operator is covariant.}$$

➢ Equation quadratic in the 4-momentum (operator), i.e. the energy E and momentum $\mathbf{p}$:

$$p_\mu\, p^\mu\, \Psi(X) \;=\; m^2\, c^2\, \Psi(X), \qquad p_\mu\, p^\mu \;=\; (i\hbar)^2\, \partial_\mu\, \partial^\mu \;=\; -\hbar^2\, \Box, \qquad \Box \;\equiv\; \frac{1}{c^2}\,\frac{\partial^2}{\partial t^2} \;-\; \Delta$$

... we search for eigenfunctions $\Psi(X)$ with eigen values $p_\mu\, p^\mu \;\equiv\; m^2\, c^2$

➢ Klein-Gordan equation: of free (non-interacting) particles

$$-\left(p_\mu\, p^\mu \;-\; m^2\, c^2\right)\; \Psi(X) \;=\; \left(\hbar^2\, \Box \;+\; m^2\, c^2\right)\; \Psi(X) \;=\; 0$$

... transforms like a Lorentz scalar (i.e. Lorentz-invariant)

6.1.b. Solutions of the free Klein-Gordon equation

Solutions from plane-wave ansatz: ... (Blackboard)

6.1.c. Lagrange density of the KG equation & current density

➢ Lagrange density and Euler-Lagrange equation for the Klein-Gordan field

$$\mathcal{L}_{\rm KG} \;=\; \frac{(\hbar c)^2}{2}\left(\partial_\mu\, \Psi\, \partial^\mu\, \Psi \;-\; \frac{m^2 c^2}{\hbar^2}\, \Psi^2\right), \qquad 0 \;=\; \partial_\mu\, \frac{\partial\, \mathcal{L}_{\rm KG}}{\partial\, (\partial_\mu\, \Psi)} \;-\; \frac{\partial\, \mathcal{L}_{\rm KG}}{\partial \Psi}$$

➢ 4-current density and continuity:

$$\Psi^*\, \left(p^\mu\, p_\mu \;-\; m^2\, c^2\right)\, \Psi \;-\; \Psi\, \left(p^\mu\, p_\mu \;-\; m^2\, c^2\right)\, \Psi^* \;=\; \partial_\mu\, \left(\Psi^*\, \partial^\mu\, \Psi \;-\; \Psi\, \partial^\mu\, \Psi^*\right) \;=\; 0 \;\equiv\; \partial_\mu\, j^\mu$$

$$j^\mu \;=\; \left(\Psi^*\, \partial^\mu\, \Psi \;-\; \Psi\, \partial^\mu\, \Psi^*\right) \qquad 4-\text{current ensures continuity}$$

4-current describes charge density and current but no probability density.

➢ In particular, time-like component of j^μ does not represent a proper probability density

$$\mathbf{j} \;=\; (\Psi\,\boldsymbol{\nabla}\,\Psi^* \;-\; \Psi^*\,\boldsymbol{\nabla}\,\Psi) \qquad \text{... agrees with current density from SE}$$

$$\rho \;\equiv\; \frac{j^0}{c} \;=\; \frac{1}{c}\,(\Psi^*\,\partial_0\,\Psi \;-\; \Psi\,\partial_0\,\Psi^*) \;=\; \frac{1}{c^2}\left(\Psi^*\,\frac{\partial\Psi}{\partial t} \;-\; \Psi\,\frac{\partial\Psi^*}{\partial t}\right) \qquad \text{... not positive definite}$$

$$\rho_{\mathrm{SE}} \;=\; \psi^*\,\psi \;=\; |\psi|^2 \;\geq\; 0 \qquad \text{... different for SE}$$

6.2. Dirac equation

6.2.a. Heuristic derivation

➢ SE with linear combination of 3-momentum operator:

$$i\hbar\,\frac{\partial}{\partial t}\,\psi(\mathrm{r},t) \;\equiv\; E\,\psi(\mathrm{r},t) \;=\; \left(\sum_{i=1}^{3} c\,\alpha^i\,p^i \;+\; \beta\,mc^2\right)\,\psi(\mathrm{r},t) \;\equiv\; H_{\mathrm{D}}\,\psi(\mathrm{r},t)$$

Dirac equation & Dirac Hamiltonian H_{D} for a free particle

➢ Expansion coefficients α^i, $i = 1..3$, and β should fulfill the relativistic energy-momentum relation:

$$\begin{aligned}
\frac{\hat{E}^2}{c^2}\,\psi(X) \;&\equiv\; \frac{E^2}{c^2}\,\psi(X) \;=\; \left(\mathbf{p}^2 \,+\, m^2\,c^2\right)\,\psi(X) \\
&=\; \frac{1}{c^2}\,H_{\mathrm{D}}^2\,\psi(X) \;=\; \left(\sum_{i=1}^{3}\alpha^i\,p^i \,+\, \beta\,mc\right)\,\left(\sum_{k=1}^{3}\alpha^k\,p^k \,+\, \beta\,mc\right)\,\psi(X) \\
&=\; \left[\sum_{i,k=1}^{3}\alpha^i\,\alpha^k\,p^i\,p^k \,+\, mc\,\sum_{i=1}^{3}\left(\alpha^i\,\beta \,+\, \beta\,\alpha^i\right)\,p^i \,+\, m^2\,c^2\,\beta^2\right]\,\psi(X) \\
&=\; \left[\frac{1}{2}\,\sum_{i,k=1}^{3}\left(\alpha^i\,\alpha^k \,+\, \alpha^k\,\alpha^i\right)\,p^i\,p^k \,+\, mc\,\sum_{i=1}^{3}\left(\alpha^i\,\beta \,+\, \beta\,\alpha^i\right)\,p^i \,+\, m^2\,c^2\,\beta^2\right]\,\psi(X)
\end{aligned}$$

➢ Comparison of coefficients for (products of momentum) eigenvalues:

$$\alpha^i\,\alpha^k \,+\, \alpha^k\,\alpha^i \;\equiv\; \left\{\alpha^i,\,\alpha^k\right\} \;=\; 2\,\delta^{ik}, \qquad\qquad \alpha^i\,\beta \,+\, \beta\,\alpha^i \;\equiv\; \left\{\alpha^i,\,\beta\right\} \;=\; 0, \qquad\qquad \beta^2 \;=\; 1$$

➢ Possible representation of α^i $(i = 1..3)$ and β :

$$\alpha^i \;=\; \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad\qquad \beta \;=\; \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\,\mathbb{1}_2 \end{pmatrix},$$

Dirac representation of the matrices α^i $(i = 1..3)$ and β

6.2.b. Covariant form of the Dirac equation

Lorentz-covariant form of Dirac equation: ... multiply with β/c

$$i\hbar\,\beta\,\partial_0\,\psi(X) \;=\; \left(\sum_{i=1}^{3}\beta\,\alpha^i\,p^i \;+\; mc\right)\,\psi(X) \qquad \Longrightarrow \qquad (\gamma^\mu\,p_\mu \;-\; mc)\;\psi(X) \;=\; (i\hbar\,\gamma^\mu\,\partial_\mu \;-\; mc)\;\psi(X) \;=\; 0$$

$$\psi(X) \;=\; (\psi_1(X),\,\psi_2(X),\,\psi_3(X),\,\psi_4(X))^T \;\ldots\; \text{4-spinor}$$

Dirac's γ^μ matrices: ... (Blackboard)

4-spinors $\psi(X) \;\equiv\; \psi(\mathbf{r},t\,)$:

➢ Since γ^μ are 4×4 matrices, so also $\psi(X)$:

$$\psi \;=\; \begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}, \qquad \ldots \qquad \begin{array}{l} 4-\text{spinor, not Lorentz } 4-\text{vector}\\ \text{different transformation behaviour}\\ \text{Dirac equation transforms like } 4-\text{spinor}\end{array}$$

➢ Hermitian-conjugate 4-spinor vs. (Dirac-) adjoint 4-spinor:

$$\psi^{+} \;=\; \left(\,\psi_1^{*},\,\psi_2^{*},\,\psi_3^{*},\,\psi_4^{*}\,\right) \qquad \longleftrightarrow \qquad \bar{\psi} \;\equiv\; \psi^{+}\,\gamma^{0}, \qquad - \;=\; +o$$

$$\psi^{+}\,\psi \;=\; \left(\,\psi_1^{*},\,\psi_2^{*},\,\psi_3^{*},\,\psi_4^{*}\,\right) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \;=\; \sum_{\alpha=1}^{4} \psi_\alpha^{*}\,\psi_\alpha \;=\; \sum_{\alpha=1}^{4} \left|\psi_\alpha\right|^2 \;>\; 0 \qquad \text{... real number but NO Lorentz} - \text{scalar}$$

$$\bar{\psi}\,\psi \;=\; \psi^{+}\,\gamma^{0}\,\psi \qquad \text{real; Lorentz} - \text{scalar;} \qquad \bar{\psi}\,\gamma^{\mu}\,\psi \;=\; \psi^{+}\,\gamma^{0}\,\gamma^{\mu}\,\psi \qquad \text{Lorentz} - \text{vector}$$

$$\psi^{+}\,\psi \;\equiv\; \psi^{+}\,\mathbb{1}\,\psi \;=\; \psi^{+}\,\left(\gamma^{0}\right)^{2}\,\psi \;=\; \bar{\psi}\,\gamma^{0}\,\psi \qquad \text{transforms as time} - \text{like } 0 - \text{component of } 4 - \text{vector}$$

6.2.c. Lagrange density of the Dirac equation. Conservation of current

➢ Dirac-Lagrange density:

$$\mathcal{L}_{\mathrm{D}} \;=\; \bar{\psi}\,\left(\not{p}c \;-\; mc^2\right)\,\psi \;\equiv\; \bar{\psi}\,\left(i\hbar c\,\not{\partial} \;-\; mc^2\right)\,\psi$$

➢ 4-current density and continuity:

$$j^\mu \equiv c\,\bar\psi\,\gamma^\mu\,\psi, \qquad \partial_\mu\, j^\mu = 0 \qquad 4-\text{current}$$

$$\rho \equiv \frac{j^0}{c} = \bar\psi\,\gamma^0\,\psi = \psi^+\left(\gamma^0\right)^2\psi = \psi^+\psi \equiv \sum_{\alpha=1}^{4}|\psi_\alpha|^2 \geq 0 \qquad \text{probability density; cf. } \rho_{\text{SE}} \equiv |\psi|^2$$

$$\mathbf{j} = c\,\bar\psi\,\boldsymbol{\gamma}\,\psi = c\,\psi^+\gamma^0\,\boldsymbol{\gamma}\,\psi = c\,\psi^+\boldsymbol{\alpha}\,\psi \qquad \text{probability}-\text{current density}$$

6.2.d. Energies (spectrum) of the free Dirac equation

Use relativistic energy-momentum relation:

➢ Ansatz linear in 4-momentum p^μ transforms the Dirac equation into an algebraic equation

$$\psi(X) = \exp\left(-\frac{i}{\hbar}p^\mu x_\mu\right)\begin{pmatrix}a_1\\a_2\\a_3\\a_4\end{pmatrix} \qquad \Longrightarrow \qquad 0 = \left(\not{p} - mc\right)\begin{pmatrix}a_1\\a_2\\a_3\\a_4\end{pmatrix} \qquad \text{or, explicitly}$$

$$0 = \begin{pmatrix}\left(p^0-mc\right)\mathbb{1}_2 & -\boldsymbol{\sigma}\cdot\mathbf{p}\\ \boldsymbol{\sigma}\cdot\mathbf{p} & \left(-p^0-mc\right)\mathbb{1}_2\end{pmatrix}\begin{pmatrix}a_1\\a_2\\a_3\\a_4\end{pmatrix} = \begin{pmatrix}p^0-mc & 0 & -p^3 & -p^1+ip^2\\ 0 & p^0-mc & -p^1-ip^2 & p^3\\ p^3 & p^1-ip^2 & -p^0-mc & 0\\ p^1+ip^2 & -p^3 & 0 & -p^0-mc\end{pmatrix}\begin{pmatrix}a_1\\a_2\\a_3\\a_4\end{pmatrix}$$

linear & homogeneous equations for coefficients $(a_1,\, a_2,\, a_3,\, a_4)$

➢ Finding solutions for p^0 :

$$0 \;=\; \det{}_{4\times 4}\left(\begin{pmatrix} (p^0 - mc)\,\mathbb{1}_2 & -\boldsymbol{\sigma}\cdot\mathbf{p} \\ \boldsymbol{\sigma}\cdot\mathbf{p} & (-p^0 - mc)\,\mathbb{1}_2 \end{pmatrix}\right) \;=\; \det{}_{2\times 2}\left\{\left[-(p^0)^2 \,+\, m^2\,c^2\right]\,\mathbb{1}_2 \,-\, (\boldsymbol{\sigma}\cdot\mathbf{p})^2\,\mathbb{1}_2\right\}$$

$$(\boldsymbol{\sigma}\cdot\mathbf{p})^2 \;=\; \sum_{i,j=1}^{3} \sigma_i\,\sigma_j\,p^i\,p^j \;=\; \frac{1}{2}\sum_{i,j=1}^{3} \{\sigma_i,\,\sigma_j\}\,p^i\,p^j \;=\; \mathbf{p}^2\,\mathbb{1}$$

$$0 \;=\; \det{}_{2\times 2}\left\{\left[-(p^0)^2 \,+\, \mathbf{p}^2 \,+\, m^2\,c^2\right]\mathbb{1}_2\right\} \;=\; \left[-(p^0)^2 \,+\, \mathbf{p}^2 \,+\, m^2\,c^2\right]^2$$

➢ Four solutions for p^0 : ... $p^0_\pm$, each two-fold degenerate; relativistic energy-momentum relation.

$$p^0_\pm \;=\; \pm\frac{E_\mathbf{p}}{c} \;=\; \pm\sqrt{\mathbf{p}^2 \,+\, m^2c^2}$$

$$\begin{cases} p^0_+ & \text{... particles; electrons} \\ p^0_- & \text{... antiparticles; positrons} \end{cases}$$

6.2.e. Spin and helicity in the Dirac equation

Dirac particles at rest: ... (Blackboard)

➢ Spin operator: ... with proper form of $\mathbf{s}^2$

$$\mathbf{s}_\mathrm{D} \;=\; \frac{\hbar}{2}\begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \qquad \Longrightarrow \quad \mathbf{s}_\mathrm{D}^2 \;=\; \frac{\hbar^2}{4}\begin{pmatrix} \boldsymbol{\sigma}^2 & 0 \\ 0 & \boldsymbol{\sigma}^2 \end{pmatrix} \;=\; \frac{\hbar^2}{4}\begin{pmatrix} 3\cdot\mathbb{1} & 0 \\ 0 & 3\cdot\mathbb{1} \end{pmatrix} \;=\; \frac{3}{4}\,\hbar^2\,\mathbb{1} \;=\; \frac{\hbar^2}{2}\left(\frac{1}{2}+1\right)$$

$$s_{\mathrm{D},z}\,\mathbf{a}_\pm^{(1,2)} \;=\; \frac{\hbar}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}\mathbf{a}_\pm^{(1,2)} \;=\; \pm\,\frac{\hbar}{2}\,\mathbf{a}_\pm^{(1,2)}, \qquad \mathbf{a}_\pm^{(1)} \;\equiv\; \mathbf{a}_\pm^{(\uparrow)}, \qquad \mathbf{a}_\pm^{(2)} \;\equiv\; \mathbf{a}_\pm^{(\downarrow)}$$

... only applies in the rest frame with $\mathbf{p}=0$; otherwise more difficult.

➢ Particles and antiparticles have a well-defined spin projection in the rest frame because $H_\mathrm{D} \;=\; c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta\,mc^2 \;=\; \beta\,mc^2 \;=\; \gamma^0\,mc^2$, and thus, $[H_\mathrm{D},\,s_z] \;=\; [mc^2\,\gamma^0,\,s_z] \;=\; 0$ only in the rest frame.

$$\left[\gamma^0,\,s_{\mathrm{D},z}\right] \;=\; \frac{\hbar}{2}\begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}\begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \;\equiv\; 0$$

➢ For a (moving) frame, $\mathbf{p}\neq 0$, in general:

$$\left[\gamma^0,\,s_{\mathrm{D},z}\right] \;=\; 0, \qquad \left[\gamma^i,\,s_{\mathrm{D},z}\right] \;\neq\; 0 \qquad \Longrightarrow \qquad [H_\mathrm{D},\,s_{\mathrm{D},z}] \;=\; [c\boldsymbol{\alpha}\cdot\mathbf{p} \;+\; mc^2\,\beta,\,s_{\mathrm{D},z}] \;\neq\; 0$$

➢ Helicity operator: ... for moving frames;

$$s_{\mathrm{D},\mathbf{p}} \;\equiv\; \mathbf{s}_\mathrm{D}\cdot\frac{\mathbf{p}}{p} \qquad \text{... component of } \mathbf{s}_\mathrm{D}\,||\,\mathbf{p}$$

helicity characterizes the spin states for arbitrary values of $\mathbf{p}$

➢ Indeed, $[H_{\mathrm{D}},\, s_{\mathrm{D},\mathbf{p}}] \,=\, 0$ ... since

$$\gamma_5 \;\equiv\; i\,\gamma^0\gamma^1\gamma^2\gamma^3 \;=\; \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \qquad \gamma_5^2 \;=\; \mathbb{1}, \qquad \{\gamma_5,\, \gamma^\mu\} \;=\; 0 \quad \forall\, \mu \;=\; 0,1,2,3$$

$$\mathbf{s}_{\mathrm{D}} \;=\; \frac{\hbar}{2}\,\gamma_5\,\boldsymbol{\alpha} \;\equiv\; \frac{\hbar}{2}\,\gamma_5\,\gamma^0\boldsymbol{\gamma} \qquad \Longrightarrow \qquad s_{\mathrm{D},\mathbf{p}} \;=\; \frac{\hbar}{2p}\,\gamma_5\,\gamma^0\,\boldsymbol{\gamma}\cdot\mathbf{p} \qquad \text{... scalar product of } 3-\text{vectors}$$

$$[H_{\mathrm{D}},\, s_{\mathbf{p}}] \;=\; [\not{p} - mc,\, s_{\mathrm{D},\mathbf{p}}] \;=\; 0$$

$H_{\mathrm{D}},\, \not{p} - mc,\, s_{\mathrm{D},\mathbf{p}}$ have common set of eigenfunctions

6.2.f. Spinors with positive and negative energy

➢ Substitution of p^μ and $p^0_+ = E_\mathbf{p}/c$ in the Dirac equation gives:

$$0 = \begin{pmatrix} E_\mathbf{p}/c - mc & 0 & -p^3 & -p^1 + ip^2 \\ 0 & E_\mathbf{p}/c - mc & -p^1 - ip^2 & p^3 \\ p^3 & p^1 - ip^2 & -E_\mathbf{p}/c - mc & 0 \\ p^1 + ip^2 & -p^3 & 0 & -E_\mathbf{p}/c - mc \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

$$a_3 = c\,\frac{p^3 a_1 + (p^1 - ip^2)\,a_2}{E_\mathbf{p} + mc^2}, \qquad a_4 = c\,\frac{(p^1 + ip^2)\,a_1 - p^3 a_2}{E_\mathbf{p} + mc^2}$$

$$\mathbf{a}^{(1)}_+ = \mathcal{N}_+ \begin{pmatrix} 1 \\ 0 \\ \frac{c\,p^3}{E_\mathbf{p}+mc^2} \\ \frac{c\,(p^1+ip^2)}{E_\mathbf{p}+mc^2} \end{pmatrix}, \qquad \mathbf{a}^{(2)}_+ = \mathcal{N}_+ \begin{pmatrix} 0 \\ 1 \\ \frac{c\,(p^1-ip^2)}{E_\mathbf{p}+mc^2} \\ \frac{-c\,p^3}{E_\mathbf{p}+mc^2} \end{pmatrix}, \qquad \mathbf{a}^{(\alpha)+}_+ \mathbf{a}^{(\beta)}_+ = 2\,E_\mathbf{p}\,\delta_{\alpha\beta}, \quad \alpha,\beta = 1,2$$

➢ Often, normalization constant is chosen as $\mathcal{N}_+ = \sqrt{E_\mathbf{p} + mc^2}$:

$$u(\mathbf{p}, m_s) = \sqrt{E_\mathbf{p} + mc^2} \begin{pmatrix} \chi_{m_s} \\ c\,\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E_\mathbf{p}+mc^2}\,\chi_{m_s} \end{pmatrix}, \qquad m_s = \pm\frac{1}{2}, \quad \chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Dirac spinor of a free particle with positive energy and spin projection $m_s = \pm 1/2$

➢ Analogue solutions for $p^0_- = -E_{\mathbf{p}}/c$ and with normalization constant $\mathcal{N}_- \equiv \mathcal{N}_+ = \sqrt{E_{\mathbf{p}} + mc^2}$:

$$\mathbf{a}^{(1)}_- = \mathcal{N}_- \begin{pmatrix} c\,\frac{p^3}{E_{\mathbf{p}}+mc^2} \\ c\,\frac{p^1+ip^2}{E_{\mathbf{p}}+mc^2} \\ -1 \\ 0 \end{pmatrix}, \qquad \mathbf{a}^{(2)}_- = \mathcal{N}_- \begin{pmatrix} -c\,\frac{p^1-ip^2}{E_{\mathbf{p}}+mc^2} \\ c\,\frac{p^3}{E_{\mathbf{p}}+mc^2} \\ 0 \\ 1 \end{pmatrix}, \qquad \mathbf{a}^{(\alpha)+}_- \mathbf{a}^{(\beta)}_- = 2\,E_{\mathbf{p}}\,\delta_{\alpha\beta}, \quad \alpha,\beta = 1,2$$

➢ Here, one often introduces:

$$\eta_{-m_s} \equiv -i\sigma_2\,\chi_{m_s}, \qquad m_s = \pm\frac{1}{2}, \qquad \eta_{1/2} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \qquad \eta_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$v(\mathbf{p}, m_s) = \sqrt{E_{\mathbf{p}} + mc^2} \begin{pmatrix} c\,\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E_{\mathbf{p}}+mc^2}\,\eta_{-m_s} \\ \eta_{-m_s} \end{pmatrix}, \qquad m_s = \pm\frac{1}{2}$$

Dirac spinor of a free particle with negative energy and spin projection $m_s = \pm 1/2$

➢ Dirac equation for antiparticles with positive energy $cp^0_+ = +E_{\mathbf{p}}$: The signs in this solution are chosen so that:

$$\left(\not{p} + mc\right)\, v(\mathbf{p}, m_s) = 0 \qquad \Longleftrightarrow \qquad \left(\not{p} - mc\right)\, v(-\mathbf{p}, m_s) = 0$$

Dirac spinors $v(\mathbf{p}, m_s)$ describes antiparticle with energy $cp^0_+ = +E_{\mathbf{p}}$
. i.e. with well-defined 3-momentum $+\mathbf{p}$ and spin projection m_s .

General solutions: ... (Blackboard)

Relation between particle spinors $u(\mathbf{p}, m_s)$ and antiparticle spinors $v(\mathbf{p}, m_s)$: ... (Blackboard)

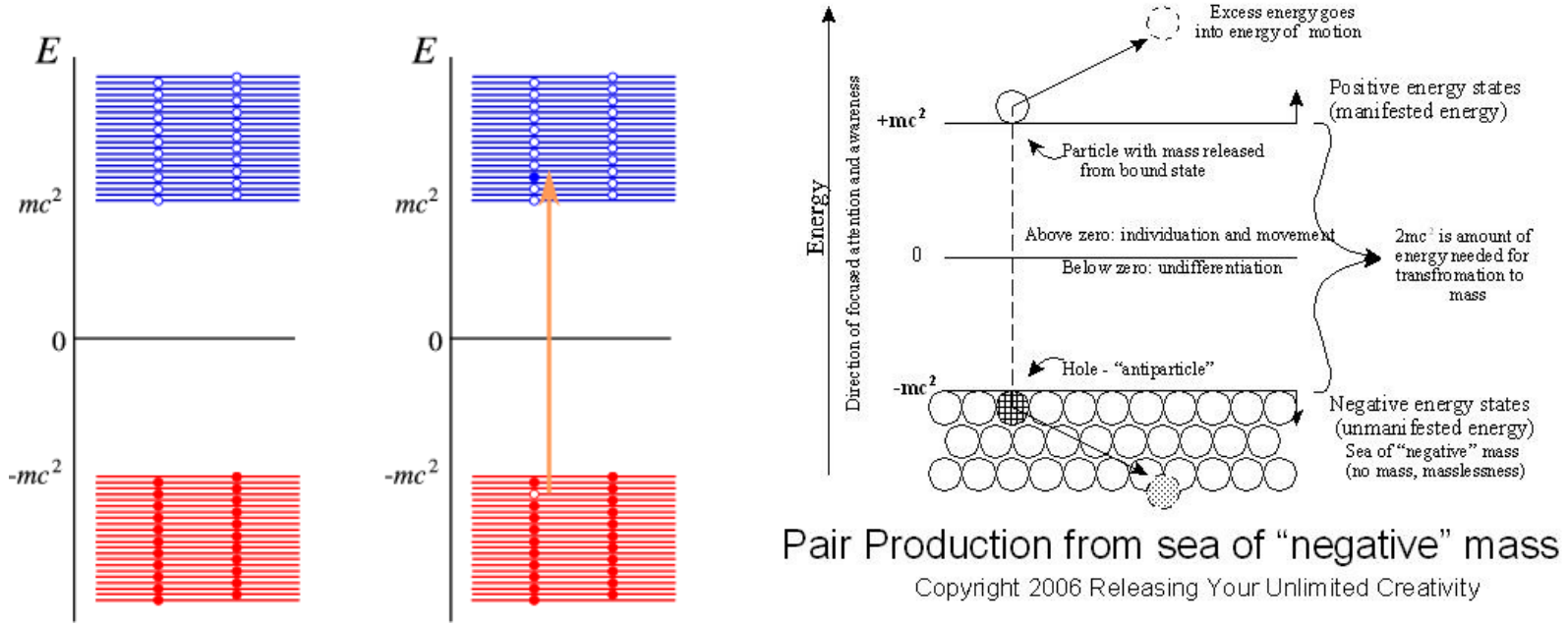


Figure 6.1.: Left: Dirac sea; right: When the particle is released, a hole is produced and that hole acts as an antiparticle.

6.2.g. Dirac's sea & hole theory

Remarks:

- ➢ Spontaneous decay should make vacuum unstable.
- ➢ Dirac 'sea': a vacuum state in which all negative-energy states are already filled by electrons; Pauli principle forbids the spontaneous decay.
- ➢ Infinite vacuum energy $\rightsquigarrow$ renormalization.
- ➢ Electron-positron creation and annihilation: particle-hole pairs; $\Delta E \geq 2mc^2$.
- ➢ Spontaneous pair creation and annihilation.

6.3. Conclusions on this lecture on QM

Richard Feynman: "Alle unsere Vorstellung in der Physik [verlangen] eine gewisse Dosis gesunden Menschenverstandes bei ihrer Anwendung; sie sind nicht rein mathematische oder abstrakte Vorstellungen."