

Computational Quantum Physics

— Lecture notes —

SS 2018

<http://www.atomic-theory.uni-jena.de/>
→ Teaching → Computational Quantum Physics

(Notes 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 misprint, etc. to s.fritzsche@gsi.de.

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0. Preliminary remarks

0.1. Schedule and agreements

Lecture period:	9. 4. 2018 – 13. 07. 2018
Lecture:	Mo 12 – 14, Max-Wien-Platz (Physik, SR 1)
Tutorial:	Mo 10 – 12, Computerpool, Physik (PAF)
Language:	German / English ??
ECTS points:	4 (inclusive the tasks and exam).
Exam:	Tasks (40 %), oral exam <u>or</u> a home task including some moderate programming.
Requirements for exam:	<i>Modulanmeldung</i> within the first 6 weeks; at least 50 % of the points from tutorials.
Home work:	Some discussion/collaboration on homework problems is encouraged; however, everyone should be able and turn in his/her written programs independently.
A few questions ahead:	Who has experience with programming ?? Which languages ?? ... Julia ?? Who makes regularly use of Maple oder Mathematica ?? Who has used the PAF computer pool before ??

0.2. Further reading

- G. Benenti, G. Casati and G. Strini: *Principles of Quantum Computation and Information; Volume I: Basic Concepts* (World Scientific, 2004).
- K. Blum: *Density Matrix Theory and Applications: Physics of Atoms and Molecules* (Plenum Press, New York, 1981, 1996).
- W. R. Johnson: *Atomic Structure Theory: Lectures on Atomic Physics* (Springer, Berlin, 2007).
- M. Metcalf, J. Reid and M. Cohen: *Fortran 95/2003 Explained: Numerical Mathematics and Scientific Computation* (Oxford University Press, Oxford, 2007).
- M. A. Nielsen and I. L. Chang: *Quantum Computation and Quantum Information* (Cambridge University Press, 2000 and later).
- W. H. Press et al.: *Numerical Recipes: The Art of Scientific Computing* (Cambridge University Press, Cambridge, 2007).
- B. Thaller: *Advanced Visual Quantum Mechanics* (Springer, Berlin, 2005).
- For Maple, moreover, you can find much material in the web: <http://www.maplesoft.com/applications/>

1. Computational physics & quantum mechanics: An overview

1.1. Scientific computing in 'physics'

Modelling physical systems by using computers:

- Solving systems of equations that **cannot be 'solved' analytically**; numerical simulations of physical systems in space and time.
- **Computational physics is often considered as a third 'pillar' of physics.**
- Many subfields of physics make heavily use of computations (dynamics of solar systems, galaxies, etc.; fluid dynamics & turbulence; molecular dynamics of fluids & gases; solving Maxwell's equations; statistical mechanics of polymers; magnetic systems, ...)
- Most of you will need to do some computational work, especially also in theoretical physics.
- **Recommendation:** Gain some proficiency in scientific computing.

1. Computational physics & quantum mechanics: An overview

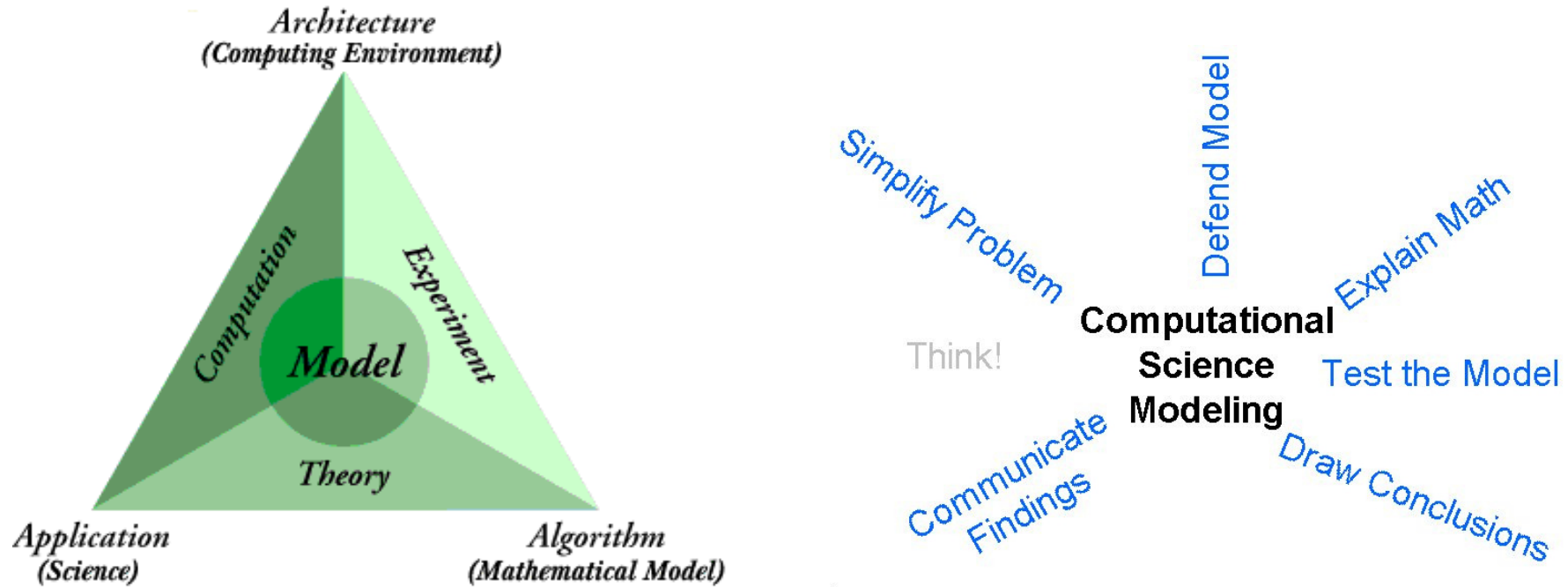


Figure 1.1.: Left: Interplay of experiment, theory and computations in science (taken from www.shodor.org/chemviz/overview). Right: Abilities to be trained in order to make use of this interplay (from www.ncsec.org/cadre2/)

1.2. Modern fields of (theoretical) quantum physics

Well-established fields of quantum physics:

- Quantum field theory (QFT: QED, QCD, string theory).
- Quantum many-body theory (nuclear structure, electronic structures of atoms and molecules, quantum chemistry).
- Quantum scattering & collision theory (nuclear reactions, atom-ion and atom-molecule collisions, electron-atom and

electron-molecule collisions, etc.).

- Solid-state theory (band structures, density functional theory, magnetism, spin chains, ...).
- Quantum optics (Rabi oscillations, field amplitudes, EIT, coherent states, ...).

Recently emerging fields:

- Quantum control theory.
- Quantum engineering (generation, tomography and use of quantum states, ...).
- Quantum information theory and processing.
- Light-matter interactions with single photons and twisted light (cavity-QED, ...).
- Metamaterials (negative refraction indices, ...).
- Electron transfer theory and photosynthesis in complex molecules.
- Parity non-conservation and electric-dipole moments.
- Ultra-cold atoms and molecules (Bose-Einstein condensation, astro chemistry, ...).
- Strong-field electron dynamics.
- ...

1.3. Programming languages in physics

1.3.a. Programming languages used in physics

- It is almost impossible to ‘overview’ all the computational languages and tools, presently available.
- Languages for doing numerics: Fortran 77/90/2008, Pascal, C, C++, Julia, ...
- Languages for scripting: python, perl, R, ...
- Computeralgebra & symbolic computations: Reduce, Maple, Mathematica, ...

High-level programming (HLP) languages; properties:

- In computer science, a programming language with strong abstraction from the details of the computer.
- HLP languages may use natural language elements or may automate (or even hide entirely) significant areas of computing systems (e.g. memory management).
- They simplify the development a programs; good readability.
- Amount of abstraction decides how “high-level” a programming language really is.
- A HLP language must always be translated into machine language by a compiler or interpreter.

The Fortran 90/2008 programming language:

- Fortran has evolved since the early days of computing (formula translation); it was introduced in 1957 and remains in many scientific computing environments the language of choice.
- Fortran 90/2008 is a quite modern programming language.
- Many useful features for scientific (numerical) computing (dynamic allocation; derived data types; modules, kind parameters, recursive subroutines, pointers, manipulation of entire arrays, ...);

- Widely used language in computational science ... but also still in engineering, etc.
- Simple control of different data types and accuracy of computations;
- Many intrinsic functions and protection of code; also **intrinsic feature for parallelization**.
- **Object-oriented features: Abstract data types – Polymorphism – Hidden code**; it misses inheritance.
- **Relatively easy to learn**;
- Many commercial and open-source compilers available; gfortran; free open source Fortran 90/95/2003/2008 compiler;
- **Disadvantages**: Case insensitive; different tricks still possible; not very strict, ...
- Enforce declarations with the **implicit none** statement; this help avoid a large fraction of all programming errors.

Some reasons for using C++:

- C++ is now one of the dominating language in Unix and Windows environments.
- It is widely available and is the language of choice for system programmers.
- C++ is very widespread for developments of non-numerical software; the C++ syntax has inspired lots of popular languages, such as Perl, Python, Java and Julia.
- Complex variables, one of Fortran's strongholds, can now also be defined in the new ANSI C++ standard.
- C++ is an object-oriented language, in contrast to C and Fortran, i.e. it supports three fundamental ideas: namely objects, class hierarchies and polymorphism.

Julia – A fresh approach to technical computing:

- Faster than other scripting languages ... as fast as C/Fortran.
- Supports rapid code development like with Python/MATLAB/R.

1. Computational physics & quantum mechanics: An overview

- Just-In-Time (JIT) compilation.
- Type-stability through [multiple-dispatch](#) allows to make efficient code.
- Built-in documentation; ? gets you to the documentation for a type, function, etc.
- Julia stands for the [combination of productivity and performance](#) through a careful language design and carefully chosen technologies.
- [Multiple dispatch](#): refers to the dynamically selected implementation and to the concept of running the right code at the right time.
- [Julia's type system](#): ... supports an aggressive code specialization against run-time types.

1.3.b. Good coding practices

- [Keep the code simple ... and always well readable.](#)
- [Use a proper set of name conventions](#) ... and maintain them uniformly throughout.
- Provide a brief description of what a variable is for and what a block of code is doing; don't be extensive and don't comment obvious issues.
- Correct errors as they occur.
- Portability.
- The size of a program has a very significant effect on error rates, programmer productivity, and the amount of management needed.
- [Physical models](#): In general, better physics is more important than better computer science.
- [Visualization](#): Visualization of large data sets is essential for debugging, problem generation and analysis of results.

- **Quality tests:** If a code is not verified and validated by proper examples, the users will not believe and see its connection to reality.
- McConnell's advice: "Every programming language has strengths and weaknesses. Be aware of the specific strengths and weaknesses of the language you're using."

A personal view [cf. Hoare (2002)]:

- Readability of the code; save your (and other people's) time with regard to mis-assignments and tricks.
- Simplicity of use.
- Keep programs modular.
- Ruggedness (difficult to misuse, kind to errors); stop when certain errors are not 'treated' internally.
- Clear, accurate, and precise user documentation.
- Reliability – efficiency – portability – parallelism.

1.4. Computer-algebra systems (CAS)

Symbolic computations:

- Computer Algebra studies the algorithms for Symbolic Computations in which one computes with symbols, rather than with numbers.
- In physics, we are mainly concerned with the practical aspects of how to use Symbolic Computations in order to solve practical mathematical problems (from QM).

1. *Computational physics & quantum mechanics: An overview*

- In CAS, the numbers are not limited to the hardware integers or floating-point numbers but can be made up of symbols, such as π , $\sqrt{2}$ or continuous fractions.
- CAS are essentially **equation crunchers** (in analogy with the number crunching algorithms of numerical analysis).
- Integration is one of the highlights of general-purpose CAS.

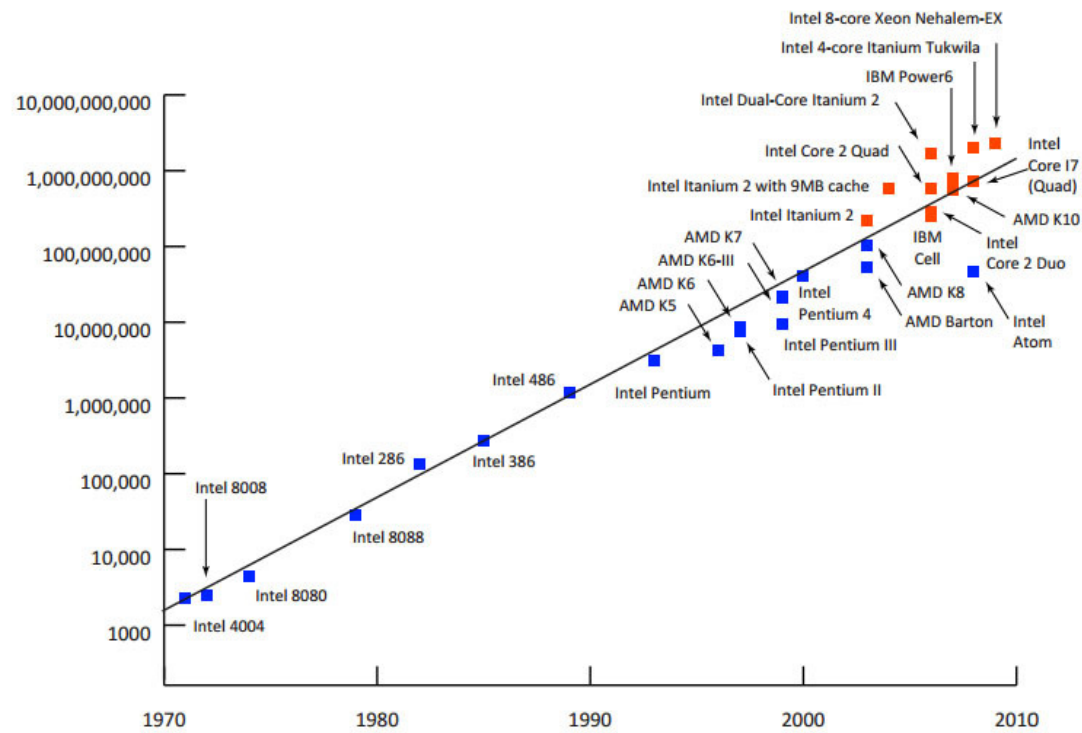


Figure 1.2.: Moore's law in term of transistors as realized on individual processor ships(from wrapidconsultingusa.com/wp-content/).

1. Computational physics & quantum mechanics: An overview

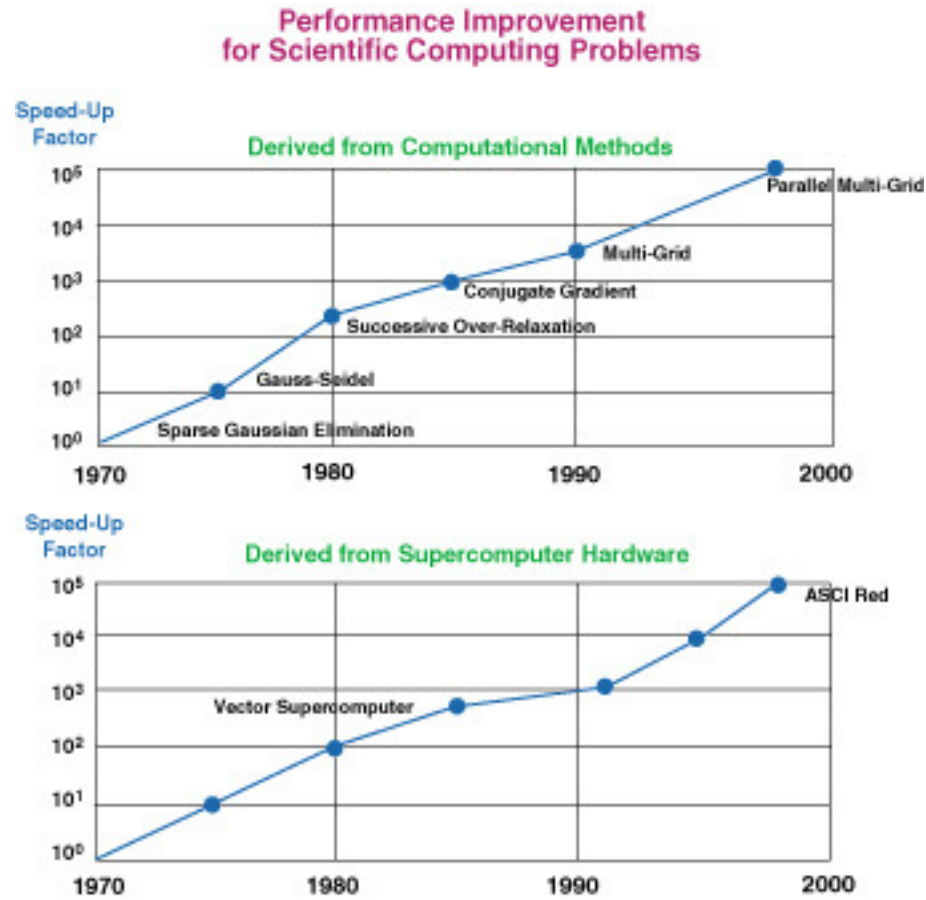


Figure 1.3.: Moore's law in term of the speed-up factor as derived from the computational methods (top panel) and the hardware of supercomputers (lower panel).

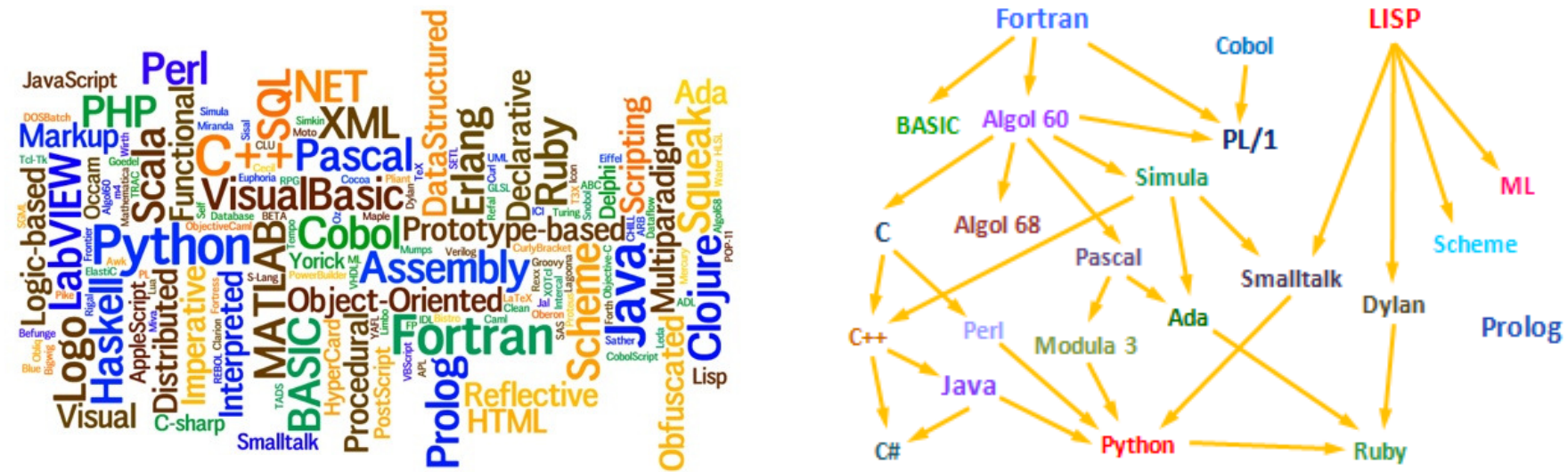


Figure 1.4.: Left: Collection of different languages, indicating the popularity (taken from blog.startapp.com/wp-content/). Right: Historical dependence of some languages (from xrds.acm.org/images)

1. Computational physics & quantum mechanics: An overview

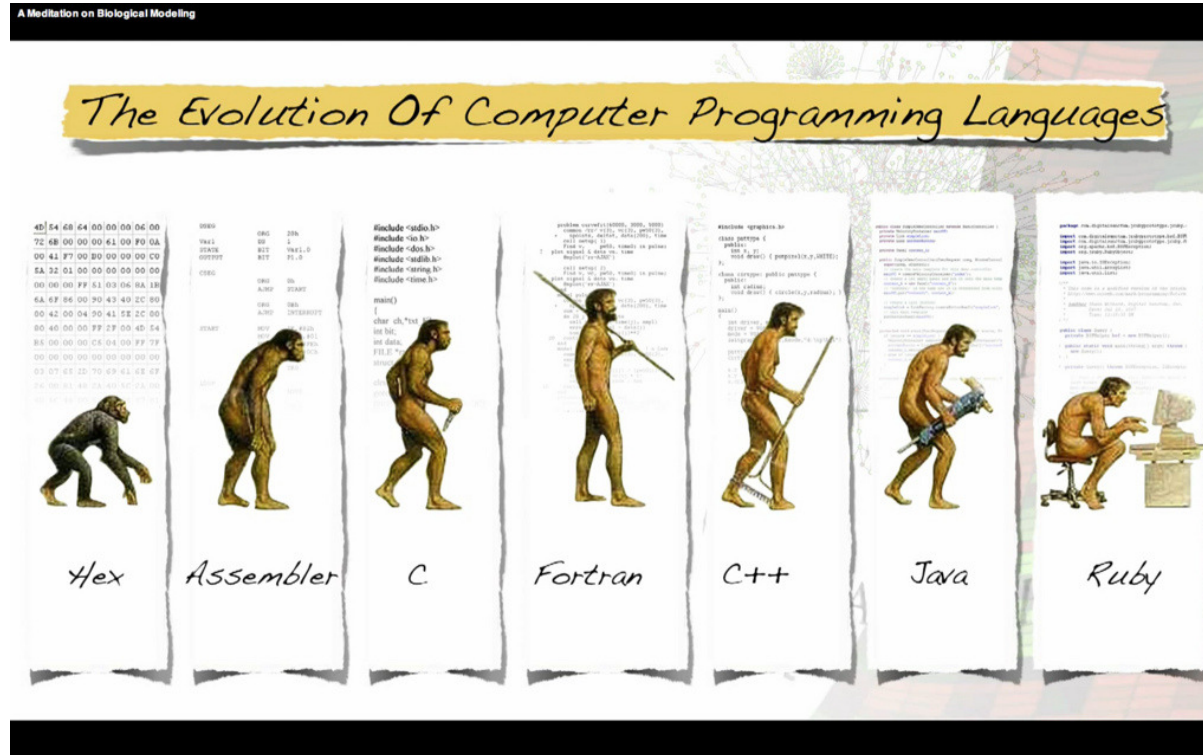


Figure 1.5.: The Evolution of Computer Programming Languages (from: ganeshkamath89.blogspot.com).

2. Julia & Maple: Some first tutorials

2.1. What is Julia standing for ??

- Julia stands for the **combination of productivity and performance** through a careful language design and carefully chosen technologies; it never forces the user to resort to C or Fortran for fast computations.
- Julia's design allows for **gradual learning of modern concepts in scientific computing**; from a manner familiar to many users and towards well-structured and high-performance code.
- **High-level languages**: Most traditional high-level languages are hampered by the overhead from the interpreter and which typically results into more run-time processing that are strictly necessary. One of these hindrances is (missing) type information, and which then results in the request for supporting vectorization.
- **Julia is a 'verb'-based language** in contrast to most object-oriented 'noun'-based language, in which the generic functions play a more important role than the datatypes.
- **Code selection**: Julia name space allows the use of the same vocabulary in different circumstances, and which makes programs easier to read.
- **Multiple dispatch**: refers to the dynamically selected implementation and to the concept of running the right code at the right time. This is achieved by overloading by multiple-argument function, a very powerful abstraction. Multiple dispatch makes it easier to structure the programs close to the underlying science.

2. Julia & Maple: Some first tutorials

- Instead of encapsulating methods inside classes, Julia's multiple dispatch is a paradigm in which methods are defined on combinations of data types (classes). Julia shows that this is remarkably well-suited for numerical computing.
- **Code re-use:** In good language design, one should be able to write a general implementation and, as long as the necessary operations are available, the code should just work.
- **Julia's type system:** Julia's expressive type system that allows optional type annotations; this type system supports an aggressive code specialization against run-time types. Over a large extent, however, Julia code can be used without any mentioning of types (in contrast to C and Fortran); this is achieved by data-flow interference.
- **Parallelization:** One of the central motivations to build Julia was the design of a parallel computing language.
- **Performance:** There are helpful macros, such as `@timing function_call(parameters)` or `@benchmark function_call(parameters)` to analyze the performance of the program and to find (and resolve) bottlenecks.
- **LAPACK:** All of LAPACK is available in Julia, not just the most common functions. LAPACK wrappers are fully implemented by 'ccall' and can be called directly from the Julia prompt.
- **Macros:** A macro is a function that runs at parse time. It takes symbolic expressions in and returns transformed expressions out, which are inserted into the code for later compilation. The output of macros is often 'inlined' into the code.

2.2. What is Maple standing for ?

Maple's internal set-up and organization:

- Maple consists of four parts: kernel, interface, library, and share library.
- While, for efficiency reasons, most kernel routines are written in C, the procedures in the library are written in the language of Maple and can be viewed: `interface(verboseproc=3);` and, for example, `print(factor);`

- A strong features of Maple is their worksheet: This can be seen a regular text document that is enhanced with computational features like a spreadsheet, or with layers and links like hypertext.
- A worksheet can be organized in sections and subsections as we would structure a technical report (see insert menu).
- An execution group in Maple is a sequence of instructions to be executed as one (similar like a paragraph).
- After loading, the worksheet is considered as plain text. We must execute the instructions (via Execute from the edit menu) to give values to the variables; the execution of an entire worksheet is analogue to running a program.
- Maple has many **composite data types** and a seemingly huge number of commands; **each command can be considered also as part of the language that enables one to built up commands at higher complexity.**
- Maple is organized in packages; instead of loading an entire package, one can always use the long form, e.g., `plots[display](...)` when only the display command from the plots package is needed.
- The internal work and memory management of Maple can be affected by `interface()`.
- There is a large library of user contributions, available online at the [Maple Application Center](http://www.mapleapps.com)
<http://www.mapleapps.com>.

2.2.a. Getting started

Web link (Some useful Maple tutorials:):

- A first Maple tutorial from the University of New South Wales (Australia):
www.maths.unsw.edu.au/sites/default/files/maplenotes.pdf
- Basic worksheets can be find at: www.peterstone.name/Maplepgs/intro.html
- Maple's Applications Center: www.maplesoft.com/applications/index.aspx/

2.2.b. Packages for Maple

Libraries & toolboxes

- There are about 120 packages and toolboxes that belong to Maple's standard distribution; among them you can find:
- **ArrayTools** – tools used for low level manipulation of Matrices, Vectors, and Arrays.
- **CodeGeneration** – tools for translating Maple code to other languages.
- **CurveFitting** – commands that support curve-fitting.
- **eBookTools** – tools to convert Maple worksheets into a book using DocBook.
- **GraphTheory** – routines for creating, drawing, manipulating, and testing graphs.
- **Maplets** – tools to create graphical user interfaces for Maple.
- **Matlab** – commands to facilitate a Matlab Link.
- **PDEtools** – tools for solving partial differential equations.
- **Physics** – a package implementing the standard mathematical physics computational objects and their operations.
- **plots** – commands for displaying graphical representations.
- **ScientificConstants** – access to physical const. and Periodic Table Element properties.
- **Student** – collection of packages covering undergraduate mathematics courses.
- **Units** – commands for converting values between units, and environments for performing calculations with units.
- **VectorCalculus** – commands for performing multivariate and vector calculus operations.

3. Quantum mechanics in finite-dimensional Hilbert spaces

3.1. Spin-1/2 quantum systems & quantum information processing

3.1.a. Need and promises of quantum computations

Computers must obey the laws of physics:

- A **computer is always a physical device** that helps us process information by executing algorithms. An **algorithm** is a finite procedure that realizes an information-processing task.
- Computers allow an efficient storage, exchange and processing of information. An information-processing task can always be translated into a physical task.
- The main difference between classical and quantum information arises from the difference between a (classical) **bit** and a **qubit**, i.e. the capability what can be represented by the corresponding physical units (systems) that are utilized to store these (qu)bits.
- Quantum Information Processing (QIP) considers how quantum physics and quantum computers can be utilized in order **to solve certain problems more efficiently than can be done with classical computers.**
- R. P. Feynman, Int. J. Theoret. Phys., 21 (1982) 467: **“Quantum Mechanics cannot be simulated efficiently on a classical PC !”**

3. Quantum mechanics in finite-dimensional Hilbert spaces

- Search for efficient algorithms for which the computational effort (time, storage) does not increase exponentially with N , the number of qubits. For example, see the factorization of large integers (Shor, 1994); search algorithm (Grover, 1995).

Read (Introduction to Quantum Computing):

- Read the article “[Whither the Future of Controlling Quantum Phenomena ?](#)” by H. Rabitz *et al.*, Science 288 (2000) 824-828; DOI: 10.1126/science.288.5467.824.
- Read the review article “[Quantum Computers](#)” by T. D. Ladd *et al.*, Nature 464 (2010) 45-53; DOI: 10.1038/nature08812.

3.1.b. Qubits and quantum registers

Classical versus quantum bits (qubits):

- Classical bit just takes values 0 or 1.
- Computational basis:

$$|0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\alpha\rangle = |\uparrow\rangle = \left| \frac{1}{2} \right\rangle = \dots, \quad |1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\beta\rangle = |\downarrow\rangle$$

- A qubit system can be in [one out of an infinite number](#) of significant states:

$$|\psi\rangle = a |0\rangle + b |1\rangle$$

- A qubit is either in a **pure** state (vector) or a **mixed** state (density matrix).
- Another commonly used basis is the **diagonal basis**

$$|+\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \quad |-\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

- Qubits are **realized by different ‘two-level’ systems**: electron spin, photon polarization, charges in a quantum dot, which-paths information, ...

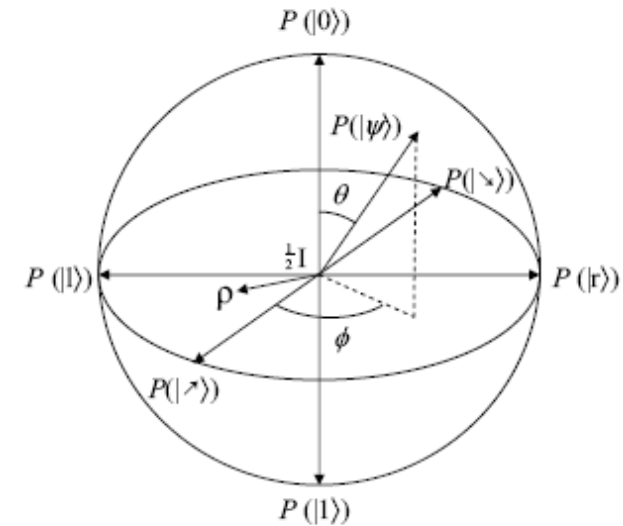


Figure 3.1.: Bloch sphere representation of the qubit. The pure qubit states lie on the periphery, known also as the Poincare-Bloch sphere. The mixed qubit states lie in the interior and are weighted convex combinations of pure states.

Quantum registers:

- **Classical:** messages are stored and processed by **sequences of bits**.
- **Quantum world:** sequence of **distinguishable qubits**; such sequences are known also as **(n -qubit) quantum registers**.
- n -qubit systems are associated with a 2^n -dimensional state space; superpositions of all 2^n basis states:
 n -qubits, linear $\iff \dim(\mathbb{H}) = 2^n$, **exponential increase, parallelism**.
- **Quantum parallelism:** certain computations can be carried out in parallel for all 2^n input values.
- An exponential increase in parallelism requires therefore only a linear increase in the amount of qubits.

3. Quantum mechanics in finite-dimensional Hilbert spaces



Figure 3.2.: From: www.labs.nec.co.jp.

- **Quantum measurements:** Difficulties arise from measurements in quantum mechanics; state reduction is never ideal.
- **Non-cloning theorem:** Quantum mechanics does not permit to generate an exact copy of an unknown state.

3.1.c. Experimental realization of qubits

Two-level systems:

- **Nuclear magnetic resonance (NMR):** ... with suitable chemical solutions; experiments with a large number of the same system; $\sim 10^{20}$ molecules; difficult to scale towards large n ; $n_{\max} \sim 7..10$).
- **Ions in traps:** Qubits are represented by the low-lying states of the corresponding quantum oscillator.
- **Neutral atoms in optical lattices:** the dimensionality, form, depth and position of optical lattices can be precisely controlled through the geometry, polarization and intensity of the external laser beams.
- **Quantum dots:** Qubits represented by elementary charges in nanostructures/dots.

Decoherence: Summarizes all processes that lead to the loss of (quantum) and phase information, for example, loss in the quantum phases due to small fluctuations in the energy. Superpositions are easily destroyed (**fragile quantum states**).

3.2. Linear vector spaces

- **General agreement:** If not stated otherwise, we consider the vector space $\mathbb{C}^n = \{(z_1, \dots, z_n); z_i \in \mathbb{C}\}$, i.e. the vector space of the complex n -tuple.
- Elements of the vector space are called (*ket*) *vectors*:

$$|\psi\rangle = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix}$$

Properties of linear vector spaces:

- addition of vectors
- multiplication with complex numbers $z \in \mathbb{C}$

$$z \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} z z_1 \\ z z_2 \\ \vdots \\ z z_n \end{pmatrix}$$

- null vector, null element: $0 \quad |v\rangle + 0 = |v\rangle \quad \forall |v\rangle$

Remember: $0 = (0, 0, \dots, 0) \in \mathbb{C}^n$

➤ associative and distributive

$$a(|v\rangle + |w\rangle) = a|v\rangle + a|w\rangle, \quad (a + b)|v\rangle = a|v\rangle + b|v\rangle$$

➤ **Basis in \mathbb{C}^n :** Every set $\{|v_1\rangle, |v_2\rangle, \dots, |v_n\rangle\}$ so that we have: $|v\rangle = \sum_i^n a_i |v_i\rangle \quad \forall |v\rangle$.

➤ **Linear independence of vectors:** $\sum_i a_i |v_i\rangle = 0$ is valid only if all $a_i = 0$; otherwise these vectors are called **linear independent**.

3.3. State vectors and operators

3.3.a. Linear Operators

➤ **Linear maps:** $A : V \rightarrow W$ or $V \rightarrow V$; ‘ A acts in/on V ’.

$$A \left(\sum_i a_i |v_i\rangle \right) = \sum_i a_i A |v_i\rangle \equiv A |v\rangle$$

➤ **Identity:** $I |v\rangle = |v\rangle \quad \forall |v\rangle$

➤ **Null operator:** $\hat{0} |v\rangle = 0 \quad \forall |v\rangle$

Apparently, the **mapping/action of an operator** is known if we know its action upon all the basis states $\{|v_i\rangle\}$.

If $A : V \rightarrow W$ and $B : W \rightarrow X$, then $(BA) : V \rightarrow X$ with $(BA) |v\rangle = B(A |v\rangle)$.

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➤ **Matrix representation of $A : V \rightarrow W$:** If $V : \{|v_1\rangle, |v_2\rangle, \dots, |v_m\rangle\}$ and $W : \{|w_1\rangle, |w_2\rangle, \dots, |w_n\rangle\}$, then

$$A |v_j\rangle = \sum_i^n A_{ij} |w_i\rangle \quad (A_{ij}) \dots (n \times m) \text{ matrix representation of } A$$

The particular matrix depends of course always on the choice of basis in V and W .

3.3.b. Pauli matrices

There are many different notations for the Pauli matrices:

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

These Pauli matrices provide a **matrix representation of 4 linear independent operators:** $\mathbb{C}^2 \rightarrow \mathbb{C}^2$ with regard to the computational basis $|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

3.3.c. Scalar product

➤ Map of $V \times V \rightarrow \mathbb{C}$ or $(|v_1\rangle, |v_2\rangle) \rightarrow \mathbb{C}$: $\langle v_1 | v_2 \rangle \equiv (|v_1\rangle, |v_2\rangle)$

➤ **Properties of the scalar product:**

- linear in the second argument: $\langle v | \sum_i a_i w_i \rangle = \sum_i a_i \langle v | w_i \rangle$

- $\langle v | w \rangle = \langle w | v \rangle^*$
- $\langle v | v \rangle \geq 0$; $\langle v | v \rangle = 0$ (only) if $|v\rangle \equiv 0$

➤ Scalar product in \mathbb{C}^n

$$\langle (y_1, y_2, \dots, y_n) | (z_1, z_2, \dots, z_n) \rangle = \sum_i y_i^* z_i$$

➤ In \mathbb{C}^n refer the terms ‘scalar product space’ and ‘Hilbert space’ to the same.

Blackboard example (Dual state and scalar product):

3.3.d. Cauchy-Schwartz and triangle inequalities

➤ Two important identities in scalar product spaces are:

$$|\langle \psi | \phi \rangle|^2 \leq \langle \psi | \psi \rangle \langle \phi | \phi \rangle \quad \text{Cauchy – Schwarz inequality}$$

$$\sqrt{\langle \psi + \phi | \psi + \phi \rangle} \leq \sqrt{\langle \psi | \psi \rangle} + \sqrt{\langle \phi | \phi \rangle} \quad \text{triangle inequality}$$

Blackboard example (Cauchy-Schwartz and triangle inequalities):

3.3.e. Orthogonality and norm

➤ **Orthogonality:** $|v\rangle$ and $|w\rangle$ are orthogonal $\iff \langle v | w \rangle = 0$

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

➤ **Unit vector:** $\|v\| = 1$

➤ Set of vectors $\{|i\rangle, i = 1, \dots, n\}$ is called **orthogonal**, if $\langle i | j \rangle = \delta_{ij} \quad \forall i, j = 1, \dots, n.$

➤ **Gram-Schmidt orthogonalization:** Let $\{|w_1\rangle, |w_2\rangle, \dots, |w_d\rangle\}$ be an arbitrary basis in V , then an **orthonormal basis** $|v_1\rangle, |v_2\rangle, \dots, |v_d\rangle$ is obtained by

$$|v_1\rangle = \frac{|w_1\rangle}{\| |w_1\rangle \|}, \quad |v_{k+1}\rangle = \frac{|w_{k+1}\rangle - \sum_i^k \langle v_i | w_{k+1}\rangle |v_i\rangle}{\| |w_{k+1}\rangle - \sum_i^k \langle v_i | w_{k+1}\rangle |v_i\rangle \|} \quad (1 \leq k \leq d - 1)$$

➤ **General agreements:**

Matrix representations of linear operators always refer to the use of some orthonormal basis if not stated otherwise.

Especially for all $A : V \rightarrow V$, the same basis is used in the input and output space

Blackboard example (Find an orthonormal state):

3.3.f. Outer product

➤ **Outer product:** For $|v\rangle \in V$, $|w\rangle \in W$, then linear operator $V \rightarrow W$

$$(|w\rangle \langle v|) |v'\rangle \equiv |w\rangle \langle v | v'\rangle, \quad \left(\sum_i a_i |w_i\rangle \langle v| \right) \left(\sum_k b_k |v_k\rangle \right) = \sum_{ik} a_i b_k |w_i\rangle \langle v | v_k\rangle$$

➤ **Completeness:** $\{|i\rangle, i = 1, \dots, n\}$... orthonormal basis in V , then

$$|v\rangle = \sum_i |i\rangle \langle i | v\rangle = \sum_i v_i |i\rangle \implies \left(\sum_i |i\rangle \langle i| \right) |v\rangle = \sum_i |i\rangle \langle i | v\rangle = |v\rangle, \quad \forall |v\rangle \iff \sum_i |i\rangle \langle i| = I$$

➤ **Matrix representation of operator $A: V \rightarrow W$**

$$A = I_w A I_v = \sum_{ik} |w_k\rangle \langle w_k | A | v_i\rangle \langle v_i| = \sum_{ik} \langle w_k | A | v_i\rangle |w_k\rangle \langle v_i| = \sum_{ik} A_{ki} |w_k\rangle \langle v_i|$$

Blackboard example (Z operator acting upon a qubit):

Example (Outer vector of two vectors):

Consider the two general qubit states $|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ and $|\phi\rangle = \begin{pmatrix} c \\ d \end{pmatrix}$ and form their outer product:

$$|\psi\rangle \langle \phi| = \begin{pmatrix} a \\ b \end{pmatrix} (c^* \ d^*) = \begin{pmatrix} ac^* & ad^* \\ bc^* & bd^* \end{pmatrix} \neq |\phi\rangle \langle \psi| = \begin{pmatrix} c \\ d \end{pmatrix} (a^* \ b^*) = \begin{pmatrix} ca^* & cb^* \\ da^* & db^* \end{pmatrix}.$$

3.3.g. Expectation value of an operator A

- **Expectation value of an operator A :** $\langle A \rangle = \langle \psi | A | \psi \rangle$... mean or average value of that operator A with respect to a given quantum state $|\psi\rangle$:
- **Measurement statistics:** Average of (a series of) measurements if the state $|\psi\rangle$ has been prepared many times, and if we measure the given operator A each time.

Blackboard example (Operator in qutrit basis):

3.4. Properties of linear operators

$A|v\rangle = v|v\rangle$... eigenvectors, eigenvalues (often useful to use the same symbol).

- **Determination of eigenvalues:** use characteristic polynomial $p(\lambda) = \det|A - \lambda I| = 0$
- **Eigenspace associated with eigenvalue v :** space spanned by all eigenvectors with eigenvalue v .
- **Diagonal form of operator:** $A = \sum_i \lambda_i |i\rangle \langle i|$... diagonalizable, if $\{|i\rangle\}$ form an orthonormal set of eigenvectors and λ_i the corresponding eigenvalues.
- A is called **diagonalizable** if such a diagonal form exist. — Diagonal form is sometimes called **orthonormal decomposition**.

Example (Eigenvalues of a matrix):

Find the eigenvalues of an operator with matrix representation $A = \begin{pmatrix} 2 & 1 \\ -1 & -1 \end{pmatrix}$:

1) Construct the matrix

$$A - \lambda I = \begin{pmatrix} 2 & 1 \\ -1 & -1 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 - \lambda & 1 \\ -1 & -1 - \lambda \end{pmatrix}$$

2) Calculate the determinant $\det |A - \lambda I| = \lambda^2 - \lambda - 1 = 0$ (!)

3) Solve the characteristic polynomial $\lambda_{1,2} = \frac{1 \pm \sqrt{5}}{2}$.

3.4.a. Adjoint and hermitean operators

$$\langle v | Aw \rangle = \langle A^+ v | w \rangle \quad \forall |v\rangle, |w\rangle \in V$$

➤ **Matrix representation:** $A^+ \equiv (A^*)^T$

- $(AB)^+ = B^+ A^+$
- $(A |v\rangle)^+ = \langle v | A^+$
- $(|w\rangle \langle v|)^+ = |v\rangle \langle w|$

➤ In physics, A^+ is called the **adjoint or hermitian conjugate operator** to A .

➤ **Hermitian (or self-adjoint) operator:** $A^+ \equiv A$

Example (Form and eigenvalues of a 2×2 hermitian matrix):

a) Show that a 2×2 hermitian matrix has the general form $H = \begin{pmatrix} a & c - id \\ c + id & b \end{pmatrix}$ with a, b, c, d being real numbers.

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b) Calculate the eigenvalues E_1 and E_2 of this matrix.

a) Let us consider the arbitrary 2×2 matrix $H = \begin{pmatrix} a + ie & c + id \\ k + if & b + ig \end{pmatrix}$ with a, b, c, d, e, f, g, k all real. From the definition of a hermitian matrix, we have $H = H^+ = (H^*)^T$ and, therefore,

$$H^+ = \begin{pmatrix} a - ie & k - if \\ c - id & b - ig \end{pmatrix} = \begin{pmatrix} a + ie & c + id \\ k + if & b + ig \end{pmatrix} = H$$

or $e = 0$, $g = 0$, $k = c$ and $d = -f$. Hence, a 2×2 hermitian matrix must have the form $H = \begin{pmatrix} a & c - id \\ c + id & b \end{pmatrix}$.

b) To calculate the eigenvalues of H , we have to solve the characteristic equation

$$\begin{aligned} \det(H - \lambda I) &= (a - \lambda)(b - \lambda) - (c + id)(c - id) = 0 \quad \rightsquigarrow \quad \lambda^2 - \lambda(a + b) + ab - c^2 - d^2 = 0 \\ &\rightsquigarrow \quad \lambda_{1,2} = \frac{a + b}{2} \pm \sqrt{\frac{(a - b)^2}{4} + c^2 + d^2} \end{aligned}$$

Example (Pauli matrices):

- a) Find the eigenvalues, eigenvectors and the diagonal representation of the Pauli matrices (definition see above).
- b) Show that the Pauli matrices are hermitian and unitary.
- c) Show that any 2×2 hermitian matrix A can always be expressed in terms of the unitary matrix I and the three

Pauli matrices as:

$$A = c_0 I + c_1 \sigma_x + c_2 \sigma_y + c_3 \sigma_z, \quad c_0, c_1, c_2, c_3 \text{ real numbers.}$$

a) For $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ we have the characteristic polynomial $\lambda^2 - 1 = 0$ and, thus, $\lambda = \pm 1$. — To find the eigenvalues, we need to solve

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lambda \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} : \quad \lambda = +1 \rightsquigarrow \mathbf{v}_{\lambda=+1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\lambda = -1 \rightsquigarrow \mathbf{v}_{\lambda=-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The diagonal representation is ... and similarly

$$\sigma_x : \quad \sum_{\lambda} \lambda |v_{\lambda}\rangle \langle v_{\lambda}| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \sigma_x$$

$$\sigma_y : \quad \lambda = \pm 1, \quad \mathbf{v}_{\lambda=+1} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix}, \quad \mathbf{v}_{\lambda=-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix}$$

$$\sigma_z : \quad \lambda = \pm 1, \quad \mathbf{v}_{\lambda=+1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{v}_{\lambda=-1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

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b) $\sigma_x^+ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x$ and $\sigma_x^+ \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \dots$ σ_y and σ_z analogue.

c)

$$\begin{aligned} c_0 I + c_1 \sigma_x + c_2 \sigma_y + c_3 \sigma_z &= \begin{pmatrix} c_0 & 0 \\ 0 & c_0 \end{pmatrix} + \begin{pmatrix} 0 & c_1 \\ c_1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -ic_2 \\ ic_2 & 0 \end{pmatrix} + \begin{pmatrix} c_3 & 0 \\ 0 & -c_3 \end{pmatrix} \\ &= \begin{pmatrix} c_0 + c_3 & c_1 - ic_2 \\ c_1 + ic_2 & c_0 - c_3 \end{pmatrix} = \begin{pmatrix} a & c - id \\ c + id & b \end{pmatrix}. \end{aligned}$$

3.4.b. Projection operators

➤ If W ... m -dimensional subspace of V and $\{|1\rangle, \dots, |m\rangle, m \leq n\}$... orthonormal basis in W , qqquad then

$$P = \sum_i^m |i\rangle \langle i|; \quad P^+ = P, \quad P^2 = P \quad \text{independent of the choice of the basis}$$

➤ Properties: $P^+ \equiv P$... always hermitian, $P^2 = P$.

➤ **Orthogonal complement:** $Q = I - P$... projector upon the (complementary) space $\{|m+1\rangle, \dots, |n\rangle\}$.

Example (Projectors upon the diagonal states): Let us construct the projection operators for the *diagonal states* $|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, which fulfill the completeness relation:

$$P_+ = |+\rangle\langle+| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad P_- = |-\rangle\langle-| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad P_+ + P_- = I$$

Alternatively, we could write

$$P_+ = |+\rangle\langle+| = \frac{1}{2} (|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|)$$

$$P_- = |-\rangle\langle-| = \frac{1}{2} (|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|),$$

and this gives rise to the same completeness: $P_+ + P_- = I$. — **These expressions allow us to write any operator in terms of different projection operators.** For example, we have seen that the Z operator is

$$Z = |0\rangle\langle 0| - |1\rangle\langle 1| = P_0 - P_1.$$

Blackboard example (Finding the i -th outcome in case of measurement):

Blackboard example (Outcome of a single-qubit measurement):

3.4.c. Normal operators and spectral decomposition

$$A \text{ is a normal operator} \iff \begin{cases} AA^+ = A^+A \\ \text{diagonalizable} \\ A = \sum_i \lambda_i |i\rangle \langle i| \end{cases}$$

Hermitian operators are always normal operators.

- **Spectral decomposition:** Every normal operator A in V is diagonalizable (with regard to some basis in V) and *vice versa* every diagonalizable operator is normal.
- **Every normal operator:** can be written in terms of eigenvalues λ_i and pairwise orthonormal eigenvectors $|i\rangle$, $\langle i|j\rangle = \delta_{ij}$.

$$A = \sum_i \lambda_i |i\rangle \langle i|, \quad A = \sum_i \lambda_i P_i, \quad \sum_i P_i = I, \quad P_i P_j = \delta_{ij} P_j$$

Here, the P_i is the projector upon the eigenspace of λ_i .

Example (Spectral decomposition of a 3×3 matrix): Consider the matrix $H = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}$.

What is the corresponding spectral decomposition ??

- 1) Determine eigenvalues and eigenvectors; calculate the characteristic polynomial ... but give eigenvectors directly:

$$e_1 = -1, |v_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix}, \quad e_2 = 1, |v_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix}, \quad e_3 = 1, |v_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

- 2) Since H is hermitian (check it !), eigenvectors are orthogonal, and we can write the operator in the form

$$H = -|v_1\rangle\langle v_1| + |v_2\rangle\langle v_2| + |v_3\rangle\langle v_3|.$$

3.4.d. Unitary operators

$$U \text{ is a unitary operator} \iff \begin{cases} UU^+ = U^+U = I \\ \text{normal} \\ U = \sum_i \lambda_i |i\rangle \langle i| \end{cases}$$

Every unitary operator is normal and has a spectral decomposition.

➤ **Unitary operator ‘conserve’ the scalar product**, i.e. distances and angles for all pairs of vectors, since

$$\langle Uv | Uw \rangle = \langle v | U^+Uw \rangle = \langle v | w \rangle$$

➤ **Notation:** Unitary operators describe generalized rotations in Hilbert space.

➤ **Especially:** $\{|v_i\rangle\}$... orthonormal basis in V , then $\{|w_i\rangle = U|v_i\rangle\}$... also orthonormal in V .

Example (Basis change from the computational to diagonal basis): We may wish to determine the transformation matrix for going from the computational basis $\{|0\rangle, |1\rangle\}$ to the diagonal basis $\{|\pm\rangle\}$; it is simply given by,

$$\text{since } \langle + | 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}$$

$$U = \begin{pmatrix} \langle + | 0 \rangle & \langle + | 1 \rangle \\ \langle - | 0 \rangle & \langle - | 1 \rangle \end{pmatrix} \implies U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We easily see $U = U^+$. — We can use this transformation matrix to transform the state

$$|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix}, \quad |\psi\rangle \longrightarrow |\psi'\rangle = U|\psi\rangle = \text{explicit} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 + \sqrt{2} \\ 1 - \sqrt{2} \end{pmatrix}.$$

Transform the $\pi/8$ -gate: :

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \quad \Longrightarrow \quad U T U^+ = \text{explicit} = \frac{1}{2} \begin{pmatrix} 1 + e^{i\pi/4} & 1 - e^{i\pi/4} \\ 1 - e^{i\pi/4} & 1 + e^{i\pi/4} \end{pmatrix}.$$

Blackboard example (Unitary transform of hermitian operator):

3.4.e. Positive operators

A is called positive $\iff \langle v | Av \rangle \geq 0$ real $\forall |v\rangle \in V$

A is positive definite $\iff \langle v | Av \rangle > 0$ real

All positive operators are hermitian and have a spectral decomposition.

$$A = \sum_i \lambda_i |i\rangle \langle i| \quad \text{with} \quad \lambda_i \geq 0 \quad \forall i.$$

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➤ **Positive operator-valued measure** or short a **POVM**: A set of positive semi-definite operators

$$\{E_1, E_2, \dots, E_m\} \quad \text{with} \quad \sum_i^k E_i = I$$

Such POVM allow another view and way of dealing with quantum measurements.

3.5. Products and functions of linear operators

3.5.a. Product spaces (tensor spaces)

➤ **Product space**: $V, W \dots$ vector spaces with dimensions m, n , then $V \otimes W \dots$ **product space** (vector space) with dimension $m n$:

$$\text{vectors (elements) :} \quad |v\rangle |w\rangle \equiv |v, w\rangle \equiv |vw\rangle, \quad |v\rangle \in V, \quad |w\rangle \in W$$

Important to describe composite systems (many-particle systems).

➤ **Orthonormal basis**: $\{|i\rangle\}$ orthonormal in V , $\{|j\rangle\}$ orthonormal in W

$$\{|i\rangle \otimes |j\rangle; \quad i = 1, \dots, m, j = 1, \dots, n\} \quad \implies \quad \text{orthonormal basis in } V \otimes W$$

➤ **Properties of tensor products:** Suppose $|v_1\rangle, |v_2\rangle \in V$, $|w_1\rangle, |w_2\rangle \in W$, $z \in \mathbb{C}$

$$1) \quad z(|v\rangle \otimes |w\rangle) = (z|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z|w\rangle)$$

$$2) \quad (|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$$

$$3) \quad |v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle$$

Example (Product space of two qubits): Let H_1 and H_2 be the \mathbb{C}^2 Hilbert spaces of two qubits. — What is a proper basis in $H = H_1 \otimes H_2$??

The basis vectors are:

$$|w_1\rangle = |0\rangle \otimes |0\rangle \equiv |00\rangle, \quad |w_2\rangle = |0\rangle \otimes |1\rangle \equiv |01\rangle, \quad |w_3\rangle = |10\rangle, \quad |w_4\rangle = |11\rangle.$$

product state of the composed system: Take the vectors $|\varphi\rangle = \sum_i a_i |u_i\rangle$ from H_1 and $|\chi\rangle = \sum_j b_j |v_j\rangle$ from H_2 , then

$$|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle = \sum_{ij} a_i b_j |u_i\rangle |v_j\rangle = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{pmatrix}$$

Components of $|\psi\rangle$ follow from the components of $|\varphi\rangle$ and $|\chi\rangle$ by taking the tensor product (see Kronecker product).

Blackboard example (Diagonal product basis):

3.5.b. Tensor product of linear operators

➤ **Definition:** ... suppose $|v_i\rangle \in V$, $|w_i\rangle \in W$ and operators $A : V \rightarrow V$, $B : W \rightarrow W$

$$(A \otimes B) (|v\rangle \otimes |w\rangle) \equiv A|v\rangle \otimes B|w\rangle \quad \Longrightarrow \quad \text{defines again linear operator } (A \otimes B) : V \otimes W \rightarrow V \otimes W$$

➤ **Generalization:**

$$\left. \begin{array}{l} A : V \rightarrow V' \\ B : W \rightarrow W' \end{array} \right\} \quad \Longrightarrow \quad C = \sum_i c_i A_i \otimes B_i \quad : \quad V \otimes W \rightarrow V' \otimes W'$$

$$C : V \otimes W \rightarrow V' \otimes W' \quad \text{with} \quad \left(\sum_i c_i A_i \otimes B_i \right) (|v\rangle \otimes |w\rangle) = \sum_i c_i A_i |v\rangle \otimes B_i |w\rangle .$$

➤ **Scalar product in $V \otimes W$:** can be naturally ‘defined/reduced to’ scalar products in V and W .

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

➤ **Kronecker product (tensor product) of matrices:** ... suppose $(m \times n)$ matrix A , $(p \times q)$ matrix B , then

$$A \otimes B = \begin{pmatrix} A_{11} B & A_{12} B & \dots & A_{1n} B \\ A_{21} B & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ A_{m1} B & \dots & \dots & A_{mn} B \end{pmatrix} \quad (mp \times nq) \text{ matrix; Kronecker product}$$

➤ **Notations:**

$$|\psi\rangle^{\otimes 2} = |\psi\rangle \otimes |\psi\rangle, \quad |\psi\rangle^{\otimes k} = |\psi\rangle \otimes |\psi\rangle \otimes \dots \otimes |\psi\rangle \quad k - \text{times}, \quad A^{\otimes k}, V^{\otimes k} \text{ similarly}$$

➤ Tensor product of two operators $A \otimes B$ has the properties:

- If A and B are hermitian, then $A \otimes B$ is also hermitian.
- If A and B are projection operators, then $A \otimes B$ is also a projection operator.
- If A and B are unitary, then $A \otimes B$ is also unitary.
- If A and B are positive, then $A \otimes B$ is also positive.

Blackboard example (Tensor product of the Pauli matrices X and Y):

Example (Eigenvalues of product eigenvectors):

Suppose $|\psi\rangle = |a\rangle \otimes |b\rangle$ and $A|a\rangle = a|a\rangle$, $B|b\rangle = b|b\rangle$. — What is $(A \otimes B)|\psi\rangle$??

$$\left. \begin{array}{l} |\psi\rangle = |a\rangle \otimes |b\rangle \\ A|a\rangle = a \\ B|b\rangle = b \end{array} \right\} \implies (A \otimes B)|\psi\rangle = (A|a\rangle) \otimes (B|b\rangle) = ab|\psi\rangle .$$

Example (Action of $(X \otimes Z)$): Determine $(X \otimes Z)|\psi\rangle$ with $|\psi\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$!!

$$(X \otimes Z) \frac{|00\rangle - |11\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} ((X \otimes Z)|00\rangle - (X \otimes Z)|11\rangle) = \frac{1}{\sqrt{2}} (|10\rangle - (-)|01\rangle) = \frac{|10\rangle + |01\rangle}{\sqrt{2}} .$$

Blackboard example (Product of two projection operators):

Example (Hadamard operator):

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For a single qubit, the Hadamard operator is often written in terms of Pauli matrices $H = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$.

- Determine how this operator acts on the vectors $|0\rangle$ and $|1\rangle$ in the 2-dimensional vector space \mathbb{C}^2 .
- Express the Hadamard operator in the outer product notation (i.e. in terms of the operators $|0\rangle\langle 0|$, $|0\rangle\langle 1|$, ...).
- Find the Hadamard operator on n qubits, $H^{\otimes n} = \underbrace{H \otimes H \otimes \dots \otimes H}_n$ in the outer product notation.

$$H = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Solution:

a)

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad H|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

b) Since $|0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, and $|1\rangle\langle 0|$, ... similar

$$H = \frac{1}{\sqrt{2}}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|) = \frac{1}{\sqrt{2}}((|0\rangle + |1\rangle)\langle 0| + (|0\rangle - |1\rangle)\langle 1|) = \frac{1}{\sqrt{2}} \sum_{i,j=0,1} (-1)^{i \cdot j} |i\rangle\langle j|.$$

c) Therefore, we may write the Hadamard operator for n qubits in the form:

$$H^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{i,j} (-1)^{\mathbf{i} \cdot \mathbf{j}} |i\rangle\langle j| \equiv \frac{1}{\sqrt{2^n}} \sum_{i,j} (-1)^{\sum_{k=1}^n i_k \cdot j_k} |\mathbf{i}\rangle\langle \mathbf{j}|$$

with $\mathbf{i} = (i_1, i_2, \dots, i_n)$, $\mathbf{j} = (j_1, j_2, \dots, j_n)$ are the ‘vectors’ due to the binary representation of \mathbf{i} and \mathbf{j} , respectively.

3.5.c. Trace of an operator

$$\text{Tr}(A) = \sum_{ii} A_{ii}$$

Properties:

- trace of an outer product $|\psi\rangle\langle\phi|$ is the inner product: $\text{Tr}(|\psi\rangle\langle\phi|) = \langle\psi|\phi\rangle$.
- invariant under unitary (similarity) transformations: $\text{Tr}(UAU^+) = \text{Tr}(AU^+U) = \text{Tr}(A)$
- trace is **basis independent**, i.e. $\text{Tr}(A) = \sum_i^n \langle v_i|A|v_i\rangle = \sum_i^n \langle w_i|A|w_i\rangle$.
- trace of an operator equals the sum of its eigenvalues: $\text{Tr}(A) = \sum_i^n \lambda_i$.
- **Properties of the trace:** If A, B, C are quadratic and of the same dimension, then
 - cyclic: $\text{Tr}(ABC) = \text{Tr}(BCA) = \text{Tr}(CAB)$
 - linear: $\text{Tr}(zA + B) = z\text{Tr}(A) + \text{Tr}(B)$
- If $|\psi\rangle$ is a unit vector, then we have

$$\text{Tr}(A|\psi\rangle\langle\psi|) = \sum_i (\langle i|A|\psi\rangle\langle\psi|i\rangle) = \langle\psi|A|\psi\rangle$$

Blackboard example (Trace of operator):

Blackboard example (Trace is equal to sum of eigenvalues):

3.5.d. Operator functions

➤ **Taylor expansion:** The function of an operator can be found by calculating its Taylor expansion

$$f(A) = \sum_{i=0}^{\infty} a_n A^n$$

$$e^{aA} = I + aA + \frac{a^2}{2!}A^2 + \frac{a^3}{3!}A^3 + \dots \quad \text{example}$$

➤ **Definition:** Suppose A is a normal operator with the spectral decomposition $A = \sum_i \lambda_i |i\rangle \langle i|$, then

$$f(A) = \sum_i f(\lambda_i) |i\rangle \langle i|$$

is a uniquely defined (operator) function.

➤ **Diagonal decomposition:** ... can be utilized in order to define/declare the roots, logarithm, exponential, sin, ... functions of linear operators.

Blackboard example (Exponent of the Pauli matrix Z):

Blackboard example (Infinitesimal unitary transformation):

Blackboard example (Exponential operator):

3.5.e. Scalar product of operators (Hilbert-Schmidt product)

- **Hilbert space of linear operators:** All (linear) operators $V \rightarrow V'$ form a linear vector space \mathbb{L}_V and together with a suitable scalar product also a Hilbert space by themselves.
- **Hilbert-Schmidt product:** $(A, B) \equiv \text{Tr}(A^+ B)$... is a map $\mathbb{L}_V \times \mathbb{L}_V \rightarrow \mathbb{C}$
 $\mathbb{L}_V \oplus$ Hilbert-Schmidt product \leftrightarrow Hilbert space of lin. operators in V
- **Basis in \mathbb{L}_V :** If V has dimension n , \mathbb{L}_V has dimension n^2 .

Example (Pauli matrices): The matrices I, X, Y and Z form a basis in $\mathbb{C}^2 \times \mathbb{C}^2$.

3.5.f. Commutators and anticommutators

- Many properties of operators can be understood by analyzing their commutators and anticommutators.

$$[A, B] = AB - BA \quad [A, B] = 0 \quad \iff \quad \text{operators 'commute' with each other}$$

$$\{A, B\} = AB + BA \quad \{A, B\} = 0 \quad \iff \quad \text{operators 'anticommute'}$$

- **Simultaneous set of eigenfunctions:** $[A, B] = 0 \iff A$ and B have a common set of eigenfunctions; diagonalizable in the same basis.
- **Distributivity of commutators:** $[A, BC] = [A, B]C + B[A, C]$.

Example (Commutation relations of the Pauli matrices):

$$\begin{aligned}
 [X, Y] &= 2iZ && \text{and cyclic} && [\sigma_j, \sigma_k] &= 2i \epsilon_{jkl} \sigma_l \\
 \{\sigma_j, \sigma_k\} &= 0 && \text{for } j \neq k && \sigma_j^2 &= I && \text{for } j = 1, 2, 3 \\
 \sigma_j \sigma_k &= \delta_{jk} I + i \epsilon_{jkl} \sigma_l
 \end{aligned}$$

3.5.g. Decomposition of linear operators

➤ Polar decomposition:

$$\begin{aligned}
 A: V \rightarrow V & \quad A = UJ = KU & \quad U \dots \text{unitary} & \quad J, K \dots \text{positive} \\
 J = \sqrt{A^+A} & \quad K = \sqrt{AA^+} & \dots \text{unique}
 \end{aligned}$$

so-called **left-polar** and **right-polar** decomposition

➤ If A^{-1} exist $\iff U$ is unique.

➤ Singular-value decomposition:

$$A \dots \text{quadratic} \iff A = UD \quad U, V \dots \text{unitary}, \quad D \dots \text{diagonal, nonnegative}$$

The diagonal elements of D are called **singular values of A** .

Example (Polar decomposition of single qubit operator):

Find the polar decomposition of matrix $A = \begin{pmatrix} a & -b \\ b & a \end{pmatrix}$!!

If we define $r = \sqrt{a^2 + b^2}$ and $\theta = \tan^{-1}(b/a)$, we can write the matrix in the form

$$A = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} = \begin{pmatrix} r \cos \theta & -r \sin \theta \\ r \sin \theta & r \cos \theta \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix},$$

i.e. in the [polar decomposition](#). This provides us also with a singular-value decomposition, if $V = I$ is taken. The (non-negative) singular values are $r = \sqrt{a^2 + b^2}$.

3.6. Postulates of quantum mechanics**3.6.a. Postulate I (State space and vectors)**

- For each quantum-mechanical systems, there is **associated a scalar product space (Hilbert space) whose unit vectors describe the system uniquely**, i.e. all these states (superpositions) represent possible states of the system.
- State of the system in position space: $\psi(\mathbf{x}, t) \in \mathcal{H}$ with $\langle \psi | \psi \rangle = \|\psi\| = 1$
- $|\psi(\mathbf{x}, t)|^2 d^3x$... probability to find the particle at time t at position \mathbf{x} within a volume d^3x .

3.6.b. Postulate II (Time evolution)

➤ Time evolution of a closed quantum system is described by a unitary transformation

$$|\psi'(t_2)\rangle = U(t_2, t_1) |\psi(t_1)\rangle \quad U \text{ ... time evolution operator; discrete time evolution}$$

➤ Schrödinger equation: ... without interaction with a classical system

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = H \psi(\mathbf{x}, t) \quad H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x})$$

SG mit Hamiltonoperator

➤ Relation for $H \neq H(t)$:

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

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

➤ Exceptions from time evolution: Quantum measurements; coupling to some bath or environment.

3.6.c. Postulate III (Quantum measurements)

➤ 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.

$$\{M_m\} \quad \mathcal{H} \rightarrow \mathcal{H} \quad \text{measurement operators}$$

➤ probability for the outcome m and state (just) after the measurement: ... $|\psi\rangle$ before the measurement

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

➤ Completeness relation:

$$1 = \sum_m p(m) = \sum_m \langle \psi | M_m^\dagger M_m | \psi \rangle \quad \forall |\psi\rangle, \quad I = \sum_m M_m^\dagger M_m$$

3.6.d. Postulate IV (Composed quantum systems)

➤ $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$

➤ 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 $\{|\psi_i\rangle, i = 1, \dots, n\}$, the overall states is:

$$|\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_n\rangle$$

... 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 environment.

➤ **Notations:** There are many different forms to describe many-particle/ multi-qubit systems; in QI, one often uses an ‘index’ to denote the subsystem, for example, X_2, Z_5, \dots

➤ **Entanglement:** Composite systems can be in (superposition) 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.

Example (Physical observables and operators in position space): A hermitian operator A is assigned to each (physical) observable [measurable entity, dynamical variable]. Functions of observables are associated with the corresponding functions of operators.

a)	observable	operator
	momentum \mathbf{p}	$\hat{\mathbf{p}} = -i\hbar \frac{\partial}{\partial \mathbf{r}}$
	position \mathbf{x}	$\hat{\mathbf{x}}$
	Hamilton function for a potential	Hamilton operator
	$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$	$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$

b) In a measurement of observable A , we always find **one of the eigenvalues** a_m of A .

Simultaneously: wave function **jumps/is reduced to** $\psi(\mathbf{x}, t_o) \longrightarrow \psi_m(\mathbf{x}, t_o)$... the corresponding eigenfunction (**state reduction or collapse of the wave functions**).

c) Expectation value (= mean value) of observable A in state ψ is obtained by: $\langle A \rangle = \langle \psi | A \psi \rangle$

Spectral decomposition: $H = \sum_E E |E\rangle \langle E|$... eigenvalues and eigenvectors of H

Remarks to the postulates:

- observable (measurable quantity) \longleftrightarrow hermitian operator.
- Observable A often refers also to the corresponding operator; the mean value of a measurement often refers just to the scalar product $\langle \psi | A \psi \rangle \equiv \langle \psi | A | \psi \rangle$ with regard to some given state $|\psi\rangle$.

➤ Fourie representation of a quantum state:

$$\psi(\mathbf{x}) = \sum_m c_m \psi_m(\mathbf{x}) = \sum_m \psi_m(\mathbf{x}) \langle \psi_m | \psi \rangle$$

➤ Normalization:

$$\langle \psi | \psi \rangle = 1 = \left\langle \sum_m c_m \psi_m(\mathbf{x}) \left| \sum_m c_m \psi_m(\mathbf{x}) \right. \right\rangle = \sum_{mn} c_m^* c_n \langle \psi_m | \psi_n \rangle = \sum_m |c_m|^2$$

➤ Expectation value:

$$\langle \psi | A \psi \rangle = \left\langle \sum_m c_m \psi_m \left| A \left(\sum_n c_n \psi_n \right) \right. \right\rangle = \sum_{mn} c_m^* c_n \langle \psi_m | A \psi_n \rangle = \sum_{mn} c_m^* c_n a_n \underbrace{\langle \psi_m | \psi_n \rangle}_{\delta_{mn}} = \sum_m |c_m|^2 a_m$$

Blackboard example (Pauli matrices):

Example (Measurement of a qubit in the computational basis):

We have $M_0 = |0\rangle\langle 0|$ and $M_1 = |1\rangle\langle 1|$... hermitian; obviously, $M_0^2 = M_0$, $M_1^2 = M_1$ and, thus, **probabilities and state after the measurement**

$$I = M_0^+ M_0 + M_1^+ M_1 = M_0 + M_1 .$$

$$p(0) = \langle \psi | M_0^+ M_0 | \psi \rangle = \langle \psi | M_0 | \psi \rangle = |a|^2 \quad p(1) = |b|^2$$

$$\frac{M_0 \psi}{|a|} = \frac{a}{|a|} |0\rangle, \quad \frac{M_1 \psi}{|b|} = \frac{b}{|b|} |1\rangle .$$

Difficulties that remain with the framework of ‘QM’:

- State vector itself is not observable.
- In classical physics, energy and momentum are the basic dynamical quantities that can be observed directly; in QM, these quantities are derived and the possible measurement outcome is determined by the state vector.
- Is there a ‘hidden world’ which we can understand only indirectly by using QM ? This issue is closely related to the Bell inequalities.
- At present, it still looks that we will have to live and learn to go around with this ‘so little intuitive quantum world’.

3.7. Tasks

See tutorials.

4. Quantum measurements & correlations. Density operators

Reminder to axiomatic QM:

➤ Postulates of QM ... this forms a 'frame' we need to learn to 'fill'.

I) State space and state vectors: \mathcal{H} ... all unit vectors in \mathcal{H} describe possible states; superpositions

II) Time evolution of closed systems ... always unitary transformations

$$|\psi(t_2)\rangle = U(t_2, t_1) |\psi(t_1)\rangle \quad \text{every } U \text{ in principle realizable}$$

$$-i\hbar \frac{\partial |\psi\rangle}{\partial t} = H |\psi\rangle, \quad U = e^{-iH(t_2-t_1)/\hbar}, \quad H \text{ hermetian}, \quad H \neq H(t)$$

Exceptions: Quantum measurements, coupling to the environment.

III) Quantum measurements $\{M_m\}$... linear, hermitian operators $\mathcal{H} \rightarrow \mathcal{H}$, often projectors. ... If system in $|\psi\rangle$

$$p(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle, \quad I = \sum_m M_m^\dagger M_m, \quad \frac{M_m |\psi\rangle}{\sqrt{p(m)}} \quad \dots \text{ post - measurement state}$$

4.1. Measurements in quantum mechanics

4.1.a. Indistinguishable quantum states

➤ In QM, nonorthogonal states cannot be distinguished with ‘certainty’.

➤ Determination of nonorthogonal states: ... task

- Alice initialize a certain $|\psi_k\rangle$ out of a given $\{|\psi_i\rangle\}$.
- Bob should figure out which $|\psi_k\rangle$ it is.

➤ Two measurement scenarios: Measurement operators and outcome for $|\psi_k\rangle$...

$$\{M_i = |\psi_i\rangle\langle\psi_i|, \quad i = 1, \dots, n \quad \text{and} \quad M_0 = I - \sum_i |\psi_i\rangle\langle\psi_i|,$$

$$p(k) = \langle\psi_k| M_i^\dagger M_i |\psi_k\rangle \begin{cases} = \delta_{ik} & \text{if } \{|\psi_i\rangle\} \text{ pairwise orthogonal; identifies } |\psi_k\rangle \text{ with ‘certainty’} \\ \neq \delta_{ik} & \text{if } \{|\psi_i\rangle\} \text{ pairwise nonorthogonal; contains other components} \end{cases}$$

➤ If $\{|\psi_i\rangle\}$ are nonorthogonal: we therefore cannot determine the state ‘with certainty’ since other $|\psi_j\rangle$ also contain some component of $|\psi_k\rangle$.

4.1.b. Projective measurements (von Neumann measurements)

➤ Measurement of some observable M : ... with hermitian operator M and the spectral decomposition

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

➤ Probability and post-measurement state:

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

Example (Action of $P_0 \otimes I$ and $I \otimes P_1$ upon two-qubit state): Let us consider the state $\psi = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$ and analyze the action of the two operators $P_0 \otimes I$ and $I \otimes P_1$ as well as the corresponding post-measurement states.

$$(P_0 \otimes I) |\psi\rangle = \frac{|01\rangle}{\sqrt{2}}, \quad |\psi'\rangle = \frac{(P_0 \otimes I) |\psi\rangle}{\sqrt{\langle \psi | P_0 \otimes I | \psi \rangle}} = \frac{|01\rangle / \sqrt{2}}{1/\sqrt{2}} = |01\rangle.$$

$$\langle \psi | P_0 \otimes I | \psi \rangle = \frac{1}{2}, \quad (I \otimes P_1) |\psi\rangle = \frac{|01\rangle}{\sqrt{2}}, \quad (I \otimes P_1) = \begin{pmatrix} 1 \cdot P_1 & 0 \cdot P_1 \\ 0 \cdot P_1 & 1 \cdot P_1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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

Properties of projective measurements:

➤ Mean value:

$$\bar{M} = \sum_m m p(m) = \sum_m m \langle \psi | P_m | \psi \rangle = \sum_m \langle \psi | m P_m | \psi \rangle = \langle \psi | M | \psi \rangle = \langle M \rangle$$

mean value = (quantum mechanical) expectation value

4. Quantum measurements & correlations. Density operators

➤ Mean quadratic deviation:

$$[\Delta(M)]^2 = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2$$

➤ Heisenberg's uncertainty principle:

$$\Delta(A) \Delta(B) \geq \frac{1}{2} |\langle \psi | [A, B] | \psi \rangle|$$

➤ Set of orthonormal projectors $\{P_m\}$: with $\sum_m P_m = I$ and $P_m P_{m'} = \delta_{mm'} P_m \iff M = \sum m P_m$.

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 (Expectation value of a two-qubit operator):

4.1.c. POVM measurements

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

POVM formalism:

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

➤ Since the probability $p(m) = \langle \psi | M_m^+ M_m | \psi \rangle \geq 0$ for the outcome m is positive, the operator

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

➤ **Positive operator:**

$$E_m \quad \dots \text{POVM elements} \quad \Longrightarrow \quad \{E_m, \sum E_m = I\} \quad \dots \text{POVM}$$

➤ **Projective measurements:** also form a POVM $\{P_m\}$

$$E_m = P_m^+ P_m = P_m \quad \Longrightarrow \quad \sum_m P_m = I, \quad P_m P_{m'} = \delta_{mm'} P_m$$

➤ Any set of positive operators $\{E_m\}$: with $\sum_m E_m = I$ also also form a POVM since:

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

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

$$\left. \begin{array}{l} \text{(i) positive} \\ \text{(ii) fulfill the completeness relation } \sum_m E_m = I \end{array} \right\} \implies \begin{array}{l} p(m) = \langle \psi | E_m | \psi \rangle \\ \text{probability for measuring outcome } m \end{array}$$

Blackboard example (POVM for a single qubit):

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

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

- If $|\psi_1\rangle = |0\rangle$, then $\text{pr}(a) = \langle \psi_1 | E_a | \psi_1 \rangle = 0 \implies$ if one measures outcome $E_a \implies |\psi\rangle = |\psi_2\rangle$.
- Analogue: Outcome of $E_b \implies |\psi\rangle = |\psi_1\rangle$.
- If outcome E_c occurs, then **no distinction is possible**.

Remarks:

- The example above shows how we can get insight into quantum measurements if we are interested only in the outcome and probability distribution.
- The frequent POVM ‘view’ on quantum measurements due to a set of (semi-) positive operators has been re-activated by QI since around 2000.
- **POVM measurements:** may help to achieve a better control of a quantum system of what is possible by projective measurements alone.
- **Advantages of POVM measurements:**
 M_m need not to be orthonormal projectors, i.e. $\sum_m M_m M_{m'} \neq \delta_{mm'} M_m$... also possible.

4.1.d. Weak measurements**Weak measurements:**

- POVM’s can be used to obtain information about a state by means of a (so-called) weak measurement, i.e. a measurement that provides **some information about the state but without enforcing a ‘collapse of the wave functions’**.
- Of course, the amount of information for such a mild disturbance is restricted.
- For a qubit in state $|\psi\rangle = a|0\rangle + b|1\rangle$ with $|a|^2 + |b|^2 = 1$, we suppose a small (positive) parameter $\varepsilon \ll 1$

4. Quantum measurements & correlations. Density operators

and two measurement operators, from which a POVM is constructed

$$M_0 = |0\rangle\langle 0| + \sqrt{1-\varepsilon}|1\rangle\langle 1|, \quad M_1 = \sqrt{\varepsilon}|1\rangle\langle 1|$$

$$E_0 = M_0^2 = |0\rangle\langle 0| + (1-\varepsilon)|1\rangle\langle 1|, \quad E_1 = M_1^2 = \varepsilon|1\rangle\langle 1| \quad \implies \quad E_0 + E_1 = I$$

eigenvalues : $E_0 \dots \{1, 1-\varepsilon\}$ $E_1 \dots \{0, \varepsilon\}$ positive semi-definite

➤ The probabilities and post-measurement state for outcomes E_0 and E_1 are

$$\langle \psi | E_0 | \psi \rangle = |a|^2 + |b|^2(1-\varepsilon) \approx 1, \quad \frac{M_0 |\psi\rangle}{\sqrt{\langle \psi | E_0 | \psi \rangle}} = \frac{a |0\rangle + b \sqrt{1-\varepsilon} |1\rangle}{\sqrt{|a|^2 + |b|^2(1-\varepsilon)}}.$$

$$\langle \psi | E_1 | \psi \rangle = |b|^2 \varepsilon \approx 0, \quad \frac{M_1 |\psi\rangle}{\sqrt{\langle \psi | E_1 | \psi \rangle}} = \frac{\sqrt{\varepsilon} b |1\rangle}{\sqrt{\varepsilon} |b|} = |1\rangle.$$

➤ **For outcome E_0 :** Although the state has been disturbed from the initial state of the wave function, a 'collapse of the wave function' to $|0\rangle$ or $|1\rangle$ did not occur ... but we still have a **superposition**.

➤ **For outcome E_1 :** Since $\varepsilon \ll 1$, the probability of obtaining this measurement result is very small. Moreover the wave function has collapsed in this case into the postmeasurement state $|1\rangle$.

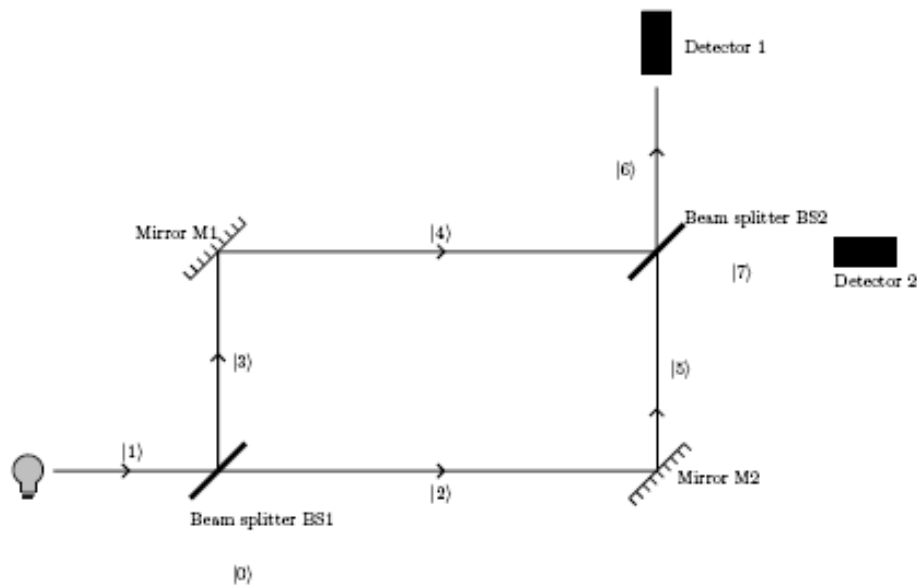


Figure 4.1.: The Mach-Zehnder interferometer. A photon is sent through a beam splitter and bounced off at two mirrors into another beam splitter. Mysteriously, **only one of the detectors registers a photon (for ideal settings)**.

4.1.e. Mach-Zehnder interferometer

Mach-Zehnder:

- The state vectors $|0\rangle$ and $|1\rangle$ can be considered as orthonormal wave packets that move along the arms of the interferometer.
- The **mirrors, beam splitters and relative phases** U_p between the two arms of the interferometer are given by:

$$U_m = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad U_{bs} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad U_p = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix}$$

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➤ For a given ρ_{in} , we need to calculate

$$\rho_{out} = U_{bs} U_m U_p U_{bs} \rho_{in} U_{bs}^+ U_p^+ U_m^+ U_{bs}^+$$

4.2. Density matrices and operators

4.2.a. Ensemble of quantum systems

➤ Ensemble of pure states & density operator:

$$\{p_i, |\psi_i\rangle\} \iff \left\{ \begin{array}{l} p_i - \text{th part of ensemble in state } |\psi_i\rangle \\ \text{system in one of the states } \{|\psi_i\rangle\} \text{ with prob. } p_i. \\ p_i \dots \text{ classical prob. distribution; } \sum_i p_i = 1 \end{array} \right\} \iff \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|.$$

ensemble representation of a quantum system in a incompletely known state

➤ 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 $|\psi_i\rangle$:

$$p(m|i) = \langle \psi_i | M_m^+ M_m | \psi_i \rangle = \text{Tr} (M_m^+ M_m | \psi_i \rangle \langle \psi_i |)$$

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

➤ State after the measurement:

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

➤ Notations: **pure states** vs. **mixed states**

$$\rho = |\psi\rangle \langle \psi|$$

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$$

$$\text{Tr}(\rho^2) = 1$$

$$\text{Tr}(\rho^2) < 1$$

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

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

➤ 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.

4.2.b. Formal definition of density operators

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

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

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

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

$$\langle \phi | \rho | \phi \rangle = \sum_i p_i \langle \phi | \psi_i \rangle \langle \psi_i | \phi \rangle = \sum_i p_i |\langle \phi | \psi_i \rangle|^2 \geq 0 \quad \dots \text{positive} \quad \iff$$

$$\text{positive } \dots \quad \rho = \sum_j \lambda_j |j\rangle \langle j|, \quad \begin{array}{l} \{|j\rangle\} \dots \text{orthonal} \\ \lambda_j \geq 0 \quad \dots \text{real} \end{array} \implies \text{Tr}(\rho) = \sum_j \lambda_j \text{Tr}(|j\rangle \langle j|) = \sum_j \lambda_j = 1$$

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

➤ Systems with the same density operator ρ are indistinguishable (same measurement statistics).

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 ??

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

As expected, we find $\text{Tr}(\rho) = 1$.

Blackboard example (Test for being a valid density operator):

Example (Expectation value of an operator): The expectation value of an operator A can be expressed also in terms of the density operator; if we consider first a pure state $|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle$, we can write

$$\langle A \rangle = \langle\psi|A|\psi\rangle = \sum_{ik} \langle\psi|u_i\rangle\langle u_i|A|u_k\rangle\langle u_k|\psi\rangle = \sum_{ik} \langle u_i|A|u_k\rangle\langle u_k|\psi\rangle\langle\psi|u_i\rangle = \sum_i \langle u_i|A\rho|u_i\rangle = \text{Tr}(A\rho) .$$

The same applies also mixture (ensemble) of state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, if we write $|\psi\rangle = \sum_i \sqrt{p_i} |\psi_i\rangle$.

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

4. Quantum measurements & correlations. Density operators

of the state $|\psi\rangle = \frac{1}{\sqrt{5}}|0\rangle + \frac{2}{\sqrt{5}}|1\rangle$ in the diagonal basis ??

$$P_- = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad \rho = |\psi\rangle\langle\psi| = \frac{1}{5} \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}, \quad p(-) = \text{Tr}(P_- \rho) = \frac{1}{10}.$$

Completely mixed state

- In contrast to pure states with just *one* state in the ensemble, there are completely mixed states where the probability to be found is equal for any possible state.
- In a n -dimensional state space, it is given by

$$\rho = \frac{1}{n} I \quad \Longrightarrow \quad \rho^2 = \frac{1}{n^2} I \quad \Longrightarrow \quad \text{Tr}(\rho^2) = \frac{1}{n}.$$

completely mixed state

4.2.c. 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 $\text{Tr}(\rho) = 1$, that acts in the state space, defines a possible state of the system. — Especially, if the system is in state ρ_i with probability 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

$$\rho' = U \rho U^\dagger = U(t_2, t_1) \rho(t_1) U^\dagger(t_2, t_1), \quad i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] \quad \dots \text{Heisenberg equation}$$

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 the system is in state ρ before the measurement, then

- Probability for outcome m : $p(m) = \text{Tr}(M_m^\dagger M_m \rho)$
- State after the measurement: $\frac{M_m \rho M_m^\dagger}{\text{Tr}(M_m \rho M_m^\dagger)}$
- Completeness: $\sum_m M_m^\dagger M_m = I$

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 prepared in the states $\{\rho_i, i = 1, \dots, n\}$, then the total state is initially:

$$\rho_{\text{tot}} = \rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_n \quad \text{but, generally, ...} \quad \rho_{\text{tot}} \neq \rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_n$$

... for interacting systems

Advantages of the density-matrix concept:

- Incomplete knowledge about the system, especially for description of quantum ensembles.
- Description of subsystems that should be considered independent of some total system.

Blackboard example (Post-measurement state):

Example (Expectation value for measuring X):

➤ Suppose a measurement is made with regard to the observable X on the state $|\psi\rangle = \frac{1}{\sqrt{6}}|0\rangle + \sqrt{\frac{5}{6}}|1\rangle$.

➤ This means: **a measurement with regard to eigenstates of X :** $|\pm\rangle$ with eigenvalues ± 1 .

➤ The corresponding projectors and probabilities are

$$|+\rangle\langle+| = \frac{1}{2}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) \quad \Longrightarrow \quad \text{Pr}(+1) = \langle\psi|P_+|\psi\rangle = \frac{6 + 2\sqrt{5}}{12}$$

$$|-\rangle\langle-| = \frac{1}{2}(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|) \quad \Longrightarrow \quad \text{Pr}(-1) = \langle\psi|P_-|\psi\rangle = \frac{6 - 2\sqrt{5}}{12}$$

➤ **Total probability & expectation value:** $\text{Pr}(+1) + \text{Pr}(-1) = 1$; $\langle X \rangle = (+1)\text{Pr}(+1) + (-1)\text{Pr}(-1) \approx 0.75$.

➤ For a single-qubit system, more generally, the **orthogonal projection operators** are given by

$$P_{\pm} = \frac{I \pm \mathbf{n} \cdot \boldsymbol{\sigma}}{2} \quad \Longrightarrow \quad \mathbf{n} = \mathbf{e}_x : \quad P_{\pm} = \frac{I \pm X}{2} = \frac{1}{2}(|0\rangle\langle 0| \pm |0\rangle\langle 1| \pm |1\rangle\langle 0| + |1\rangle\langle 1|),$$

again, **the projectors upon the $|\pm\rangle$ states**

4.2.d. Uniqueness of the density operator

Unitary freedom:

- Different ensemble $\{p_i, |\psi_i\rangle\}$ may have the same density operator, i.e. they **behave uniquely with regard to all measurements**.
- The **particular ensemble** $\rho = \sum_i \lambda_i |i\rangle \langle i|$, which is associated with the eigenvalues and eigenvectors, is **physically not distinguished**.
- **Notation:** A set of (non-normalized and generally non-orthogonal) vectors $\{\widetilde{|\psi_i\rangle}\}$ is said to ‘create’ a density operator:

$$\rho = \sum_i \widetilde{|\psi_i\rangle} \widetilde{\langle\psi_i|} \quad \Longrightarrow \quad \left\{ p_i, \frac{\widetilde{|\psi_i\rangle}}{\sqrt{p_i}} \dots \text{normalized} \right\}.$$

4.2.e. Bloch-sphere representation of qubits

Frequently applied qubit bases:

- **Computational basis:**

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |\psi\rangle = a|0\rangle + b|1\rangle \quad a, b \in \mathbb{C}, \quad |a|^2 + |b|^2 = 1.$$

- **Conjugate basis:** Two bases are called **conjugate** to each other if the corresponding pairs of antipodal points on the Bloch sphere are 90° apart from each other. For two conjugated bases $|0\rangle, |1\rangle$ and $|0'\rangle, |1'\rangle$, the probability of a qubit in the state $|0\rangle$ or $|1\rangle$ to be found in the state $|0'\rangle$ or $|1'\rangle$ is always $1/2$ and *vice versa*.

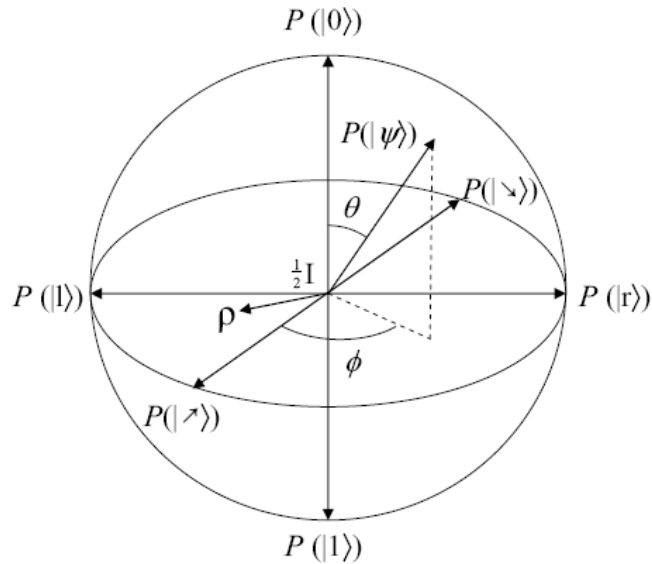


Figure 4.2.: Statistical operators represented in the unit Bloch ball, a **real-valued representation** of the space of qubit states via the expectation values, S_i , of the Pauli operators σ_i , $i = 1, 2, 3$. $P(|x\rangle) = |x\rangle\langle x|$. Orthogonal quantum states are antipodal in this representation; 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 counter-clockwise about the diagonal-basis axis by 90° with respect to the one here; taken from wikipedia.

➤ **Diagonal basis:**

$$|\nearrow\rangle \equiv |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |\searrow\rangle \equiv |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

This basis is **conjugate** to the computational basis. utilized in the BB84 quantum key distribution (QKD) protocol.

➤ **Circular basis:**

$$|R\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle), \quad |L\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle).$$

This basis is **conjugate** to both, the computational and diagonal basis. It is also useful in quantum cryptography and in many quantum-optical realizations and experiments.

4. Quantum measurements & correlations. Density operators

➤ **Breitbart or ‘intermediate’ basis:**

$$\left(\cos \frac{\pi}{8} |0\rangle + \sin \frac{\pi}{8} |1\rangle \right), \quad \left(-\sin \frac{\pi}{8} |0\rangle + \cos \frac{\pi}{8} |1\rangle \right).$$

This basis lies on the $\varphi = 0$ plane ($x - z$ plane) and is used in QKD for eavesdropping.

➤ **Bloch-sphere or spinor representation:**

$$|\psi\rangle = e^{i\gamma} \left(\cos \frac{\vartheta}{2} |0\rangle + e^{i\varphi} \sin \frac{\vartheta}{2} |1\rangle \right) \quad \begin{cases} (\vartheta, \varphi) & \dots \text{ polar angles on a unit sphere} \\ \vartheta = 0, \pi & \longrightarrow \varphi = 0, \text{ by convention} \end{cases}$$

Example (Stern-Gerlach filter): A beam of electrons ($s = 1/2$), polarized completely in the y direction, is sent through a Stern-Gerlach filter. This filter admits only particles which have a spin projection $+1/2$ along the z -axis.

— **From physical insight:** What is the probability that the electron will pass the filter ?

Apply the projector operator technique in order to find the probability that an electron from the beam will penetrate the filter.

For this, we need to know either the state $|\psi_y\rangle$ or the density matrix matrix ρ_y . Using the **Bloch-sphere representation**, we find the density matrix of a pure single-qubit state and, especially, $\rho_y(\vartheta = \pi/2, \varphi = \pi/2)$ as

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos \frac{\vartheta}{2} \\ e^{i\varphi} \sin \frac{\vartheta}{2} \end{pmatrix} \begin{pmatrix} \cos \frac{\vartheta}{2} & e^{-i\varphi} \sin \frac{\vartheta}{2} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \cos \vartheta & e^{-i\varphi} \sin \vartheta \\ e^{i\varphi} \sin \vartheta & 1 - \cos \vartheta \end{pmatrix} \implies \rho_y = \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}.$$

From the given Stern-Gerlach filter (problem with $\boldsymbol{\nu} = \mathbf{e}_z$), we know the projector as well as the probability

$$P_+ = (I + \mathbf{v} \cdot \boldsymbol{\sigma})/2 \quad \longrightarrow \quad P_{\mu_z=+1/2} = (I + \sigma_z)/2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$W(\mu_z = +1/2) = \text{Tr}(\rho_y P_{\mu_z=+1/2}) = \text{Tr} \begin{pmatrix} 1/2 & 0 \\ i & 0 \end{pmatrix} = 1/2.$$

4.2.f. Stokes parameters

Stokes parameters

➤ Stokes parameters and density matrix: ... **homomorphic** to each other and related by

$$\rho = \frac{1}{2} \sum_{\mu=0}^3 P_\mu \sigma_\mu = \frac{1}{2} \begin{pmatrix} P_0 + P_3 & P_1 - iP_2 \\ P_1 + iP_2 & P_0 - P_3 \end{pmatrix} \quad \Longleftrightarrow \quad P_\mu = \text{Tr}(\rho \sigma_\mu)$$

Pauli representation of the density operator

The Stokes parameter are often normalized to $P_0 = 1$... as a measure of the total (quantum) probability.

Blackboard example (Stoke's parameters of a single-qubit state):

Blackboard example (Pauli representation for two qubits):

Blackboard example (Mixed state density operators):

Example (Density matrix of spin-1/2 particle):

Let a spin-1/2 particle be in the spin state

$$|\psi\rangle = \sum_{\mu=\pm 1/2} a_{\mu} |\chi_{\mu}\rangle .$$

- a) Find the density matrix which describe the spin state of this particle.
 b) Find the polarization vector $\mathbf{P} = \langle \psi | \boldsymbol{\sigma} | \psi \rangle$ in terms of the coefficients a_{μ} .

a)

$$\rho = |\psi\rangle \langle \psi| = \sum_{\mu\mu'} a_{\mu} a_{\mu'}^* |\chi_{\mu}\rangle \langle \chi_{\mu'}| \quad \Longrightarrow \quad \langle \chi_{\mu} | \rho | \chi_{\mu'} \rangle = \begin{pmatrix} |a_{1/2}|^2 & a_{1/2} a_{-1/2}^* \\ a_{1/2}^* a_{-1/2} & |a_{-1/2}|^2 \end{pmatrix} \quad \dots \text{densitymatrix}$$

b)

$$\langle \psi | \sigma_x | \psi \rangle = a_{1/2} a_{-1/2}^* + a_{1/2}^* a_{-1/2} = P_x, \quad \langle \psi | \sigma_y | \psi \rangle = i a_{1/2} a_{-1/2}^* - i a_{1/2}^* a_{-1/2} = P_y,$$

$$\langle \psi | \sigma_z | \psi \rangle = |a_{1/2}|^2 - |a_{-1/2}|^2 = P_z$$

If the electrons in a beam are in the state $|\psi\rangle = |+1/2\rangle$, then $a_{1/2} = 1$ and $a_{-1/2} = 0$ and, thus, $P_x = P_y = 0$ and $P_z = 1$.

4.2.g. Reduced density operators and partial trace

➤ **Reduced density operator of subsystem A:** ρ^{AB} ... density operator of two subsystems A and B; then

$$\rho^A = \text{Tr}_B(\rho^{AB}) \quad \dots \text{partial trace over system } B$$

➤ **Partial trace:** density matrix ρ^{AB} of a composed system with regard to two orthonormal bases $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$,

$$\rho^{AB} = \sum_{ik}^{n_A} \sum_{jl}^{n_B} \rho_{ij,kl} |i_A\rangle |j_B\rangle \langle k_A| \langle l_B| \quad \Longrightarrow \quad \text{Tr}_B(\rho^{AB}) = \sum_{ik}^{n_A} \left(\sum_m^{n_B} \rho_{im,km} \right) |i_A\rangle \langle k_A| .$$

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

$$\rho = \frac{|00\rangle \langle 00| + |11\rangle \langle 00| + |00\rangle \langle 11| + |11\rangle \langle 11|}{2}$$

$$\rho_1 = \text{Tr}_2(\rho) = \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|) = \frac{I}{2} = \rho_2 \quad \Longrightarrow \quad \text{Tr}(\rho_1^2) = \text{Tr}(\rho_2^2) = \frac{1}{2} \leq 1 .$$

➤ Although the total system is in a pure state, the reduced density matrix of any subsystem represents in general a mixed state.

Blackboard example (Reduced density matrix of a product state):

4.2.h. 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

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle, \quad \lambda_i \geq 0, \quad \text{real}, \quad \sum_i \lambda_i = 1$$

Schmidt coefficients λ_i

➤ Reduced density operators for subsystems A and B

$$\rho^A = \sum_i \lambda_i^2 |i_A\rangle \langle i_A|, \quad \rho^B = \sum_i \lambda_i^2 |i_B\rangle \langle i_B|, \quad \rho^A, \rho^B \quad \dots \text{ with same eigenvalues } \{\lambda_i^2\}$$

(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:

$$|\psi^{AB}\rangle \text{ is product state; separable} \iff \text{Tr}[(\rho^A)^2] = \text{Tr}[(\rho^B)^2] = 1; \quad \text{Schmidt - No. is 1; } \rho^A, \rho^B \dots \text{ pure}$$

Blackboard example (Schmidt decomposition of two-qubit states):

4.2.i. Purification of reduced density operators

- **Given:** ρ^A of a quantum system A .
- **Look for** pure state $|AR\rangle$ with: $\rho^A = \text{Tr}_R(|AR\rangle\langle AR|)$.

This pure state is to be obtained from the ‘composed’ system A together with some chosen reference system R .

- Suppose,

$$\rho^A = \sum p_i |i_A\rangle\langle i_A| \quad \text{and} \quad \text{reference system } R \text{ in same state space with basis } \{|i_R\rangle\}$$

$$|AR\rangle = \sum_i \sqrt{p_i} |i_A\rangle |i_R\rangle .$$

- Obviously,

$$\text{Tr}_R(|AR\rangle\langle AR|) = \text{Tr}_R\left(\sum_{ik} \sqrt{p_i p_k} |i_A\rangle\langle k_A| (|i_R\rangle\langle k_R|)\right) = \sum_i p_i |i_A\rangle\langle i_A| = \rho^A .$$

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

$$|AR_1\rangle = (I_A \otimes U_R) |AR_2\rangle .$$

4.3. The EPR paradoxon and Bell's inequality

(Einstein, Podolsky und Rosen, 1935)

4.3.a. Bohr–Einstein debate (1926–35)

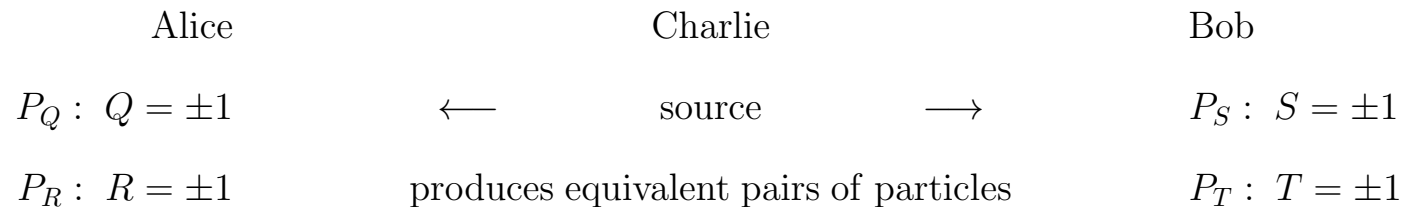
The Bohr-Einstein debate refers to a series of public disputes about quantum mechanics between Albert Einstein and Niels Bohr, and it was later summarized by Bohr in an article titled *Discussions with Einstein on Epistemological Problems in Atomic Physics*.

Historical remarks:

- In 1925, remember, Werner Heisenberg introduced matrix equations that replaced the Newtonian elements of space and time, such as a well-defined trajectory of quantum particles or the simultaneous assignment of a position and velocity at every time t , etc.
- In 1926, Max Born then proposed that the mechanics was to be understood as a probability without any causal reasoning.
- Bohr himself accepted the ‘philosophical’ problems with quantum mechanics by proposing a Principle of Complementarity that emphasized the role of the observer over the system that is to be observed.
- At the sixth Congress of Solvay in 1930, Einstein attacked again Heisenberg’s indeterminacy relation and proposed an experimental apparatus which was subsequently re-designed by Bohr to emphasize the essential elements and the key points which he would use in his response.

4.3.b. EPR 'gedanken' experiment

- Idea of the EPR paper: ... show that quantum mechanics is not a 'complete theory'
- '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:



with P_X property and X the outcome of a measurement.

- How to interpret and understand such an experiment classically and quantum mechanically ??

Correlations of entangled–Bell states:

- Two spin-1/2 particles of a prior (total) spin-0 state if they are in the (so-called) singlet state

$$|\psi\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}} \quad S = 0, \quad \text{spin – singlet state}$$

- Next, we make an measurement of Z on the first particle and leave the second untouched: $Z \otimes I$
 - if first qubit in $|0\rangle$, the second qubit in $|1\rangle$ with certainty
 - if first qubit in $|1\rangle$, again the second qubit is fully correlated.

4.3.c. Classical vs. quantum mechanical ‘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	$ \psi\rangle = \frac{ 01\rangle + 10\rangle}{\sqrt{2}}$	Bob	
$P_Q : Z_1$	← source →	$P_S : \frac{-Z_2 - X_2}{\sqrt{2}},$	$\langle QS \rangle = \left\langle \psi \left Z \otimes \left(\frac{-Z - X}{\sqrt{2}} \right) \right \psi \right\rangle$
$P_R : X_1$		$P_T : \frac{Z_2 - X_2}{\sqrt{2}},$	$\langle RS \rangle = \left\langle \psi \left X \otimes \left(\frac{-Z - X}{\sqrt{2}} \right) \right \psi \right\rangle$

- **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 a 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 :

- At least one of the assumptions about the **elements of reality are not fulfilled by Nature**; either
- **'physical reality' of properties** ... assumption that the properties P_Q, \dots, P_T exist independently from the observation is wrong ??
 - or
 - **'locality' of events**, causal independent events cannot influence each other is wrong ??
- Apparently, the **quantum world is not local-realistic**.

4.3.d. Bipartite systems and the Bell basis

➤ **Bipartite system** ... two subsystems of Alice and Bob

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B, \quad |a_i\rangle \otimes |b_j\rangle \equiv |a_i b_j\rangle \quad \dots \text{basis in } \mathcal{H}, \quad \langle a_i b_j | a_k b_l \rangle = \delta_{ik} \delta_{jl}$$

$$\text{Pr}(a_i b_j) = |\langle a_i b_j | \psi \rangle|^2, \quad A = \sum_{ijkl} |a_i b_j\rangle \langle a_i b_j | A | a_k b_l \rangle \langle a_k b_l | = \sum_{ijkl} |a_i b_j\rangle \langle a_k b_l | A_{ijkl}$$

for the scalar product, probability and representation of an operator in this product basis.

4. Quantum measurements & correlations. Density operators

➤ Bell basis for two-qubit systems:

$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \quad |\beta_{01}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \quad |\beta_{10}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}} \quad (\text{triplet state; can be symmetrized})$$

$$|\beta_{11}\rangle = \frac{|10\rangle - |01\rangle}{\sqrt{2}} \quad (\text{singlet state; anti - symmetric})$$

$$|\beta_{xy}\rangle = \frac{|0y\rangle + (-1)^x |1\bar{y}\rangle}{\sqrt{2}}, \quad \bar{y} = \text{NOT}(y) \quad y \quad \begin{cases} x \dots \text{phase bit} \\ y \dots \text{parity bit} \end{cases} \quad \dots \text{compact form}$$

Example ($Z \otimes Z |\beta_{xy}\rangle$): Let's consider the parts of $|\beta_{xy}\rangle = \frac{|0y\rangle + (-1)^x |1\bar{y}\rangle}{\sqrt{2}}$ separately:

$$Z \otimes Z |0y\rangle = (-1)^y |0y\rangle$$

$$Z \otimes Z (-1)^x |1\bar{y}\rangle = (-1)^x Z |1\rangle \otimes Z |\bar{y}\rangle = (-1)^{x+1+\bar{y}} |1\bar{y}\rangle = (-1)^{x+y} |1\bar{y}\rangle$$

$$Z \otimes Z |\beta_{xy}\rangle = \frac{(-1)^y |0y\rangle + (-1)^y (-1)^x |1\bar{y}\rangle}{\sqrt{2}} = (-1)^y |\beta_{xy}\rangle.$$

Blackboard example (Is the state $H \otimes H |00\rangle$ entangled ??):

4.3.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

$$\rho = \sum_{i,j=1,2} c_{ij} |\beta_{ij}\rangle \langle \beta_{ij}| = c_{00} |\beta_{00}\rangle \langle \beta_{00}| + c_{01} |\beta_{01}\rangle \langle \beta_{01}| + c_{10} |\beta_{10}\rangle \langle \beta_{10}| + c_{11} |\beta_{11}\rangle \langle \beta_{11}|.$$

➤ Outer products in this expansion: ... in terms of the Pauli matrices

$$|\beta_{00}\rangle\langle\beta_{00}| = \frac{1}{4} (I \otimes I + X \otimes X - Y \otimes Y + Z \otimes Z)$$

$$|\beta_{01}\rangle\langle\beta_{01}| = \frac{1}{4} (I \otimes I + X \otimes X + Y \otimes Y - Z \otimes Z)$$

$$|\beta_{10}\rangle\langle\beta_{10}| = \frac{1}{4} (I \otimes I - X \otimes X + Y \otimes Y + Z \otimes Z)$$

$$|\beta_{11}\rangle\langle\beta_{11}| = \frac{1}{4} (I \otimes I - X \otimes X - Y \otimes Y - Z \otimes Z).$$

➤ When expressible in this form, a density operator ρ is separable if and only if: $c_{00} \leq \frac{1}{2}$.

4.4. Concluding remarks

4.5. Tasks

See tutorials.

5. Schrödinger equations

5.1. Finite-difference techniques

5.1.a. Second- and fourth-order central difference formula

- Discrete regular grid: x_0, x_1, \dots, x_n with $x_k = x_0 + k \Delta_x$ $k = 1, \dots, n$, Δ_x step size.
- Discretization of differential operators: ... need to be replaced by finite-difference approximations.

$$\left. \frac{df(x)}{dx} \right|_{x=x_0} = \lim_{\Delta x \rightarrow 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x_0}$$

- Second-order finite difference formulas ... based on 3 points; error $\sim \Delta_x^2$

$$f'(x_i) \approx \frac{1}{\Delta_x} \left(-\frac{1}{2} f(x_i - \Delta_x) + \frac{1}{2} f(x_i + \Delta_x) \right) = \frac{1}{2\Delta_x} (-f(x_{i-1}) + f(x_{i+1}))$$

$$f''(x_i) \approx \frac{1}{\Delta_x^2} (f(x_i - \Delta_x) - 2f(x_i) + f(x_i + \Delta_x)) = \frac{1}{\Delta_x^2} (f(x_{i-1}) - 2f(x_i) + f(x_{i+1}))$$

5. Schrödinger equations

➤ **Fourth-order finite difference formulas** ... based on 5 points; error $\sim \Delta_x^4$

$$\begin{aligned} f'(x_i) &\approx \frac{1}{\Delta_x} \left(\frac{1}{12} f(x_i - 2\Delta_x) - \frac{2}{3} f(x_i - \Delta_x) + \frac{2}{3} f(x_i + \Delta_x) - \frac{1}{12} f(x_i + 2\Delta_x) \right) \\ &= \frac{1}{12 \Delta_x} (f(x_{i-2}) - 8 f(x_{i-1}) + 8 f(x_{i+1}) - f(x_{i+2})) \end{aligned}$$

$$f''(x_i) \approx \frac{1}{\Delta_x} \left(-\frac{1}{12} f(x_i - 2\Delta_x) + \frac{4}{3} f(x_i - \Delta_x) + \frac{4}{3} f(x_i + \Delta_x) - \frac{1}{12} f(x_i + 2\Delta_x) \right) = \dots$$

➤ **Symmetry of the central finite difference formulas:** ... preserves that the Hamiltonian matrix is hermitian; these schemes typically reduce the SE to a large but finite matrix equation that need to be solved for their eigenvalues and vectors.

5.1.b. Numerical solution of the free SE

Use of 2nd-order central finite-difference scheme:

➤ Application of 2nd-order central finite-difference formula to 1-dim SE:

$$-\frac{1}{2m} \frac{d^2 \psi(x)}{dx^2} = E \psi(x)$$

➤ **Eigenvalue problem with Hermitian matrix:** ... with periodic boundary conditions; ... obtain solution with

5. Schrödinger equations

- **Numerical mathematics:** Further analytical considerations possible; ... however, numerically often simpler,
 $\Delta p = 2\pi \hbar/n \Delta x$

$$E_j = \frac{2 \hbar^2}{m_o \Delta_x^2} \sin^2 \left(\frac{\pi j}{n} \right) = \frac{2 \hbar^2}{m_o \Delta_x^2} \sin^2 \left(\frac{\Delta_x p_j}{2 \hbar} \right)$$

- **Harmonic oscillator:** very similar, apart from additional diagonal matrix:

$$q \begin{pmatrix} \dots & & & & \\ & \phi(x_{i-1}) & & & \\ & & \phi(x_i) & & \\ & & & \phi(x_{i+1}) & \\ & & & & \dots \end{pmatrix}$$

5.1.c. Numerov's method

- **1-dim SE:** $\psi''(x) = f(x) \psi(x)$
- **Uniform grid in x :** $x_k = k \Delta_x$, Δ_x ... step size.
- **Taylor expansion for $\psi(x_{k\pm 1}) = \psi(x_k \pm \Delta_x)$:**

$$\psi(x_{k+1}) = \psi(x_k) + \sum_n \frac{(-1)^n}{n!} \Delta_x^n \psi^{(n)}(x_k)$$

$$\psi(x_{k-1}) = \psi(x_k) + \sum_n \frac{(-1)^n}{n!} (-\Delta_x)^n \psi^{(n)}(x_k)$$

$$\psi(x_{k+1}) + \psi(x_{k-1}) = 2 \psi(x_k) + \Delta_x^2 \psi''(x_k) + \frac{1}{12} \Delta_x^4 \psi^{(4)}(x_k) + \mathcal{O}(\Delta_x^6) \quad (*)$$

➤ Central difference operator δ , acting on general function $g(x)$:

$$\delta g(x) = g(x + \Delta_x/2) - g(x - \Delta_x/2)$$

$$\delta^2 g(x) = \delta [\delta g(x)] = g(x + \Delta_x) - 2g(x) + g(x - \Delta_x)$$

➤ Equation (*) can be transformed into:

$$\delta^2 \psi(x_k) = \Delta_x^2 \psi''(x_k) + \frac{1}{12} \Delta_x^2 \delta^2 \psi''(x_k) + \mathcal{O}(\Delta_x^6)$$

➤ For 1-dim SE above, we can replace $\psi''(x) \rightarrow f(x) \psi(x)$ and define a new function:

$$\phi(x_k) = \psi(x_k) (1 - \Delta_x^2 f(x_k)/12)$$

$$\phi(x_{k+1}) = 2\phi(x_k) - \phi(x_{k-1}) + \Delta_x^2 \underbrace{f(x_k) \psi(x_k)}_{\text{rhs of SE}} + \mathcal{O}(\Delta_x^6)$$

$$\phi_{k+1} = 2\phi_k - \phi_{k-1} + \Delta_x^2 f_k \psi_k + \mathcal{O}(\Delta_x^6), \quad g_k = g(x_k)$$

Numerov formula: elegant fifth-order integration scheme for 2nd order ode, error $\sim \mathcal{O}(\Delta_x^6)$

Integration in a box with boundary conditions:

➤ $\psi(x)$ defined for all $-\infty < x < \infty$: ... need to be restricted to a finite range; apply **boundary conditions**.

finite at $r \rightarrow 0$

for $r \rightarrow \infty$: use asymptotic form to construct starting values for $\psi(x_{\max})$

5. Schrödinger equations

- **Shooting techniques:** ... since energy is not known, make a trial ... improve it successively.
- **Soft potentials:** ... asymptotic behaviour known up to a constant ... normalization.
- **Initial-value problems:** ... just forward integration.

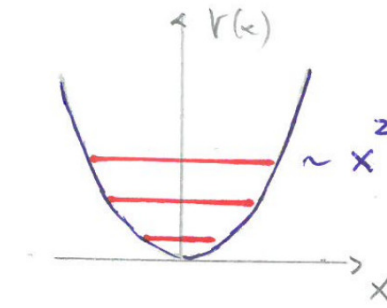
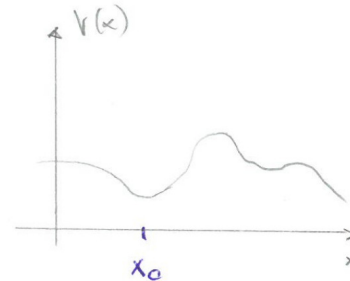
5.2. Harmonic oscillator

5.2.a. Reminder

- General potential $V(x)$

$$V(x) = V(x_0) + \left. \frac{dV}{dx} \right|_{x_0} (x - x_0) + \frac{1}{2} \left. \frac{d^2V}{dx^2} \right|_{x_0} (x - x_0)^2 + \approx \text{const.} + \frac{1}{2} \left. \frac{d^2V}{dx^2} \right|_{x_0} (x - x_0)^2 +$$

$$V(x) = \frac{a}{2} x^2 = \frac{m}{2} \omega^2 x^2, \quad \omega = \sqrt{\frac{a}{m}}$$



- **Time-independent SE:**

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m}{2} \omega^2 x^2 \right) \psi(x) = E \psi(x)$$

Importance of harmonic potentials

- **Looking for:** ... allowed energies E and stationary states $\psi(x)$.

➤ Substitution of variables: ... simplifies SE $u(y) = \psi(x(y))$

$$\alpha = \frac{2E}{\hbar\omega}; \quad y = \sqrt{\frac{m\omega}{\hbar}} x = \frac{x}{b}, \quad b = \sqrt{\frac{\hbar}{m\omega}} \quad \Longrightarrow \quad \left[\frac{d^2}{dy^2} + (\alpha - y^2) \right] u(y) = 0$$

Behavior form $y \rightarrow \pm\infty, \quad y^2 \gg \alpha$

$$u''(y) \approx y u(y) \quad \Longleftrightarrow \quad u(y) \sim e^{\pm y^2/2} \quad (y \rightarrow \pm\infty) \quad \text{normalizable only } e^{-y^2/2}$$

➤ Solution by power series:

- Energies of harmonic oscillator: $E = \frac{\hbar\omega}{2} (2n + 1) = (n + \frac{1}{2}) \hbar\omega, \quad n = 0, 1, 2, \dots$

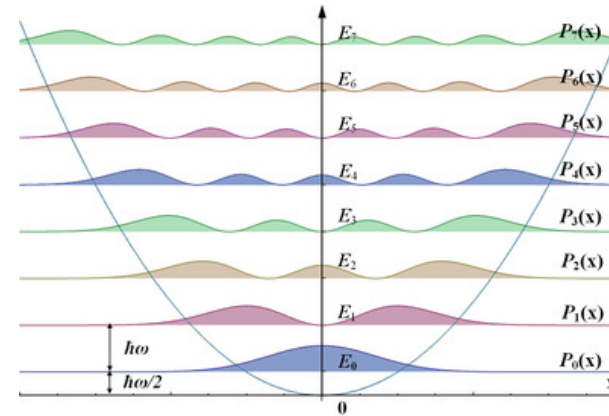
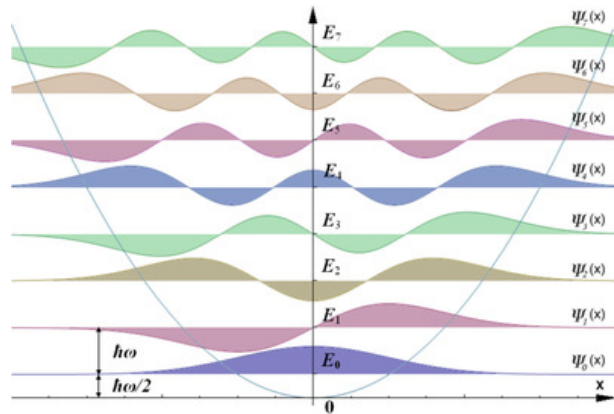
- Eigenfunctions:

$$\begin{aligned} \psi_n(x) = u(y(x)) = e^{-y^2/2} H_n(y(x)) \\ \int dx |\psi_n(x)|^2 = 1 \end{aligned} \quad \Longleftrightarrow \quad \psi_n(x) = \frac{c_n}{\sqrt{b}} H_n\left(\frac{x}{b}\right) e^{-\frac{x^2}{2b^2}}, \quad b = \sqrt{\frac{\hbar}{m\omega}}$$

- Two lowest (normalized) solutions:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right), \quad \psi_1(x) = \left(\frac{4}{\pi}\right)^{1/4} \left(\frac{m\omega}{\hbar}\right)^{3/4} x \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

5. Schrödinger equations



Wave functions $\psi_n(x)$ and probability $p_n(x) = |\psi_n(x)|^2$ for the lowest solutions of the harmonic oscillator. From: <https://de.wikipedia.org/wiki>.

➤ Short remarks:

- **Ground-state energy:** $\frac{1}{2} \hbar \omega$
- **Two-atomic molecules:** Vibration spectra due to vibrations around the equilibrium position of the atoms; absorbed and emitted photons have multiple energies of $\hbar \omega$.

➤ 3-dimensional harmonic oscillator: ... potential and solutions

$$V(x, y, z) = \frac{a}{2} x^2 + \frac{b}{2} y^2 + \frac{c}{2} z^2 = \frac{m}{2} (\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 X(x)}{\partial x^2} + \frac{m_e}{2} \omega_1^2 x^2 X(x) = E_1 X(x), \quad \omega_1 = \frac{a}{m}; \quad \dots$$

$$E_{n_1 n_2 n_3} = \hbar \omega_1 \left(n_1 + \frac{1}{2} \right) + \hbar \omega_2 \left(n_2 + \frac{1}{2} \right) + \hbar \omega_3 \left(n_3 + \frac{1}{2} \right)$$

$$\psi_{n_1 n_2 n_3}(x, y, z) = H_{n_1}(\tilde{x}) H_{n_2}(\tilde{y}) H_{n_3}(\tilde{z}) e^{-\frac{1}{2}(\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2)} \quad H_n \quad \dots \text{ Hermite polynomials}$$

$$\tilde{x} = \sqrt{\frac{m \omega_1}{\hbar}} x; \quad \tilde{y} = \sqrt{\frac{m \omega_2}{\hbar}} y; \quad \tilde{z} = \sqrt{\frac{m \omega_3}{\hbar}} z;$$

5.3. Variational techniques

5.3.a. Rayleigh-Ritz method

Variation of energy functional:

- Trial function $\psi_{\{p_i\}}(\mathbf{x})$: ... real parameter $\{p_i\}$
- Energy functional: ... energy expectation value

$$E[\psi_{\{p_i\}}] = \frac{\langle \psi_{\{p_i\}} | H | \psi_{\{p_i\}} \rangle}{\langle \psi_{\{p_i\}} | \psi_{\{p_i\}} \rangle} \iff \frac{d E[\psi_{\{p_i\}}]}{d p_i} = 0 \quad \text{for all } p_i$$

- **Minimization:** variation of the the energy functional with regard to $\{p_i\}$.
This is typically a very complex (formidable) task.
- Expansion in basis states $\{\phi_i(\mathbf{x})\}$:

$$\psi_{\{p_i\}}(\mathbf{x}) = \sum_{i=1}^N p_i \phi_i(\mathbf{x}) \iff \text{secular equation}$$

5.3.b. Variational calculations in an orthonormal basis

Matrix form of the SE in a discrete orthonormal basis:

➤ Orthonormal basis $\{|m\rangle\}$: $\langle m | n \rangle = \delta_{mn}$

➤ SE: $H |\psi\rangle = E |\psi\rangle$, $|\psi\rangle = \sum_n c_n |n\rangle \implies \sum_n c_n H |n\rangle = E \sum_n c_n |n\rangle$

➤ Projection upon $\langle m|$ to the left:

$$\sum_n H_{mn} c_n \equiv \sum_n \langle m | H | n \rangle c_n = E c_m, \quad \text{for all } m = 1 \dots n$$

$$\begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \quad n \times n \text{ eigenvalue problem}$$

$$\sum_n \langle m | H - E I | n \rangle c_n = 0 \quad \iff \quad (\mathbf{H} - E \mathbf{I}) \mathbf{c} = 0$$

Secular equation: Diagonalization of Hamiltonian matrix.

Variational computations: Condition for energy minimization is equivalent to fulfill the matrix SE.

Discretization in a finite box:

- Diagonalization in a finite box with periodic boundary conditions: V ... volume of the box

$$\mathbf{k} \equiv \phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} \exp(-i \mathbf{k} \cdot \mathbf{x}) \quad \Longrightarrow \quad c_{\mathbf{k}} = \frac{1}{\sqrt{V}} \int d^3x \exp(-i \mathbf{k} \cdot \mathbf{x}) \psi(\mathbf{x})$$

Fourier transform of the wave function.

- Allowed wave vectors satisfying the periodic boundary conditions:

$$\mathbf{k} = (k_x, k_y, k_z) = \left(n_x \frac{2\pi}{L_x}, n_y \frac{2\pi}{L_y}, n_z \frac{2\pi}{L_z} \right), \quad n_x, n_y, n_z \quad \dots \text{integers}$$

5.3.c. Variational calculations in an non-orthonormal basis

- Nonorthonormal basis $\{|m\rangle\}$: $\langle m | n \rangle = S_{mn} \neq \delta_{mn}$

- Projection upon $\langle m |$ to the left:

$$\sum_n H_{mn} c_n \equiv \sum_n \langle m | H | n \rangle c_n = E \sum_n \langle m | n \rangle c_n = E \sum_n S_{mn} c_n, \quad \text{for all } m = 1 \dots n$$

$$\begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} S_{11} & S_{12} & \dots \\ S_{21} & S_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \quad \Longleftrightarrow \quad \mathbf{H} \mathbf{c} = E \mathbf{S} \mathbf{c}$$

Generalized eigenvalue equation: overlap matrix \mathbf{S} .

- Can be traced back to matrix diagonalization, if the overlap matrix is first diagonalized by means of a similarity transformation: $\mathbf{B}^{-1} \mathbf{S} \mathbf{B} = \mathbf{S}_D$
- **Numerical libraries** ... routines for generalized eigenvalue problem are often available.

5.4. Solution of time-dependent SE

5.5. Tasks

See tutorials.

6. Hydrogenic atoms

6.1. Separation of the Schrödinger equation in spherical coordinates

➤ Many physical systems are approximately spherical-symmetric and, thus, can be described in **spherical coordinates**.

➤ **Spherical-symmetric potentials, central fields:** $V = V(r)$... (r, ϑ, φ) spherical coordinates

➤ **Laplacian in spherical coordinates:**

$$\begin{aligned}\frac{\partial}{\partial \mathbf{r}^2} &= \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{r^2 \sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{\mathbf{L}^2}{\hbar^2 r^2}\end{aligned}$$

6. Hydrogenic atoms

➤ SE in spherical coordinates:

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right\} \psi(\mathbf{x}) = E \psi(\mathbf{x})$$

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\mathbf{L}^2}{2m r^2} + V(r) \right] \psi(r, \vartheta, \varphi) = E \psi$$

➤ $Y_{\ell m}$'s are EF for \mathbf{L}^2 , ... separation is therefore possible

$$\psi(r, \vartheta, \varphi) = R(r) Y_{\ell m}(\vartheta, \varphi)$$

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\hbar^2 \ell(\ell+1)}{2m r^2} + V(r) \right] R(r) = E R(r) \quad \text{bzw. mit} \quad R(r) = \frac{P(r)}{r}$$

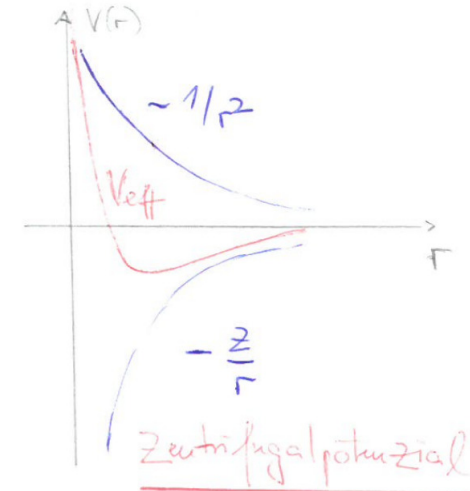
$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2m r^2} + V(r) \right] P(r) = E P(r)$$

radiale SG

➤ Remarks:

- H is invariant (scalar) w.r.t. rotations, hence: $[H, \mathbf{L}] = [H, \mathbf{L}^2] = [H, L_z] = 0$
 H, \mathbf{L}^2, L_z have a common system of eigenfunctions (together diagonalizable).
- Analogue to 1-dim SE ... if terms are interpreted as

$$\frac{\hbar^2 \ell(\ell+1)}{2m r^2} + V(r) = V_{\text{eff}} \quad \dots \text{effective potential}$$



- Boundary conditions and normalization for $P(r)$:

$$\lim_{r \rightarrow \infty} |P(r)| \leq \frac{a}{r^{(1/2+\epsilon)}} \quad \text{mit } \epsilon > 0$$

$P(r \rightarrow 0) = 0$, since otherwise $\Delta \psi = \nabla^2 \frac{P(r)}{r} \Big|_{r=0} \approx \delta(\mathbf{r}) P(0)$ infinite.

- $|P(r)|^2 dr$... probability to find particle in the intervall $r \dots r + dr$, since

$$|P(r)|^2 dr = |R(r)|^2 r^2 dr \underbrace{\int_0^\pi d\vartheta \sin \vartheta \int_0^{2\pi} d\varphi |Y_{\ell m}(\vartheta, \varphi)|^2}_{\text{normalization of spherical harmonics}}$$

6.2. Radial Schrödinger equation

➤ Coulomb potential: $V(r) = -\frac{Z e^2}{4\pi \epsilon_0 r}$

➤ Assumption: Elektron bewegt sich im Kraftfeld des im Koordinatenursprung **festgehaltenen Kernes**; gleiche Form der radialen SG gilt jedoch auch, wenn für die Elektronenmasse $m_e \rightarrow \mu = \frac{m_e m_N}{m_e + m_N} \lesssim m_e$ verwendet wird.

6. Hydrogenic atoms

➤ **Solution by power series:** ... substitution gives ode for $F(\rho)$

$$F(\rho) = \sum_{k=0}^{\infty} a_k \rho^k \quad \Longrightarrow \quad \rho \frac{d^2 F(\rho)}{d\rho^2} + 2(\ell + 1 - \rho) \frac{dF}{d\rho} + (\rho_0 - 2(\ell + 1)) F = 0$$

➤ **Energies:**

$$E_n = -\frac{m Z^2 e^4}{2 \hbar^2 n^2} \quad n = 1, 2, \dots; \quad \ell = 0, 1, \dots, n - 1;$$

➤ **Degenerate energies E_n**

- principal quantum numbers: $n = 1, 2, \dots$
- orbital angular momentum QN: $\ell = 0, 1, \dots, n - 1$
- magnetic quantum number: $m = -\ell, -\ell + 1, \dots, \ell$

$$\sum_{\ell=0}^{n-1} (2\ell + 1) = 2 \frac{n(n-1)}{2} + n = n^2 \quad \left\{ \begin{array}{lll} n = 1 & \ell = 0 \text{ (s - Orbital)} & m = 0 & E_1, \text{ 1 - fold} \\ n = 2 & \ell = 0 \text{ (s)} & m = 0 & \\ & \ell = 1 \text{ (p)} & m = -1, 0, 1 & E_2, \text{ 4 - fold} \\ n = 3 & \ell = 0 \text{ (s)} & m = 0 & \\ & \ell = 1 \text{ (p)} & m = -1, 0, 1 & \\ & \ell = 2 \text{ (d)} & m = -2, -1, 0, 1, 2 & E_3, \text{ 9 - fold} \end{array} \right.$$

n^2 -fold degenerate energies in a (pure) Coulomb field

- **Spin:** allows 2 electrons for each $\psi_{n\ell m}(r, \vartheta, \varphi)$
 $2n^2$ electrons for each n ; $2(2\ell + 1)$ for each ... (electron) shell ($n \ell$)
- Restrictions for the allowed quantum numbers ... due to (generating) ODE for Laguerre and associated Laguerre polynomials
 - (i) **radial function** $N = n - \ell - 1$... positive zeros (knots).
 - (ii) $R_{n\ell}(r) = \frac{P_{n\ell}(r)}{r}$... does not depend on m in any spherical potential.
 - (iii) $|\psi_{n\ell m}|^2 d^3x = |\psi_{n\ell m}(r, \vartheta, \varphi; t)|^2 r^2 dr d\Omega$... probability distribution in dr and $d\Omega$;
 $|R_{n\ell}(r)|^2 r^2 dr \equiv P_{n\ell}^2 dr$... radial distribution function

6.3. B-splines

6.4. Numerical solution of radial Coulomb problem

6.4.a. Finite-difference approach

6.4.b. B-spline approach

6.5. Realistic atomic potentials

6.5.a. Further corrections for hydrogenic atoms

6. Hydrogenic atoms

- i) **H-atom is already a two-body problem:** nucleus + electron \rightsquigarrow coordinate transformation into the center-of-mass system gives rise to a **one-body problem with reduced mass:**

$$\mu = \frac{m_e m_p}{m_e + m_p} = \frac{m_e}{1 + m_e/m_p} \approx \underbrace{\frac{m_e}{1.000545}}_{\text{correction in 4. digit}} \quad \text{but : positronium } e^- e^+ : \mu = \frac{m_e}{2}$$

- ii) **'Relativistic' effects cause fine-structure,** i.e. splittings and corrections of order α^2

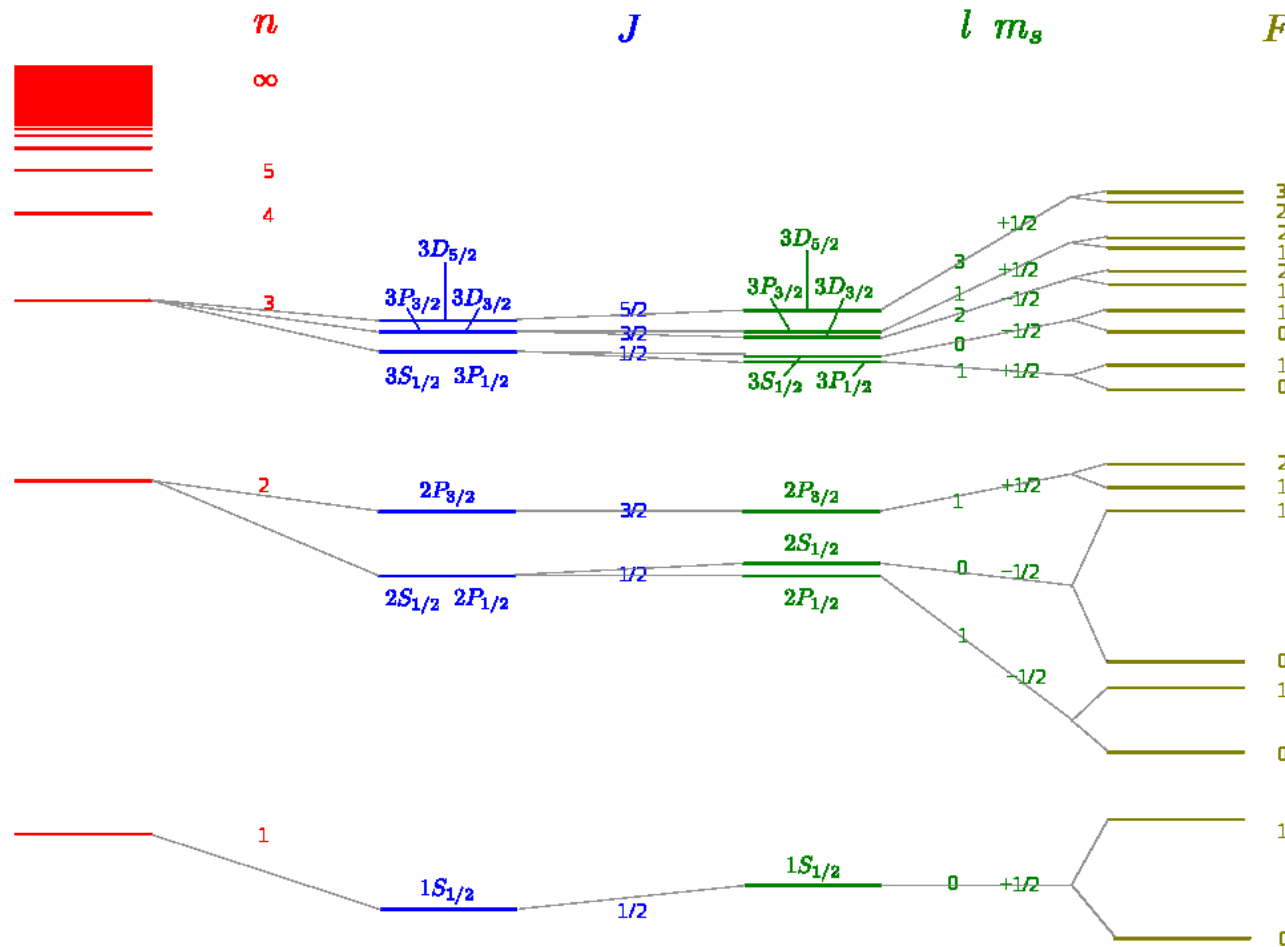
- relativistic correction (increase) of the electron mass
- Darwin term
- spin-orbit coupling ... or
- simply apply: ... **Dirac's equation**

- iii) **Lamb-shift:** quantum-field theoretical correction of order $\alpha^3 \ln \alpha$; requires QED-description.

$$E_{2s} - E_{2p_{1/2}} \approx 4.3 \cdot 10^{-6} \text{ eV}$$

- iv) **Hyperfine structure:** Interaction of the magnetic moments of the electrons and nucleons (nucleus); important only for ns -orbitals, $\simeq 1/n^3$.

$$\Delta E_{1s}^{(\text{HFS})} = 5.8 \cdot 10^{-6} \text{ eV} \quad \rightarrow \quad 21 \text{ cm}^{-1} \text{ (H - atom) line in radio astronomy}$$



6.5.b. Numerical estimation of the finite-nuclear size contribution

Bohr

Feinstruktur

Lamb-Verschiebung

Hyperfeinstruktur

6.6. Central-field approximations

Lösungen der Schrödingergleichung ohne Spin. Entartung: n^2

Spin-Bahn-Kopplung und relativistische Korrektur.

Strahlungs-korrektur (QED)

Spin-Spin-Kopplung (Energieskala 100-mal gestreckt)

6.6.a. The central-field model

6. Hydrogenic atoms

➤ Coulomb Hamiltonian:

$$\begin{aligned}
 H_C &= H_o + H' \\
 &= \sum_i \left(-\frac{\nabla_i^2}{2} - \frac{Z}{r_i} \right) + \sum_{i < j} \frac{1}{r_{ij}} = \sum_i \left(-\frac{\nabla_i^2}{2} - \frac{Z}{r_i} + u(r_i) \right) + \sum_{i < j} \frac{1}{r_{ij}} - \sum_i u(r_i).
 \end{aligned}$$

Choose: $u(r_i)$, such that the repulsion with the $N - 1$ other electrons, when averaged over time, is well described.

➤ Independent-particle model (IPM):

Each electron moves independent of all other electrons in the central field of the nucleus and the $N - 1$ remaining electrons.

Hope: $H_o \gg H'$, i.e. H' can be treated later by perturbation theory.

➤ Solutions to H_o ... product functions of one-electron orbital functions

$$\phi_k(\mathbf{r}, \sigma) = \frac{1}{r} P_{n_k \ell_k}(r) Y_{\ell_k m_{\ell_k}}(\vartheta, \varphi) \chi_{m_{s_k}}(\sigma) = |n_k \ell_k m_{\ell_k}, m_{s_k}\rangle$$

➤ Spin-orbitals: one-electron functions

$$\langle \phi_k | \phi_p \rangle = \langle n_k \ell_k m_{\ell_k}, m_{s_k} | n_p \ell_p m_{\ell_p}, m_{s_p} \rangle = \delta_{kp} = \delta_{n_k n_p} \delta_{\ell_k \ell_p} \delta_{m_{\ell_k} m_{\ell_p}} \delta_{m_{s_k} m_{s_p}}$$

6.6.b. Product functions and Slater determinants

➤ H_o has one-particle character: ... each product function is solution for H_o .

$$\psi = \phi_1(\mathbf{x}_1) \phi_2(\mathbf{x}_2) \dots \phi_N(\mathbf{x}_N) \quad \mathbf{x} = (\mathbf{r}, \sigma)$$

- **Pauli principle:** No two electrons may agree in all quantum numbers, $n l, m_l, m_s$
- $[H, P_{ij}] = 0$ for all $i \neq j$. **Solutions must be totally antisymmetric.**
- **Slater determinants:** ... simplest form of antisymmetric solutions

$$\psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1) & \phi_1(2) & \dots & \phi_1(N) \\ \phi_2(1) & \phi_2(2) & \dots & \phi_2(N) \\ \dots & \dots & \dots & \dots \\ \phi_N(1) & \phi_N(2) & \dots & \phi_N(N) \end{vmatrix} = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \phi_1(k_1) \phi_2(k_2) \dots \phi_N(k_N)$$

$N!$ terms; this form is nevertheless quite simple for practical computations.

- **Remark:** There are (much) more complicated functions ψ possible which fulfill the requirements from above since H_o and $\{P_{ij}, i \neq j\}$ do NOT describe a complete set of operators.
- **Norm:**

$$\begin{aligned} \langle \psi | \psi' \rangle &= \frac{1}{N!} \sum_{PP'} (-1)^{P+P'} \langle \phi_1(k_1) \phi_2(k_2) \dots \phi_N(k_N) | \phi'_1(k'_1) \phi'_2(k'_2) \dots \phi'_N(k'_N) \rangle \\ &= \frac{1}{N!} \sum_P (-1)^{2P} \delta_{\psi\psi'} = \delta_{\psi\psi'} \end{aligned}$$

- For free atoms, however, also

$$[H, \mathbf{J}^2] = [H, J_z] = 0; \quad \mathbf{J} = \sum_{i=1}^N (\mathbf{l}_i + \mathbf{s}_i)$$

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i.e. solutions to H (or H_0) can be classified by the J, M quantum numbers, while **determinants are in general NO eigenfunctions for \mathbf{J}^2** , only to J_z with eigenwert $M = \sum_i (m_{\ell_i} + m_{s_i})$.

- The complete classification of the **many-electron quantum states require** further quantum numbers; usually **$4N$ quantum numbers.**

6.6.c. Equivalent electrons. Electron configurations and the PSE

- **Electron orbitals:** $\phi_k(\mathbf{r}, \sigma); \quad k = (n \ell m_\ell, m_s)$

➡ all functions with equal quantum numbers $(n\ell)$ but different (m_ℓ, m_s) are degenerate in any central-field potential. They are called **equivalent electron orbitals** or short **equivalent electrons.**

- Set of (maximal) $q = 2(2\ell + 1)$ equivalent electrons form a subshell: **$(n\ell)^w$**

- **Electron configuration:**

$$(n_1 \ell_1)^{q_1} (n_2 \ell_2)^{q_2} \dots (n_r \ell_r)^{q_r} \quad 0 \leq q_i \leq 2(2\ell_i + 1) \quad \sum_{i=1}^r q_i = N$$

- **Shell notations in atomic spectroscopy:**

K-shell:	$n = 1$	$(1s)$
L	$n = 2$	$(2s + 2p)$
M	$n = 3$	$(3s + 3p + 3d)$
N	$n = 4$	$(4s + 4p + 4d + 4f)$
O	$n = 5$	$(5s + 5p + 5d + 5f + 5g)$

➤ **Atomic shell model:** ... total charge density of a filled subshell is **spherical symmetric**, since

$$\rho_{subshell} = e \frac{1}{r^2} |P_{n\ell}|^2 \sum_{m=-\ell}^{\ell} \sum_{m_s} |Y_{\ell m}|^2 |\chi_{m_s}|^2 = \frac{2(2\ell + 1)}{4\pi r^2} |P_{n\ell}|^2$$

i.e. the equivalent electrons of any filled subshell form indeed a **spherical symmetric shell (Unsöld's theorem)**.

➤ **Central-field model (approximation):** ... theoretical basis for the periodic table of elements

➤ **Rydberg series (of configurations):** $2p^5 3p$, $2p^5 4p$, $2p^5 5p$, ...

The fully occupied core is typically omitted from the notation.

➤ **Aufbau principle:** Electron shells ($n\ell$) are filled successively due to their energy, from shells with large binding energies to those with lower energy. In practice, deviations from this principle occur already for $Z \gtrsim 18$ (argon):

- $(n + 1)s$ and $(n + 1)p$ are often filled before the nd shell \rightsquigarrow **transition metals**.

$3d$... iron group $Z = 21, \dots, 28$

$4d$... palladium group $Z = 39, \dots, 46$

$5d$... platinum group $Z = 71, \dots, 78$

- nf -shells are filled 'afterwards' ($4f$... lanthanides, $5f$... actinides);
- filled and half-filled shells are particularly stable.

Blackboard example (Low-lying electron configurations of light elements):

Blackboard example (Alkali atoms):

6. Hydrogenic atoms

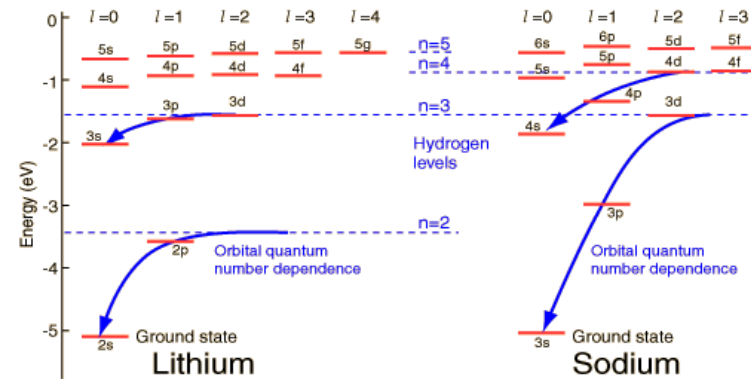


Figure 6.1.: For alkali atoms, a rather strong orbital angular momentum dependence is found for the low-lying energy levels; from <http://hyperphysics.phy-astr.gsu.edu>.

6.6.d. Thomas-Fermi model

Thomas-Fermi model & equation:

➤ **Thomas-Fermi model:** Electrons form a Fermi gas (Fermi-Dirac statistic)

electron density \rightarrow electrostatic potential

➤ **Phase space volume of electrons:** $\frac{4\pi}{3} p^3 dV$

V ... volume, p ... isotropically distributed momentum of the electrons.

➤ Pauli's principle: max. 2 electrons / ($h^3 \times$ phase space volume)

➤ Maximum electron number with $p \leq p_o$ per unit volume (at zero temperature):

$$u = \frac{2}{h^3} \frac{4\pi}{3} p_o^3 = \frac{8\pi}{3h^3} (2mT_o)^{2/3}$$

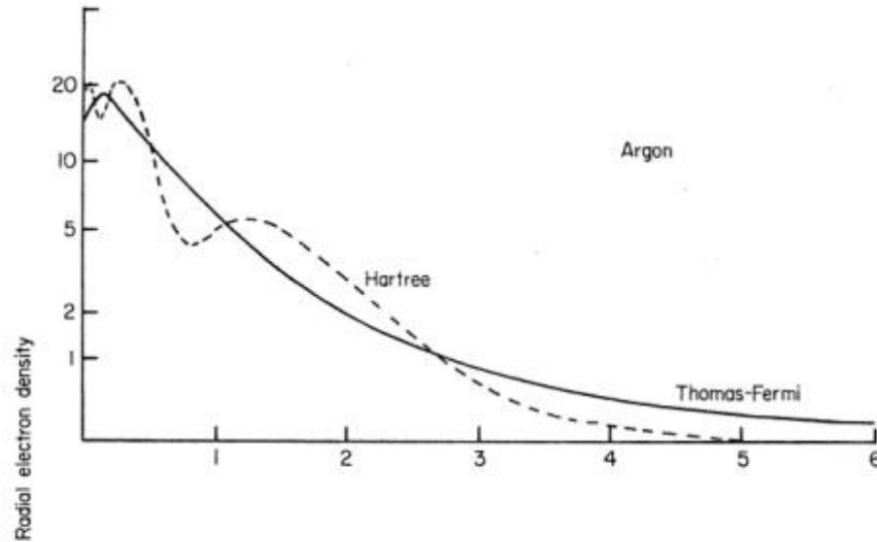


Figure 6.2.: Comparison between the Thomas-Fermi electron densities (from which the potential can be derived) and more accurate quantum-mechanical Hartree densities, obtained in the independent-electron approximation.; from <http://www.virginia.edu/ep/Interactions/>.

- Bound electrons: $T - e\phi \leq 0 \rightsquigarrow T_o = T_{max} = e\phi$
- Charge density $\rho = -en = -\frac{8\pi}{3h^3} e (2me\phi)^{3/2}$
- Potential and charge density are related to each other via the Poisson equation $\Delta\phi = -\rho/\epsilon_o$ and by applying the proper boundary conditions as well as the substitutions below:

$$\Delta\phi = \frac{8\pi}{3h^3\epsilon_o} e (2me\phi)^{3/2}, \quad \lim_{r \rightarrow 0} \phi(r) = -\frac{Ze}{4\pi\epsilon_o r}, \quad \lim_{r \rightarrow \infty} r\phi(r) = 0$$

$$\phi(r) = \chi(r) \frac{Ze}{4\pi\epsilon_o r} \quad r = bx \quad \text{with} \quad b = \left(\frac{3\pi^2}{2^7}\right)^{1/3} \frac{4\pi\epsilon_o \hbar^2}{me^2} Z^{-1/3} \approx 0.885 a_o Z^{-1/3}$$

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➤ **Thomas-Fermi equation:**

$$\frac{d^2\chi}{dx^2} = x^{-1/2} \chi^{3/2}$$

Universal equation for all atoms (within the TF model) which can be solved numerically; $\chi(r)$ describes the screening of the nuclear charge and b a weak Z -dependent scaling factor.

6.6.e. Effective potentials

6.6.f. Self-consistent-fields

6.7. Tasks

See tutorials.

6.8. Atomic theory and computations in a nut-shell

6.8.a. Atomic spectroscopy: Level structures & collisions

Atomic processes & interactions:

- **Spontaneous emission/fluorescence:** ... occurs without an ambient electromagnetic field; related also to absorption.
- **Stimulated emission:** ... leads to photons with basically the same phase, frequency, polarization, and direction of propagation as the incident photons.
- **Photoionization:** ... release of free electrons.
- **Rayleigh and Compton scattering:** ... Elastic and inelastic scattering of X-rays and gamma rays by atoms and molecules.
- **Thomson scattering:** ... elastic scattering of electromagnetic radiation by a free charged particle (electrons, muons, ions); low-energy limit of Compton scattering.
- **Multi-photon excitation, ionization and decay:** ... non-linear electron-photon interaction.
- **Autoionization:** ... nonradiative electron emission from (inner-shell) excited atoms.
- **Electron-impact excitation & ionization:** ... excited and ionized atoms; occurs frequently in astro-physical and laboratory plasmas.
- **Elastic & inelastic electron scattering:** ... reveals electronic structure of atoms and ions; important for plasma physics.
- **Pair production:** ... creation of particles and antiparticles from the internal of light with matter (electron-positron pairs).

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- **Delbrück scattering:** ... deflection of high-energy photons in the Coulomb field of atomic nuclei; a consequence of vacuum polarization.
- ...
- In practice, the distinction and discussion of different atomic and electron-photon interaction processes also depends on the particular community/spectroscopy.

6.8.b. Atomic theory

Covers a very wide range of many-body methods and techniques, from the simple shell model of the atom to various semi-empirical method to mean-field approaches ... and up to advanced ab-initio and quantum-field theories. The aim of ab-initio atomic structure and collision theory is to describe the (electronic) level structure, properties and dynamical behaviour on the basis of the (many-electron) Schrödinger equation or by even applying field-theoretical techniques.

Well, ... this is quite an ambitious task, and with a lot of surprises when it comes to details.

Atomic theory is a great playground, indeed.

Requires good physical intuition, or this is typically beneficial, at least.

Theoretical models:

- **Electronic structure of atoms and ions:** is described quantum mechanically in terms of wave functions, energy levels, ground-state densities, etc., and is usually based on some atomic (many-electron) Hamiltonian.
- **Interaction of atoms with the radiation field:** While the matter is treated quantum-mechanically, the radiation is — more often than not (> 99 % of all case studies) — described as a classical field.
- This semi-classical treatment is suitable for a very large class of problems, sometimes by incorporating ‘ad-hoc’ quantum effects of the em field (for instance, spontaneous emission).
- Full quantum treatment: of the radiation field is very rare in atomic and plasma physics and requires to use quantum-field theoretical techniques; for example, atomic quantum electrodynamics (QED).

Combination of different (theoretical) techniques:

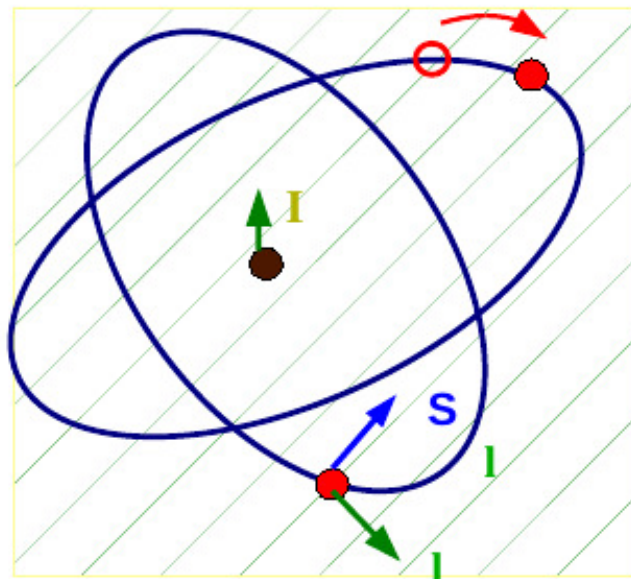
- Special functions from mathematical physics (spherical harmonics, Gaussian, Legendre- and Laguerre polynomials, Whittaker functions, etc.).
- Racah’s algebra: Quantum theory of angular momentum.
- Group theory and spherical tensors.
- Many-body perturbation theory (MBPT, coupled-cluster theory, *all-order* methods).
- Multiconfigurational expansions (CI, MCDF).
- Density matrix theory.

6.9. Need of (accurate) atomic theory and data

- **Astro physics:** Analysis and interpretation of optical and x-ray spectra.
- **Plasma physics:** Diagnostics and dynamics of plasma; astro-physical, fusion or laboratory plasma.
- **EUV lithography:** Development of UV/EUV light sources and lithographic techniques (13.5 nm).
- **Atomic clocks:** Design of new frequency standards; requires accurate data on hyperfine structures, atomic polarizabilities, light shift, blackbody radiation, etc.
- **Search for super-heavy elements:** beyond fermium ($Z = 104$); ‘island of stability’; better understanding of nuclear structures and stabilities.
- **Nuclear physics:** Accurate hyperfine structures and isotope shifts to determine nuclear parameters; formation of the medium and heavy elements.
- **Surface & environmental physics:** Attenuation, autoionization and light scattering.
- **X-ray science:** Ion recombination and photon emission; multi-photon processes; development of x-ray lasers; high-harmonic generation (HHG).
- **Fundamental physics:** Study of parity-nonconserving interactions; electric-dipole moments of neutrons, electrons and atoms; ‘new physics’ that goes beyond the standard model.
- **Quantum theory:** ‘complete’ experiments; understanding the frame and boundaries of quantum mechanics ?
- ...

Hierarchy of inner-atomic interactions

-- self-consistent fields vs. perturbation theory



External fields

★ Motion of the nucleus: Reduced mass and mass polarization

- Nuclear potential
- Instantaneous Coulomb repulsion between all pairs of electrons
- Spin-orbit interaction
- Relativistic electron velocities; magnetic contributions and retardation
- QED: radiative corrections
- Hyperfine structure
- Electric and magnetic nuclear moments (isotopes)

Figure 6.3.: Atomic interactions that need to be considered for a quantitative description/prediction of atoms.

6. Hydrogenic atoms

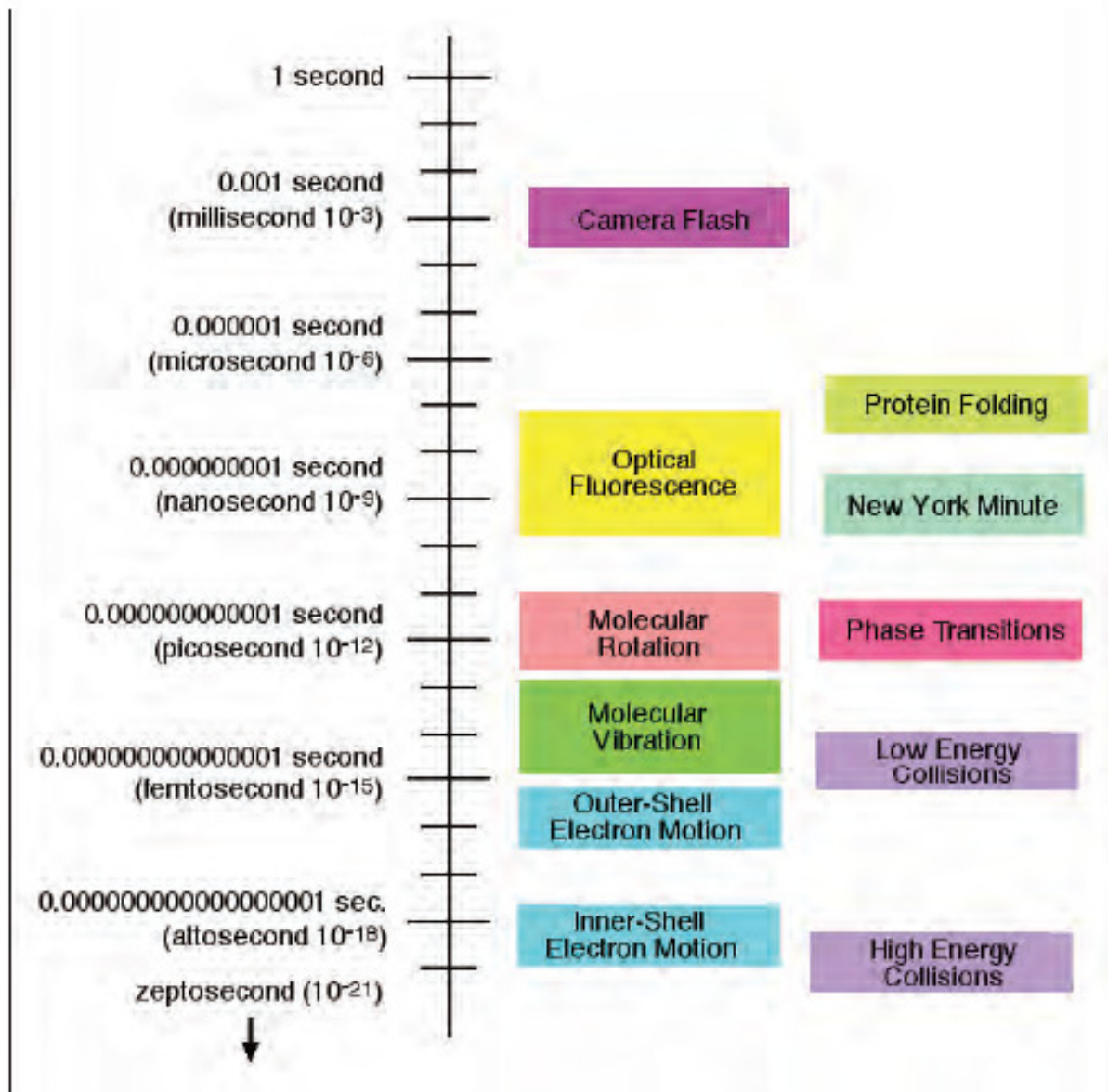


Figure 6.4.: Characteristic time scales of atomic and molecular motions; taken from: *Controlling the Quantum World*, page 99.