Computational Quantum Physics

— Lecture script —

WS 2014/2015

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

(Script and additional material)

Stephan Fritzsche

Helmholtz-Institut Jena &

Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena

Fröbelstieg 3, D-07743 Jena, Germany

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

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Contents

0. Preliminary remarks

0.1. Schedule and agreements

Lecture period:	20. 10. 2014 – 10. 02. 2015
Lecture:	Fr 8 – 10, Max-Wien-Platz (Physik, SR 1)
Tutorial:	Thu 10 – 12, Computerpool, Physik (...)
Language:	German / English ??
ECTS points:	4 (inclusive the tasks and exam).
Exam:	Tasks (40 %), oral exam or a home task including some moderate programming.
Requirements for exam:	*Modulanmeldung* 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 ?? Who makes regularly use of Maple oder Mathematica ?? Who has used the PAF computer pool ??

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.

1.2. Modern fields of (theoretical) quantum physics

Well-established fields of quantum physics: ... (Blackboard)

Recently emerging fields:

- ➢ Quantum control theory.
- ➢ Quantum engineering (generation, tomography and use of quantum states, ...).
- ➢ Quantum information theory and processing.
- ➢ Light-matter interaction 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.
- ➢ ...

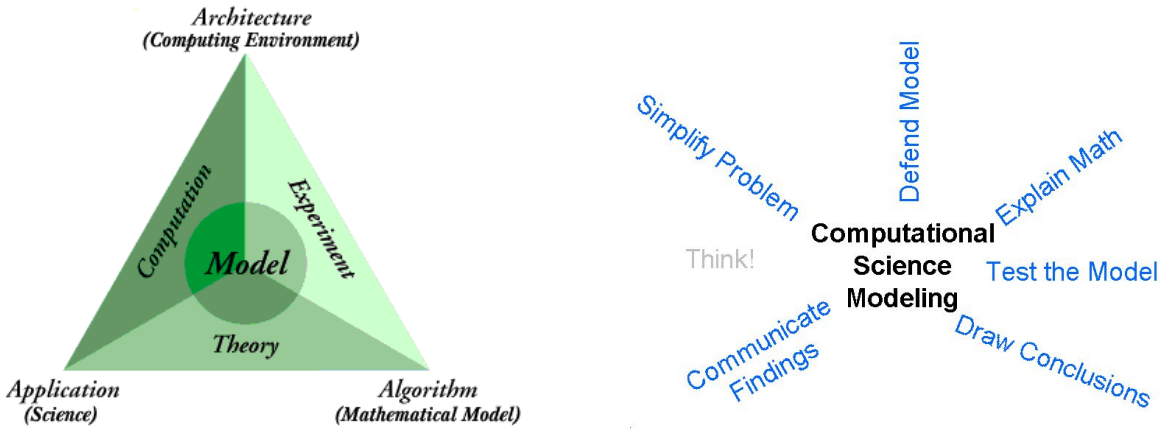


Figure 1.1.: Left: Interplay of experiment, theory and computations in science (taken from www.shodor.org/chemviz/overview). Right: Abilities to be trained in order to make use of this interplay (from www.ncsec.org/cadre2/)

1.3. Programming languages in physics

Programming languages used in physics: ... (Blackboard)

High-level programming (HLP) languages; properties: ... (Blackboard)

The Fortran 90 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 very modern programming language, perhaps the most modern;
- ➢ 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 intrinsice functions and protection of code;
- ➢ Object-oriented features: Abstract data types – Polymorphism – Hidden code;
  it misses inheritance.
- ➢ Intrinsic feature for parallelization;
- ➢ Relatively easy to learn;
- ➢ Many commercial and open-source compilers available;
  gfortran; free open source Fortran 90/95/2003/2008 compiler;
- ➢ ...

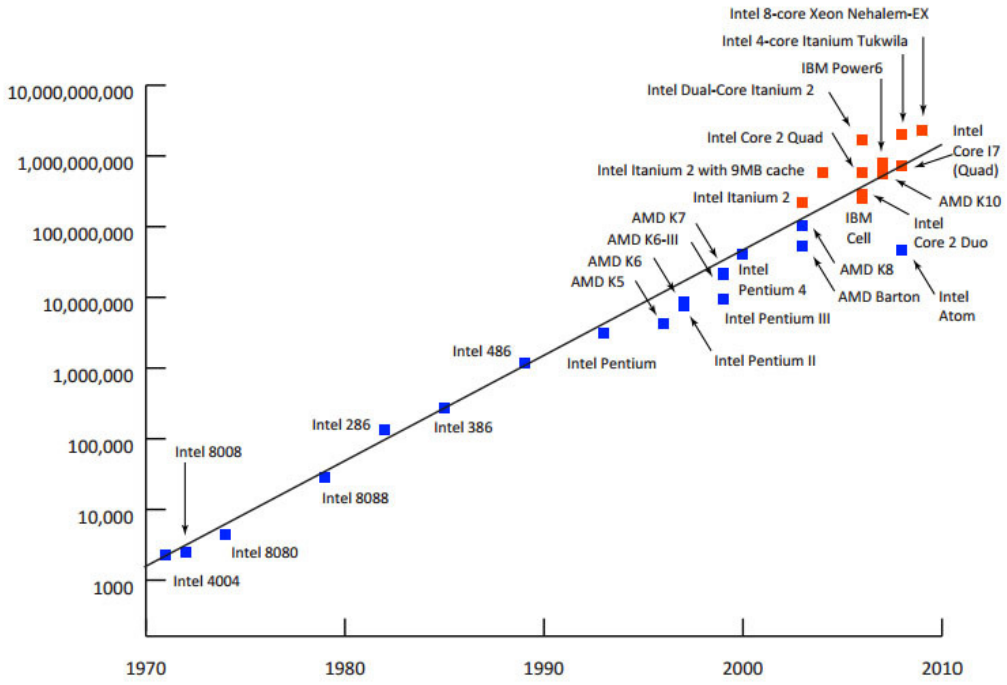


Figure 1.2.: Moore's law in term of transitors as realized on individual processor ships (from wrapidconsultingusa.com/wp-content/).

Variables and declarations in Fortran: ... (Blackboard)

Some reasons for using C++: ... (Blackboard)

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.
- ...
- 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)]: ... (Blackboard)

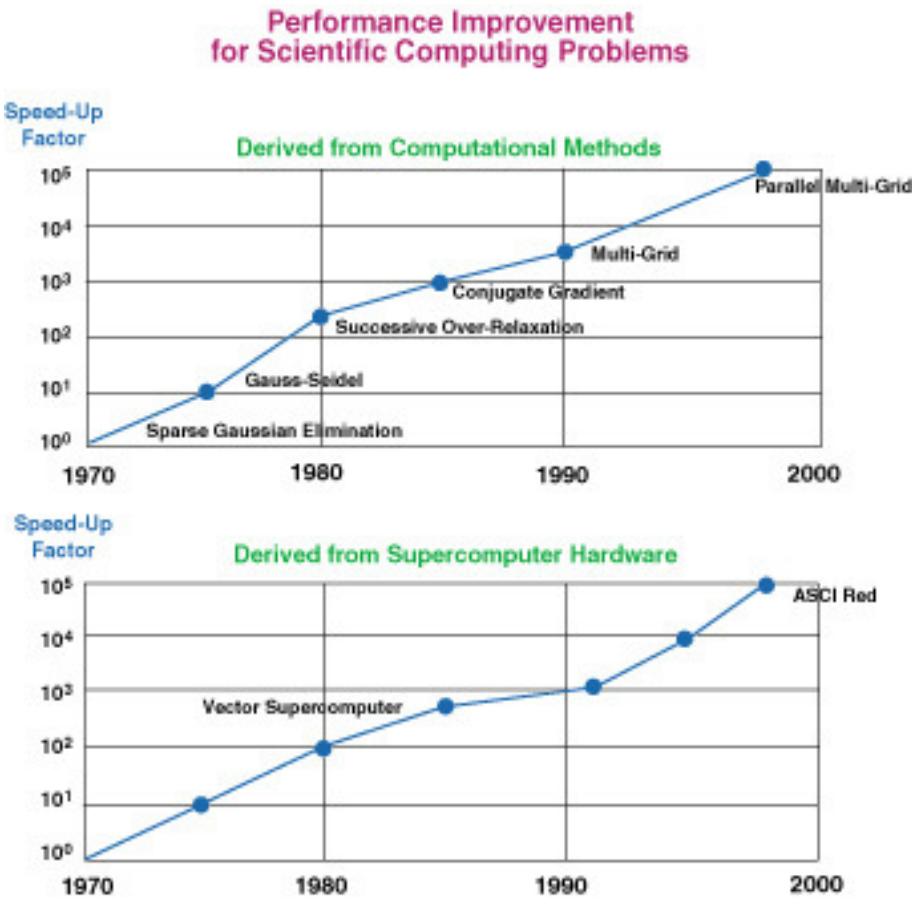


Figure 1.3.: Moore's law in term of the speed-up factor as derived from the computational methods (top panel) and the hardware of supercomputers (lower panel).

1.4. Computer-algebra systems (CAS)

Symbolic computations: ... (Blackboard)

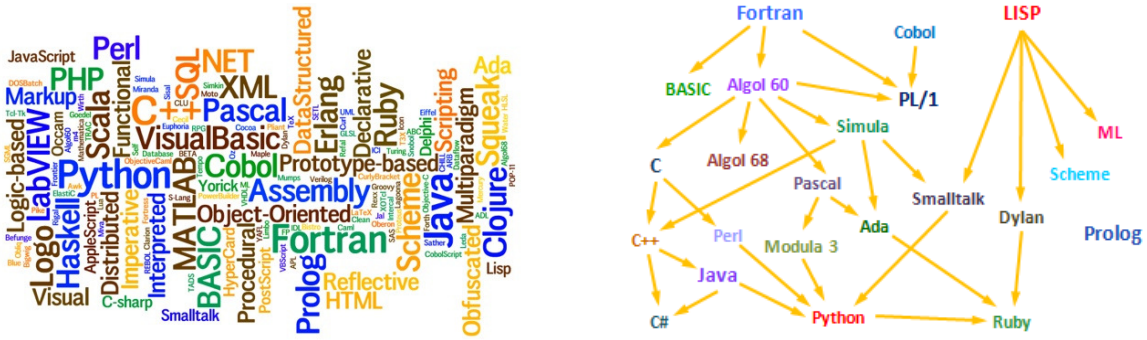


Figure 1.4.: Left: Collection of different languages, indicating the popularity (taken from blog.startapp.com/wp-content/). Right: Historical dependence of some languages (from xrds.acm.org/images)

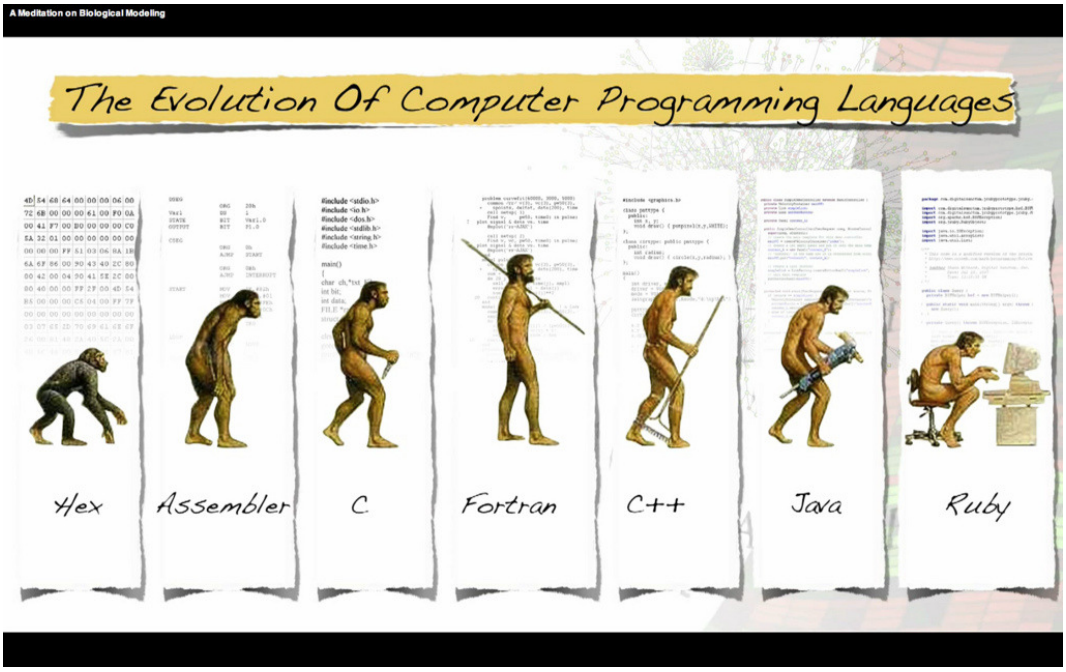


Figure 1.5.: The Evolution of Computer Programming Languages (from: ganeshkamath89.blogspot.com).

2. Maple: A first tutorial

2.1. What is Maple ?

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.

2.2. Getting started

Web link (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/

2.3. A simple example from physics

2.4. A short tour into programming with Maple

Web link (How does Maple differ from other CAS ?):

➢ www.wikivs.com/wiki/Maple_vs_Mathematica

2.5. 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.

➢ Grid – a package for multi-process parallel computation.

➢ GroupTheory – collection of routines for working with groups.

➢ LinearAlgebra – commands for manipulating Matrices and Vectors as rtable structures.

➢ ListTools – tools for manipulating lists.

➢ 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.

2.6. More advanced example: ...

2.7. CAS and quantum physics

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 bit and a qubit, i.e. the capability what can be represented by the corresponding physical units 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 !"
- ➢ 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).

Further reading (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.
- ➢ Listen to the GoogleTechTalk: http://www.youtube.com/watch?v=I56UugZ_8DI
- ➢ 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:

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

- A qubit system can be in one out of an infinite number of significant states:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

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

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

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

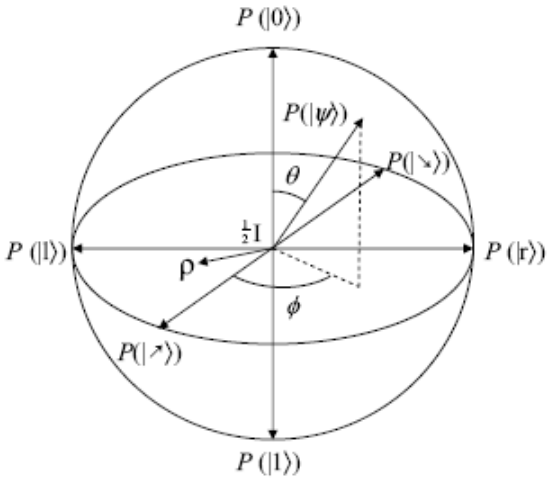


Figure 3.1.: Bloch sphere representation of the qubit. The pure qubit states lie on the periphery, known also as the Poincare-Bloch sphere. The mixed qubit states lie in the interior and are weighted convex combinations of pure states (c-03-bloch-sphere.eps).

Quantum registers:

- Classical: messages are stored and carried by sequences of bits.
- Quantum world: sequence of distinguishable qubits; such sequences are called ($n-$qubit) quantum registers.

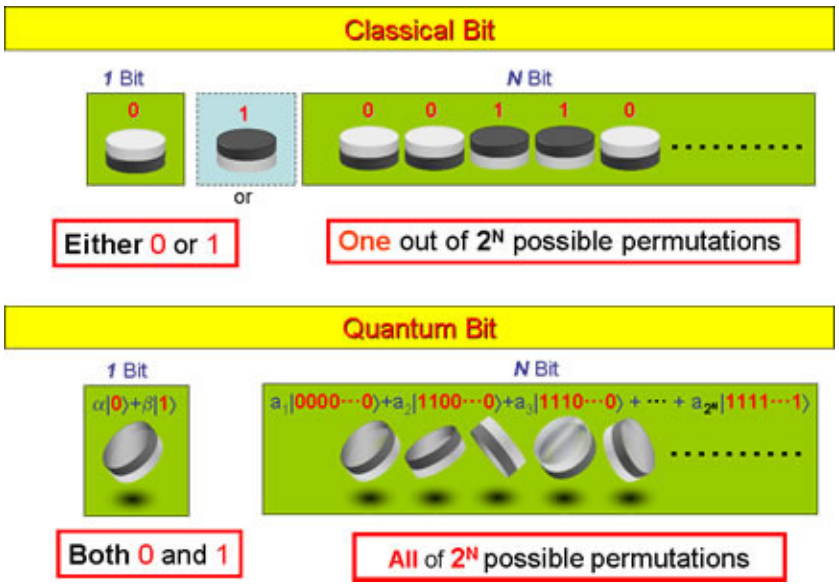


Figure 3.2.: From: www.labs.nec.co.jp (c-02-cbit-qubit.eps).

- $n-$qubit systems are associated with a 2^n-dimensional state space; in general, superpositions of all 2^n basis states are possible.
- Quantum parallelism: certain computations can be carried out in parallel for all 2^n input values. This follows directly from the superposition principle but is, by far, not easy to utilize (see quantum algorithms).
- In quantum systems, therefore, an exponential increase in parallelism requires only a linear increase in the amount of space needed, i.e. the qubits [cf. Fig. 1.5].
- Diffuculties arise from measurements in quantum mechanics; state reduction is never ideal.
- Quantum mechanics does not permit to generate an exact copy of an unknown state (non-cloning theorem).

Experimental realization of qubits: ... (Blackboard)

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 $\mathbb{C}^n = \{(z_1, ..., z_n);\ z_i \in \mathbb{C}\}$, i.e. the vector space of the complex n-tupel.

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: ... (Blackboard)

Basis in $\mathbb{C}^n$: Every set $\{|v_1\rangle\,,\,|v_2\rangle\,,\,...,|v_n\rangle\}$ so that we have

$$|v\rangle \;=\; \sum_i^n a_i\,|v_i\rangle \qquad \forall\;|v\rangle\;.$$

Linear indepedence 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.

Problem (Linear independence): How can we determine the linear dependence or independence of a given set of vectors ?

Many mathematical difficulties of 'quantum mechanics', that one encounters in studying atoms, molecules, the solid state, etc., are associated with the need to treat $\infty-$ dimensional Hilbert spaces; this is not the case if we consider a finite number of distinguishable qubits ($\mathbf{C}^{2^n}$ if n is the number of qubits).

3.3. State vectors and operators

3.3.a. Linear Operators

Linear maps: $A : V \;\to\; W$ or $V \;\to\; V$; '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: $\qquad I\,|v\rangle \;=\; |v\rangle \qquad \forall\;|v\rangle$

Null operator: $\qquad \hat{0}\,|v\rangle \;=\; 0 \qquad \forall\;|v\rangle$

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

If $A : V \;\to\; W$ and $B : W \;\to\; X$, then $(BA) : V \;\to\; X$ with

$$(BA)\,|v\rangle \;=\; B\,(A\,|v\rangle)\;.$$

Matrix representation of $A : V \to W$: If $V : \{|v_1\rangle, |v_2\rangle, ..., |v_m\rangle\}$ and $W : \{|w_1\rangle, |w_2\rangle, ..., |w_n\rangle\}$, we can write also

$$A|v_j\rangle = \sum_i^n A_{ij} |w_i\rangle$$

with (A_{ij}) being a $(n \times m)$ matrix representation of A. The particular matrix depends of course always on the choice of basis in V and W.

Problem (Matrix in $\mathbb{C}^2$): Suppose V is a vector space with the basis vectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and $A : V \to V$ is a linear operator such that $A|0\rangle = |1\rangle$ and $A|1\rangle = |0\rangle$. Give the matrix representation of A.

3.3.b. Pauli matrices

There are many different notations for the Pauli matrices:

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma_1 = \sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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

These Pauli matrices provide a matrix representation of 4 linear independent operators $\mathbb{C}^2 \to \mathbb{C}^2$ 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 $V \times V \to \mathbb{C}$ or $(|v_1\rangle, |v_2\rangle) \to \mathbb{C}$:

$$\langle v_1 | v_2 \rangle \equiv (|v_1\rangle, |v_2\rangle)$$

Properties of the scalar product:

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

- $\langle v \,|\, w \rangle \;=\; \langle w \,|\, v \rangle^*$
- $\langle v \,|\, v \rangle \;\geq\; 0; \qquad\qquad = 0 \quad \text{(only) if} \qquad |v\rangle \equiv 0$

Scalar product in $\mathbb{C}^n$:

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

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 the Cauchy-Schwarz inequality

$$|\, \langle \psi \,|\, \phi \rangle \,|^2 \;\leq\; \langle \psi \,|\, \psi \rangle \; \langle \phi \,|\, \phi \rangle$$

and the triangle inequality

$$\sqrt{\langle \psi + \phi \,|\, \psi + \phi \rangle} \;\leq\; \sqrt{\langle \psi \,|\, \psi \rangle} \;+\; \sqrt{\langle \phi \,|\, \phi \rangle}\,.$$

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 $\{|i\rangle\,,\; i = 1, ...n\}$ is called orthogonal, if

$$\langle i \,|\, j \rangle \;=\; \delta_{ij} \qquad \forall\; i, j = 1, ..., n\,.$$

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

$$|v_1\rangle \;=\; \frac{|w_1\rangle}{||\,|w_1\rangle\,||}$$

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

➢ General agreements:
Matrix representations of linear operators always refer to the use of some orthonormal basis if not stated otherwise.
Especially for all $A : V \to V$, the same basis is used in the input and output space

Blackboard example (Find an orthonormal state):

Problem (Gram-Schmidt procedure): Construct an orthonormal basis from the three vectors

$$|v_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \qquad |v_2\rangle = \begin{pmatrix} 1 \\ 3 \\ 1 \end{pmatrix}, \qquad |v_3\rangle = \begin{pmatrix} 2 \\ 2 \\ 3 \end{pmatrix},$$

using the standard scalar product in $\mathbb{R}^3$.

3.3.f. Outer product

If we have $|v\rangle \in V$ and $|w\rangle \in W$, then

$$(|w\rangle \langle v|)\ |v'\rangle \equiv |w\rangle\ \langle v \mid v'\rangle$$

defines a linear operator $V \to W$ and is known as the outer product $(|w\rangle \langle v|)$:

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

i.e. linear: $V \to W$.

Completeness: Let's $\{|i\rangle, i = 1, .., n\}$ be an orthonormal basis in V,
i.e. $|v\rangle = \sum_i |i\rangle \langle i \mid v\rangle = \sum_i v_i\, |i\rangle$, then we have

$$\left(\sum_i |i\rangle \langle i|\right) |v\rangle = \sum_i |i\rangle \langle i \mid v\rangle = |v\rangle \qquad \forall\ |v\rangle$$

$$\sum_i |i\rangle \langle i| = I$$

Matrix representation of operator $A : V \to W$:

$$\begin{aligned} A = I_w\, A\, I_v &= \sum_{ik} |w_k\rangle \langle w_k |A| v_i\rangle \langle v_i| \\ &= \sum_{ik} \langle w_k |A| v_i\rangle\, |w_k\rangle \langle v_i| \\ &= \sum_{ik} A_{ki}\, |w_k\rangle \langle v_i| \end{aligned}$$

Blackboard example (Z operator acting upon a qubit):

Blackboard example (Outer vector of two vectors):

3.3.g. Expectation value of an operator A

The expectation value of an operator A is the mean or average value of that operator A with respect to a given quantum state $|\psi\rangle$:

$$< A > = \langle\psi|A|\psi\rangle \ .$$

It tells us the 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 polynomal

$$p(\lambda) = \det|A - \lambda I| = 0$$

- ➢ 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.

Blackboard example (Eigenvalues of a matrix):

Problem (Eigenvalues and eigenvectors of the $\pi/8-$gate):
Find the eigenvalues and eigenvectors for the $\pi/8-$gate with the matrix representation

$$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} .$$

3.4.a. Adjoint and hermitean operators

$$\langle v \,|\, Aw \rangle \;=\; \left\langle A^{+} v \,|\, w \right\rangle \qquad \forall\; |v\rangle, |w\rangle \in V$$

➢ 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: $A^{+} \;\equiv\; A$

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

Blackboard example (Pauli matrices):

3.4.b. Projection operators

If W denotes a m-dimensional subspace of V and $\{|1\rangle, ..., |m\rangle,\; m \leq n\}$ an orthonormal basis in W, then

$$P \;=\; \sum_{i}^{m} |i\rangle\,\langle i|\,; \qquad P^{+} \;=\; P, \quad P^{2} \;=\; P$$

is called the projection operator (projector) on W and is independent of the choice of the basis.

Properties: $P^{+} \;\equiv\; P$ is always hermitian and $P^{2} \;=\; P$.

Orthogonal complement: $\quad Q \;=\; I - P$

... projector upon the (complementary) space $\{|m+1\rangle, ..., |n\rangle\}$.

Blackboard example (Projectors upon the diagonal states):

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

$$A \text{ is a normal operator} \quad \Longleftrightarrow \quad \begin{cases} AA^{+} \;=\; A^{+}A \\ \text{diagnalizable} \\ A \;=\; \sum_{i} \lambda_{i}\, |i\rangle\,\langle i| \end{cases}$$

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.

Moreover, every normal operator can be written as

$$A = \sum_i \lambda_i \, |i\rangle \langle i|$$

where λ_i are the eigenvalues and $|i\rangle$ the pairwise orthonormal eigenvectors, $\langle i \,|\, j\rangle = \delta_{ij}$.

Also:

$$A = \sum_i \lambda_i \, P_i \,, \qquad \sum_i P_i = I \,, \qquad P_i P_j = \delta_{ij} P_j$$

where the P_i is the projector upon the eigenspace of λ_i.

Blackboard example (Spectral decomposition of a 3×3 matrix):

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, if $\{|v_i\rangle\}$ is an orthonormal basis in V, then $\{|w_i\rangle = U\,|v_i\rangle\}$ is also orthonormal in V.

Blackboard example (Basis change from the computational to diagonal basis):

Blackboard example (Unitary transform of hermitian operator):

3.4.e. Positive operators

$$\begin{aligned} A \text{ is called positive} &\iff \langle v \,|\, Av\rangle \geq 0 \quad \text{, real} \quad \forall\ |v\rangle \in V \\ A \text{ is positive definite} &\iff \langle v \,|\, Av\rangle > 0 \quad \text{, real} \end{aligned}$$

All positive operators are hermitian and have a spectral decomposition

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

POVM: A set of positive semi-definite operators

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

is called a positive operator-valued measure or short a POVM. Such POVM allow another view and way of quantum measurements.

3.5. Products and functions of linear operators

3.5.a. Product spaces (tensor spaces)

If V and W are vector spaces with dimensions m and n, then $V \otimes W$ is called the product space with dimension mn; the vectors (elements) of this space are:

$$|v\rangle\,|w\rangle \equiv |v, w\rangle \equiv |vw\rangle$$

with $|v\rangle \in V$ and $|w\rangle \in W$.

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

Especially, if $\{|i\rangle\}$ denotes an orthonormal basis in V and $\{|j\rangle\}$ an orthonormal basis in W, then

$$\{\, |i\rangle \otimes |j\rangle\,; \quad i = 1, ..., m,\ j = 1, ..., n\,\}$$

an orthonormal basis in $V \otimes W$.

Properties of tensor products:

Suppose, we have $|v_1\rangle\,,\ |v_2\rangle \in V$, $|w_1\rangle\,,\ |w_2\rangle \in W$ and $z \in C$, then

- $z\,(|v\rangle \otimes |w\rangle) = (z\,|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z\,|w\rangle)$
- $(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$
- $|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle$

Blackboard example (Product space of two qubits):

Blackboard example (Diagonal product basis):

3.5.b. Tensor product of linear operators

Definition: Suppose, we have the vectors $|v_i\rangle \in V$, $|w_i\rangle \in W$ and the operators $A : V \to V$ and $B : W \to W$. Then

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

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

Generalization: If $A : V \to V'$ and $B : W \to W'$ define two maps between different vector spaces, then every operator

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

defines also a linear operator $C : V \otimes W \to V' \otimes W'$ with

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

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

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

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

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

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

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

Notations:

$$|\psi\rangle^{\otimes 2} \ = \ |\psi\rangle \otimes |\psi\rangle$$

$$|\psi\rangle^{\otimes k} \;=\; |\psi\rangle \otimes |\psi\rangle \otimes ... \otimes |\psi\rangle \quad k - \text{times}$$

and, similarly, $A^{\otimes k}$ or $V^{\otimes k}$.

Blackboard example (Eigenvalues of product eigenvectors):

Blackboard example (Action of $(X \otimes Z)$):

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 (Product of two projection operators):

Problem (Two hermitian operators $A,\ B$): Suppose that A and B are hermitian. Show that $A \otimes B$ is then also hermitian.

Blackboard example (Hadamard operator):

3.5.c. Trace of an operator

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

Properties:

➢ trace of an outer product $|\psi\rangle\langle\phi|$ is the inner product: $\quad \mathrm{Tr}\,|\psi\rangle\langle\phi| \;=\; \langle\psi\,|\,\phi\rangle$.

➢ invariant under unitary (similarity) transformations:

$$\mathrm{Tr}(UAU^{+}) \;=\; \mathrm{Tr}(AU^{+}U) \;=\; \mathrm{Tr}(A)$$

and, therefore, independent of the choice of the basis.

➢ trace is *basis independent*, i.e.

$$\mathrm{Tr}A \;=\; \sum_{i}^{n} \langle v_i\,|A|\,v_i\rangle \;=\; \sum_{i}^{n} \langle w_i\,|A|\,w_i\rangle \;.$$

➢ trace of an operator equals the sum of its eigenvalues: $\quad \mathrm{Tr}A \;=\; \sum_{i}^{n} \lambda_i \,.$

➢ If A, B, C are quadratic and of the same dimension, then the trace has the properties:

- cyclic: $\quad \mathrm{Tr}(ABC) \;=\; \mathrm{Tr}(BCA) \;=\; \mathrm{Tr}(CAB)$

- linear: $\mathrm{Tr}(zA+B) \;=\; z\,\mathrm{Tr}(A)+\mathrm{Tr}(B)$

➢ If $|\psi\rangle$ is a unit vector, then we have

$$\mathrm{Tr}(A\,|\psi\rangle\,\langle\psi|) \;=\; \sum_i \left(\langle i\,|A|\,\psi\rangle\;\langle\psi\,|\,i\rangle\right) \;=\; \langle\psi\,|A|\,\psi\rangle$$

Blackboard example (Trace of operator):

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

3.5.d. Operator functions

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

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

for instance,

$$e^{aA} \;=\; I \;+\; aA \;+\; \frac{a^2}{2!}A^2 \;+\; \frac{a^3}{3!}A^3 \;+\; \ldots$$

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 and 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):

Problem (Single-qubit rotation):

Let $\mathbf{v} \;=\; (v_1, v_2, v_3)$ be any real, three-dimensional unit vector and θ a real number. Prove that

$$\exp(i\theta\,\mathbf{v}\cdot\sigma) \;=\; \cos\theta\,I \;+\; i\sin\theta\,\mathbf{v}\cdot\sigma\,,$$

where $\sigma \;=\; (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices.

Blackboard example (Exponential operator):

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

All (linear) operators $V \to V'$ form a linear vector space $\mathbb{L}_V$ and together with a suitable scalar product also a Hilbert space by themself.

Hilbert-Schmidt product: $(A, B) \equiv \mathrm{Tr}(A^+ B)$

is a map $\mathbb{L}_V \times \mathbb{L}_V \to \mathbb{C}$ and fulfills all properties of the scalar product:

$$\mathbb{L}_V \oplus \text{Hilbert-Schmidt product} \hookrightarrow \text{Hilbert space of lin. operators in } V$$

If V has dimension n, the vector space $\mathbb{L}_V$ has dimension n^2; in general, we can choose any set of n^2 orthonormal hermitian matrices as a basis in $\mathbb{L}_V$.

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

$$[A, B] = AB - BA \qquad [A, B] = 0 \iff \text{operators 'commute'}$$

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

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

Simultaneous set of eigenfunctions:

$$[A, B] = 0 \iff A \text{ and } B \text{ have a common set of eigenfunctions;}$$
$$\text{they are diagonalizable in the same basis.}$$

Distributivity of the commutator:

$$[A, BC] = [A, B]C + B[A, C]\,.$$

Example (Commutation relations of the Pauli matrices):

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

3.5.g. Decomposition of linear operators

Polar decomposition: If $A : V \to V$ is given, then we can always find a unitary operator U and two positive operators J and K so that we have

$$A = U\,J = K\,U\,.$$

These decompositions are called left-polar and right-polar decomposition, respectively.

Moreover, the operators J and K are unique and are given by

$$J = \sqrt{A^+A} \qquad \text{and} \qquad K = \sqrt{AA^+}$$

$$\text{If } A^{-1} \text{ exist} \quad \Longleftrightarrow \quad U \quad \text{is unique.}$$

Singular-value decomposition: If A is a quadratic matrix, then there exist two unitary matrices U and V (with the same dimension) and a diagonal matrix D with non-negative eigenvalues

$$A = U\,D\,V$$

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

Blackboard example (Polar decomposition of single qubit operator):

3.6. Postulates of quantum mechanics

3.6.a. Postulate I (State space & state 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.

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

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

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

U ... time evolution operator; discrete time evolution

Example (Pauli matrices):

- X : NOT gate, spin-flip (in analogy to the classical case); $|0\rangle \to |1\rangle\,,\ |1\rangle \to |0\rangle$
- Z : phase-flip; $|0\rangle \to |0\rangle\,,\ |1\rangle \to -|1\rangle$

- Hadamard: $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad H^2 = I$

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

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

Schrödinger equation: alternative description with contineous time evolution

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

... hermitian Hamilton operator H

The knowledge of the Hamilton operator typically requires physical intuition and experimental information; in QI, the Hamiltonian is itself often less in the focus of interest but assumed to be a known (and given by an) hermitian matrix.

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

... eigenvalues and eigenvectors of H

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

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

K hermitian $\iff$ $U = \exp(iK)$ is unitary

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

Exceptions:

➢ Quantum measurements.

➢ Coupling to some bath or environement.

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

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

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

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

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

and the state (just) after the measurement

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

Completeness relation:

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

$$I = \sum_m M_m^+ M_m$$

Blackboard example (Measurement of a qubit in the computational basis):

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

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

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

... total state in the interaction free case

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

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

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.

Problem (Bell state): Prove that the entangled state $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ cannot be represented in the form $|\psi\rangle = |a\rangle\,|b\rangle$ where $|a\rangle$ and $|b\rangle$ are single-qubit states.

Difficulties that remain with the framework of 'QM': ... (Blackboard)

3.7. Measurements in quantum mechanics

3.7.a. Indistinguisable quantum states

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

Blackboard example (Determination of nonorthogonal states):

3.7.b. Projective measurements (von Neumann measurements)

Projective measurements usually refer to measuring some observable (hermitian operator) M with the spectral decomposition

$$M \;=\; \sum_m m\, P_m$$

where P_m denotes the projectors upon the eigenspace associated with eigenvalue m. The probability to find this result and the state after the measurement are:

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

This result follows immediately from postulate III, if we assume the measurement operators to be hermitian and orthogonal projectors, $M_m = M_m^+$ and $M_m M'_m = \delta_{mm'} M_m$, respectively.

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

Problem (Measurement of the three-qubit state): A three-qubit system is in the state

$$|\psi\rangle \;=\; \left(\frac{\sqrt{2}+i}{\sqrt{20}}\,|000\rangle \;+\; \frac{1}{\sqrt{2}}\,|001\rangle \;+\; \frac{1}{\sqrt{10}}\,|011\rangle \;+\; \frac{i}{2}\,|111\rangle\right)$$

a) Is this state normalized ?? What is the probability that the system is found in the state $|000\rangle$ if all 3 qubits are measured ?

b) What is the probability that a measurement on the first qubit only gives 0 ? What is the postmeasurement state of the system in this case ?

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

Properties of projective measurements: ... (Blackboard)

The description of the measurement by means of hermitian operators (observables) also implies Heisenberg's uncertainty principle

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

Instead of the observable M, one can start equivalently also from a set of orthonormal projectors $\{P_m\}$ with $\sum_m P_m = I$ and $P_m P'_m = \delta_{mm'} P_m$; the corresponding observable is then of course $\sum m\, P_m$.

Other notions: Measurement in an (orthonormal) Basis $\{|m\rangle\}$ always refers to a projective measurement with projector $P_m = |m\rangle\langle m|$.

Blackboard example (Measurement of Z):

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

Problem (Projectors of $\mathbf{v}\cdot\sigma$):

a) Show that the operator $\mathbf{v}\cdot\sigma = v_x\sigma_x + v_y\sigma_y + v_z\sigma_z$ has eigenvalues ± 1 and that the projectors upon the corresponding eigenspaces are given by $P_\pm = (I \pm \mathbf{v}\cdot\sigma)/2$.

b) Apply the projector $P_\pm$ to calculate the probability that, for a measurement of the operator $\mathbf{v}\cdot\sigma$, one obtains the result ± 1, if the state prior to the measurement was $|0\rangle$. What is the state of the qubit just after the measurement if the outcome $+1$ was obtained ?

3.7.c. POVM measurements

..... positive operator-valued measure;
i.e., with non-negative eigenvalues or a positive operator norm

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

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

$$E_m = M_m^+ M_m$$

must be a positive operator, and we have

$$\sum_m E_m = I,\ p(m) = \langle\psi\,|E_m|\,\psi\rangle\ .$$

This means, however, that any set of positive operators $\{E_m\}$ is sufficient to characterize uniquely the probabilities for some possible outcome of an experiment; the operators E_m are called the POVM elements and the set $\{E_m\}$ is called POVM.

Note: The projectors $\{P_m\}$ with $\sum_m P_m = I$ and $P_m P'_m = \delta_{mm'} P_m$ from a projective measurement form a POVM (POVM elements = measurement operators), since

$$E_m = P_m^+ P_m = P_m\,.$$

If we have a set of positive operators $\{E_m\}$ with $\sum_m E_m = I$, they also form a POVM since, with $M_m = \sqrt{E_m}$, we can always write

$$\sum_m M_m^+ M_m = \sum_m E_m = I\,.$$

Alternative definition: A POVM is a set of operators $\{E_m\}$ that are
(i) positive,
(ii) fulfill the completeness relation $\sum_m E_m = I$.
The probability for measuring the outcome m is then given by $p(m) = \langle\psi|E_m|\psi\rangle$.

Blackboard example (POVM for a single qubit):

Blackboard example (Transmission of non-orthogonal states):

Remarks: ... (Blackboard)

Problem (Construct a POVM): A given source produces a system either in one of two nonorhtogonal states, either $|\psi\rangle$ or $|\phi\rangle$ with scalar product $|\langle\psi|\phi\rangle| = \cos\theta$. — Construct a POVM that help distinguish these states.

3.7.d. Weak measurements

Use a POVM in order to extract some information about the state but without enforcing a 'collapse of the wave functions'.

Blackboard example (Weak measurements):

POVMs are more general and enable us to do things in quantum mechanics that are not possible using ordinary projective measurements; they are often helpful if we do not need or cannot know the postmeasurement state.

While every projective (and, hence, repeatable) measurement can be treated also as a POVM measurement, POVM's provide us with more freedom in that its elements need not to be projectors and to describe especially measurements on the system without concern of the postmeasurement state.

Problem (Weak measurements): Do the operators

$$A_0 = |0\rangle\langle 0| + \sqrt{1-\varepsilon}\,|1\rangle\langle 1|, \qquad A_1 = \sqrt{\varepsilon}\,|1\rangle\langle 1|$$

form a POVM ??

3.7.e. Mach-Zehnder interferometer

Set-up: A collimated beam is split by a half-silvered mirror. The two resulting beams (the sample beam and the reference beam) are each reflected by a mirror. The two beams then

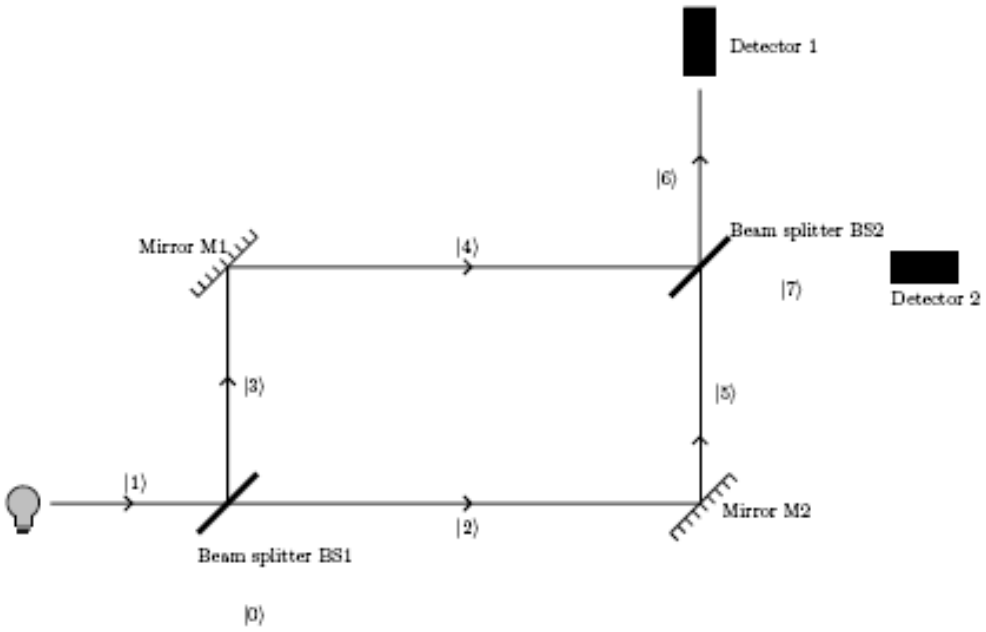


Figure 3.3.: The Mach-Zehnder interferometer. A photon is sent through a beam splitter and detectors registers a photon (from: ...).

pass a second half-silvered mirror and enter two detectors (1 and 2).

It is important that the fully-silvered and half-silvered surfaces of all mirrors, except the last, face the inbound beam, and that the half-silvered surface of the last mirror faces the outbound beam exiting in the same orientation as the original collimated beam. That is, if the original beam is horizontal, the half-silvered surface of the last mirror should face the horizontally outbound beam.

In quantum mechanics, the Mach-Zehnder interferometer can be described by a two-dimensional Hilbert space which is associated to the photon pathes. The state vectors $|0\rangle$ and $|1\rangle$ can be considered as orthonormal wave packets that move along the arms of the interferometer, and where the mirrors, beam splitters and relative phases U_p are given by

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

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

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

For the density matrix

$$\rho_{in} = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

one obtains

$$\rho_{out} = \frac{1}{2} \begin{pmatrix} 1+\cos\phi & i\sin\phi \\ -i\sin\phi & 1-\cos\phi \end{pmatrix} .$$

For the intensity along the path $|0\rangle$ (detector 2), we find

$$I \propto 1 + \cos\phi\,,$$

or in other words, the relative phase U_p can be observed in the output signal of the interferometer. The intensity vanishes for a phase $\phi = \pi$.

3.8. Density matrices and operators

3.8.a. Ensemble of quantum systems

The density operator formalism provides a suitable language if the state of a system is not completely known, for example

$$\{p_i,\ |\psi_i\rangle\}$$

Ensemble of pure states: p_i-th part of the Ensemble is in state $|\psi_i\rangle$ or

System is in one of the states $\{|\psi_i\rangle\}$ with probability p_i.

The density operator is then given by:

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

Time evolution of a closed quantum system:

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

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

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

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

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

$$= \mathrm{Tr}(\ M_m^+\ M_m\,\rho\ )$$

and the state after the measurement:

$$|\psi_i^m\rangle = \frac{M_m\,|\psi_i\rangle}{\sqrt{p(m|i)}}$$

$$\rho_m = \sum_i p(i|m)\ |\psi_i^m\rangle\,\langle\psi_i^m|$$

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

where use is made that $p(i|m) = p(m|i) \cdot p_i/p(m)$ (Bayes theorem)

Comparison:

pure states	mixed states
$\rho = \|\psi\rangle\langle\psi\|$	$\rho = \sum_i p_i \|\psi_i\rangle\langle\psi_i\|$
$\mathrm{Tr}(\rho^2) = 1$	$\mathrm{Tr}(\rho^2) < 1$

Mixture of density operators: is again a valid density operator since with

$$\rho_i = \sum_k q_k \|\psi_{ik}\rangle\langle\psi_{ik}|$$

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

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

3.8.b. Properties of density operators

Beside of the ensemble interpretation of the density matrix, there is an independent definition that does not rely on the term of the state vector.
An operator ρ is a valid density operator, i.e. the density operator for ensemble $\{p_i, |\psi_i\rangle\}$, if

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

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

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

$$\langle\phi|\rho|\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0\,.$$

and vice versa: Since ρ is positive, there alway exist a spectral decomposition

$$\rho = \sum_j \lambda_j \|j\rangle\langle j|$$

with $\{|j\rangle\}$ orthonormal and $\lambda_j \geq 0$, real.

Moreover

$$\mathrm{Tr}(\rho) = \sum_j \lambda_j \,\mathrm{Tr}(|j\rangle\langle j|) = \sum_j \lambda_j = 1\,,$$

that is ensemble $\{\lambda_i,\ |\psi_i\rangle\}$ has density operator ρ.

Blackboard example (Density matrix of a pure state):

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

Blackboard example (Expectation value of an operator):

Blackboard example (Probability for finding the $|-\rangle$ state):

Blackboard example (Completely mixed state):

Problem (Mixed state density operators): Proof that $\mathrm{Tr}(\rho^2) < 1$ for mixed state !

Problem (Pure vs. mixed states): There are given the following density matrices:

$$a)\ \rho = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}, \qquad b)\ \rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix},$$

$$c)\ \rho = \begin{pmatrix} 1/2 & 1/4 \\ 1/4 & 1/2 \end{pmatrix}, \qquad d)\ \rho = \begin{pmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{pmatrix},$$

$$e)\ \rho = \begin{pmatrix} 1/2 & \frac{1-i}{2\sqrt{2}} \\ \frac{1+i}{2\sqrt{2}} & 1/2 \end{pmatrix}.$$

Which of these density operators represent pure and which one mixed states ? — If the state is pure, then determine the state vector, and find an ensemble representation otherwise.

3.8.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 operator ρ with $\mathrm{Tr}\rho = 1$, that acts in the state space, defines a possible state of the system. Especially, if the system is in state ρ_i with probablility p_i, then $\rho = \sum_i p_i \rho_i$.

Postulate II (Time evolution of closed systems):

Every (discrete) time evolution of a closed system can be described by a unitary transformation

$$\rho' = U \rho U^+ = U(t_2, t_1)\ \rho(t_1)\ U^+(t_2, t_1)\ .$$

Postulate III (Quantum measurements and measurement operators):

Quantum measurements are described by a set of measurement operators $\{M_m\}$, that act in the state space and where m denotes the possible outcomes.

If, before the measurement, the system is in state ρ, then

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

Postulate IV (Composite systems and entanglement):

The state space of a composed system is the product space of the state spaces of the subsystems; if the n subsystems are in the state $\{\rho_i,\ i = 1, .., n\}$, then the total state is

$$\rho_{\mathrm{tot}} = \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_n$$

Advantages of the density-matrix concept:

- ➢ Incomplete knowledge about the system
- ➢ Description of subsystems that should be considered independent of some total system.

Blackboard example (Post-measurement state):

Blackboard example (Expectation value for measuring X):

3.8.d. Uniqueness of the density operator

Problem (Density operator of a pure state): Let ρ denote a density operator. Show that $\mathrm{Tr}(\rho^2) \leq 1$ and that $= 1$ applies if and only if ρ represents a pure state.

Different ensemble $\{p_i, |\psi_i\rangle\}$ may have the same density operator, i.e. the behave uniquely with regard to all measurements. The particular ensemble $\rho = \sum_i \lambda_i |i\rangle \langle i|$, that is associated with the eigenvalues and eigenvectors, is physically not distinguished.

Notation: A set of (non-normalized) vectors $\{\widetilde{|\psi_i\rangle}\}$ is said to 'create' the density operator $\rho = \sum_i \widetilde{|\psi_i\rangle}\widetilde{\langle\psi_i|}$, then we refer to the ensemble

$$\left\{ p_i, \frac{\widetilde{|\psi_i\rangle}}{\sqrt{p_i}} \dots \text{normalized} \right\} .$$

Suppose $\rho = \sum_i \widetilde{|\psi_i\rangle}\widetilde{\langle\psi_i|}$ is valid density operator, then

$$\Longrightarrow \left\{ p_i, \frac{\widetilde{|\psi_i\rangle}}{\sqrt{p_i}} \dots \text{normalized} \right\} \Longrightarrow \widetilde{|\psi_i\rangle} \quad \text{is said ...}$$

to 'create' the density operator $\rho = \sum_i \widetilde{|\psi_i\rangle}\widetilde{\langle\psi_i|}$.

Unitary freedom: Two set of vectors $\{\widetilde{|\psi_i\rangle}\}$ and $\{\widetilde{|\phi_i\rangle}\}$ create the same density operator, if

$$\widetilde{|\psi_i\rangle} = \sum_j u_{ij} \widetilde{|\phi_j\rangle}$$

are related to each other via a unitary matrix, $U = (u_{ij})$ If the number of $\{\widetilde{|\psi_i\rangle}\}$ and $\{\widetilde{|\phi_i\rangle}\}$ vectors are different, then a corresponding number of 'null vectors' can be added.

If two ensemble $\{p_i, |\psi_i\rangle\}$ and $\{q_j, |\phi_j\rangle\}$ are given, then they have the same density operator if

$$\sqrt{p_i}\,|\psi_i\rangle = \sum_j u_{ij} \sqrt{q_j}\,|\phi_j\rangle$$

is fulfilled for some unitary matrix.

3.8.e. Bloch sphere representation of a qubit

Computational basis: ... eigenstates of σ_z

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle \qquad a, b \in \mathbb{C}; \qquad |a|^2 + |b|^2 = 1$$

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

Diagonal basis: ... eigenstates of σ_x

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

This basis is conjugate to the computational basis. The computational and diagonal bases are used together to provide the pairs of 'signal states' that are utilized in the BB84 quantum key distribution (QKD) protocol.

Circular basis: ... eigenstates of σ_y

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

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.

Breitbart or 'intermediate' basis:

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

This basis lies on the $\phi = 0$ plane and is used in QKD for eavesdropping.

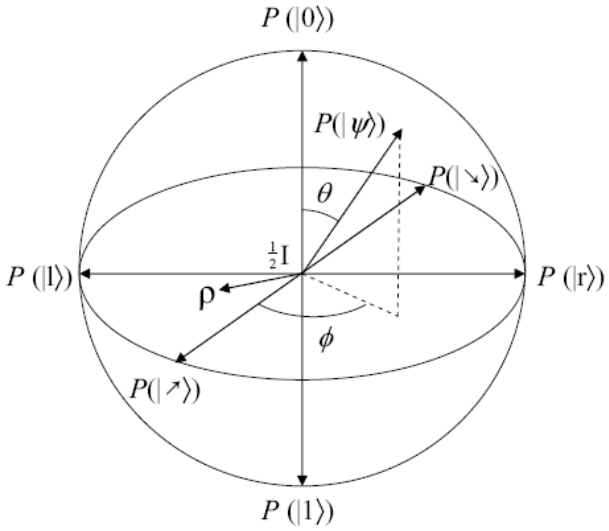


Figure 3.4.: Statistical operators represented in the unit Bloch ball, a real-valued representation of the space of qubit states via the expectation values, P_i, of Pauli operators σ_i, $i = 1, 2, 3$. (from: ...).

Bloch-sphere or spinor representation:

$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}\,|0\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|1\rangle\right),$$

and where (θ, ϕ) refers to the polar angles on a unit sphere. If $\theta = 0$ or π, then ϕ is taken to be zero by convention. The effect of a general operation on a qubit can be viewed as a (possibly stochastic) transformation within this (Bloch) ball.

Unfortunately, there is no simple picture for several qubits.

General representation for mixed states:

$$\rho \;=\; \frac{I \,+\, \mathbf{r}\cdot\sigma}{2}\;,$$

where $\mathbf{r} \;=\; (r_x, r_y, r_z)$ is any 3−dimensional vector with $|\mathbf{r}| \leq 1$. For $|\mathbf{r}| \;=\; 1$, ρ describes a pure state.

Blackboard example (Stern-Gerlach filter):

Problem (Stern-Gerlach filter): A beam of electrons, prepared as a 50:50 statistical mixture with spin projections $\mu_z = \pm 1/2$ (along the $z-$axis), is sent through a Stern-Gerlach filter which admits only particles with spin projection $+1/2$ on the $z-$axis.

Determine the probability that an electron will penetrate the filter. — Compare this result with the solution from above. How can one distinguish the pure and mixed electron states by using the Stern-Gerlach technique ?

3.8.f. Stokes parameters

- Instead to the three real parameters (r_x, r_y, r_z) in $\rho \;=\; \frac{I+\mathbf{r}\cdot\boldsymbol{\sigma}}{2}$, four Stokes parameters P_μ are often utilized that have the advantage of being more closely related to empirical quantities, such as photon-counting rates in selective measurements.
- Three of these parameters $(\mu = 1, 2, 3)$ correspond to measurements in the computational, diagonal and circular basis (which are all orthogonal on the Bloch sphere).

Stokes parameters and density matrix:

- both representations are homomorphic to each other, since the density matrix and the Stokes four-vector P_μ are related to each other via the Pauli (and unit) matrices by

$$\rho \;=\; \frac{1}{2}\sum_{\mu=0}^{3} P_\mu\,\sigma_\mu$$

  with $\sigma_0 \;\equiv\; I$. This representation of the density operator is known also as Pauli representation.
- The Stokes parameters P_μ also enables one to directly visualize the qubit state geometrically in the Bloch ball

$$\rho \;=\; \frac{1}{2}\begin{pmatrix} P_0 + P_3 & P_1 - iP_2 \\ P_1 + iP_2 & P_0 - P_3 \end{pmatrix}.$$

  The Stokes parameter are often normalized to $P_0 = 1$ ... the total quantum probability.
- Stokes parameters are expressed in terms of the density matrix as

$$P_\mu \;=\; \mathrm{Tr}(\rho\sigma_\mu)\,.$$

➢ If the state of a qubit is given in the spinor representation $\begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$, then the Stokes are $P_0 = 1,\ P_1 = \sin\theta\cos\phi,\ P_2 = \sin\theta\sin\phi$ and $P_3 = \cos\theta$.

➢ The four-vectors formed by the Stokes parameters provide a basis in Minkowski space $\mathbb{R}^4_{1,3}$ in which the σ_μ are the generators of rotations and hyperbolic rotations in this space.

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

Blackboard example (Pauli representation for two qubits):

Problem (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 $\mathbf{P} \;=\; \langle\psi\,|\sigma|\,\psi\rangle$ in terms of the coefficients a_μ.

3.8.g. Reduced density operators and partial trace

Reduced density operator: Let ρ^{AB} be the density operator of a composite system that consists out of two subsystems A and B. Then, the reduced density operator of system A

$$\rho^A \;=\; \mathrm{Tr}_B(\rho^{AB})$$

is given by the partial trace over system B.

Partial trace: Suppose the density matrix of a composed system is given by

$$\rho^{AB} \;=\; \sum_{ik}^{n_A}\sum_{jl}^{n_B} \rho_{ij,kl}\ |i_A\rangle\,|j_B\rangle\,\langle k_A|\,\langle l_B|$$

with respect to two orthonormal bases $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$, then the partial trace is defined as

$$\mathrm{Tr}_B\left(\rho^{AB}\right) \;=\; \sum_{ik}^{n_A}\left(\sum_{m}^{n_B}\rho_{im,km}\right)\ |i_A\rangle\,\langle k_A|\ .$$

The partial trace is independent of the basis $\{|j_B\rangle\}$ and, thus, suitable to describe observations and measurements for subsystem A.

Example (Reduced density matrix of a product state):

Suppose $\rho^{AB} = \sigma \otimes \tau = \rho^A \otimes \rho^B$, then

$$\rho^A = \mathrm{Tr}_B(\sigma \otimes \tau) = \sigma\,\mathrm{Tr}(\tau) = \sigma \qquad \text{since} \qquad \mathrm{Tr}(\tau) = 1\,.$$

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

Problem (Reduced density matrix of other Bell states):

Find the reduced density operators also for the Bell states $|\Psi^{\pm}\rangle = \frac{1}{2}(|01\rangle \pm |10\rangle)$.

3.8.h. Schmidt decomposition of pure states

Schmidt decomposition: Suppose $|\psi\rangle$ is a pure state of a bipartite system AB. Then, there always exist orthonormal states $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$ so that m

$$|\psi\rangle = \sum_i \lambda_i\, |i_A\rangle\, |i_B\rangle$$

with $\lambda_i \geq 0$, real and $\sum_i \lambda_i = 1$. The λ_i are called the Schmidt coefficients.

The reduced density operators for the subsystems A and B are given by

$$\rho^A = \sum \lambda_i^2\, |i_A\rangle\langle i_A|\,, \qquad \rho^B = \sum \lambda_i^2\, |i_B\rangle\langle i_B|\,,$$

that is the ρ^A and ρ^B have the same eigenvalues $\{\lambda_i^2\}$. For a proof, see Nielsen & Chuang (2002), section 2.5; applies the singular-value decomposition (proof see Nielsen/Chuang, 2002).

The bases $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$ are called Schmidt bases.

Schmidt number: Number of non-zero eigenvalues $\lambda_i > 0$ measure for entanglement between A and B.

For composed systems:

$$\left|\psi^{AB}\right\rangle \text{ is a pure product state} \qquad \Longleftrightarrow \qquad \mathrm{Tr}(\rho^{A^2}) = \mathrm{Tr}(\rho^{B^2}) = 1$$

separable — Schmidt number is 1. ρ^A and ρ^B are pure.

Problem (Schmidt decomposition of two-qubit states):

Find the Schmidt decomposition for the following two-qubit states:

(a) $(|00\rangle + |11\rangle)/\sqrt{2}$ and

(b) $(|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$.

3.8.i. Purification of reduced density operators

Given: mixed state ρ^A of a quantum system A: $\rho^A = \sum_i p_i \, |a\rangle \langle a|$

Looking for: Pure state $|AR\rangle$, so that compsed system $|AR\rangle$

$$\rho^A = \mathrm{Tr}_R(|AR\rangle \langle AR|) \, .$$

This pure state is to be obtained by considering the 'composed' system A together with some particularly chosen reference system R.

Indeed, such a pure state exist for every valid density operator ρ^A. Suppose, we have $\rho^A = \sum p_i \, |i_A\rangle \langle i_A|$ and a reference system in the same state space and with the basis $\{|i_R\rangle\}$. Then,

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

Obviously,

$$\begin{aligned} \mathrm{Tr}_R(|AR\rangle \langle AR|) &= \sum_{ik} \sqrt{p_i p_k} \, |i_A\rangle \langle k_A| \, |i_R\rangle \, \mathrm{Tr}(|i_R\rangle \langle k_R|) \\ &= \sum_i p_i \, |i_A\rangle \langle i_A| = \rho^A \, . \end{aligned}$$

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

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

3.9. The EPR paradoxon and Bell's inequality

(Einstein, Rosen und Podolsky, 1935)

3.9.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 who were two of its founders. Their debates are remembered because of their importance to the philosophy of science. It was summarized by Bohr in an article titled *Discussions with Einstein on Epistemological Problems in Atomic Physics.*

A few (historical) remarks:

- ➢ See, for example, wikipedia (Bohr-Einstein debate) for details.
- ➢ In 1925, remember, Werner Heisenberg introduced matrix equations that removed the Newtonian elements of space and time from any underlying reality; in 1926, Max Born then proposed that the mechanics was to be understood as a probability without any causal explanation. — Einstein, in contrast, believed that the reasons for the 'new' mechanics still needed to be understood.
- ➢ Bohr himself accepted the 'philosophical' problems with quantum mechanics by proposing a Principle of Complementarity that emphasized the role of the observer over the observed.
- ➢ A first serious attack by Einstein took place during the Fifth Conference of Physics at the Solvay Institute in 1927 where he argued from the viewpoint of the (universally accepted) laws of conservation of energy and of impulse (momentum).
- ➢ Bohr's replied quickly and showed the impossibility of using Einstein's apparatus to violate the principle of indeterminacy depends crucially on the fact that the macroscopic system also obeys quantum laws.
- ➢ At the sixth Congress of Solvay in 1930, Einstein attacked again the indeterminacy relation; he 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.
- ➢ Finally, the discussion culminated in 1935 in the famous EPR paper which stated the paradoxon of quantum-mechanically entangled states in a very clear way and which, since then, has lead to numerous experiments to (dis-)prove the consequences of non-locality.

3.9.b. EPR 'gedanken' experiment

The idea of the EPR paper was to show that quantum mechanics is not a 'complete theory' in the sense that it provides only an imcomplete description of Nature.

'Elements of reality' (local realism):

- ➢ every complete theory must be able to predict the physical properties of an object with certainty.
- ➢ Physical events and measurements must be independent if they are causal unrelated to each other.

Core value of EPR: was that the properties of physical systems have definite values (an objective reality) whether you observe the system or not. That is, a given property of a system has (should have) a defined value already before a measurement is made, or even if no measurement is made. Quantum mechanics, however, tells a different story: Prior to measurement, a property of the system does not have a definite or sharply defined value.

Classical experiment:

Alice		Charlie		Bob
$P_Q:\ Q=\pm 1$	$\longleftarrow$	source	$\longrightarrow$	$P_S:\ S=\pm 1$
$P_R:\ R=\pm 1$	produces equivalent pairs of particles			$P_T:\ T=\pm 1$

with P_X property and X the outcome of a measurement.

The scenario drawn by EPR is difficult to test experimentally (for mainly technical reasons). A simpler version of this seminal thought experiment was put forward by David Bohm in 1952 and involved particles with correlated spins; he considered a spin-0 particle that decays into two spin-1/2 particles (like in the two-photon decay of an atom).

Example (Correlations of–entangled–Bell states):

Two spin-1/2 particles for a (total) spin-0 state if they are in the(so-called) singulet state of two spin-1/2 particles (singulett state)

$$|\psi\rangle \;=\; \frac{|01\rangle \;-\; |10\rangle}{\sqrt{2}}\,.$$

If we make an measurement of Z on the first particle and leave the second untouched, we need to apply $Z\otimes I$, and see:

– if we find the first qubit in $|0\rangle$, the second qubit is with certainty found in $|1\rangle$;
– if we find the first qubit in $|1\rangle$, again the second qubit is fully correlated.

Well, this seems clear by looking at the given state; however, if we measure in the diagonal basis $|\pm\rangle$, we find with

$$|0\rangle \;=\; \frac{|+\rangle \;+\; |-\rangle}{\sqrt{2}}, \qquad |1\rangle \;=\; \frac{|+\rangle \;-\; |-\rangle}{\sqrt{2}}$$

that the Bell state takes the form:

$$|\psi\rangle \;=\; \frac{|+-\rangle \;-\; |-+\rangle}{\sqrt{2}}\,.$$

Therefore, by making a measurement in this basis, we obtain again a full correlation between the measurement outcome. Actually, the same happens in for any choice of basis ... or, simply, this is just a property of the fully entangled Bell states.

3.9.c. Bell' inequalities

Analyze classically the outcomes Q, ..., T as random variables gives rise to equation:

$$QS \,+\, RS \,+\, RT \,-\, QT \;=\; (Q+R)S - (R-Q)T \;=\; \pm 2\,.$$

for all possible combinations of the random variables.
Suppose, $p(q,r,s,t)$ is the probability to find $Q=q$, $R=r$, ..., then the:

Classical expectation value (average) is:

$$\begin{aligned} 2 \;\geq\; E(QS+RS+RT-QT) \;&=\; \sum_{qrst} p(q,r,s,t)\,(qs+rs+rt-qt) \\ &\leq\; 2\sum_{qrst} p(q,r,s,t) \;=\; 2\,. \end{aligned}$$

John Bell's ineqality: classical expectation has certain upper/lower limits ... which are violated by QM.

Therefore, since expectation values is linear, we obtain

$$E(QS) \,+\, E(RS) \,+\, E(RT) \,+\, E(QT) \;\leq\; 2$$

Bell's inequality: Classical expectation for any experiment has under the assumptions above an 'upper limit'.

3.9.d. Quantum mechancical 'anticorrelations' in the EPR experiment

Consider the two-qubit (Bell) state

$$|\psi\rangle \;=\; \frac{|01\rangle \,+\, |10\rangle}{\sqrt{2}}\,,$$

i.e. an entangled singulet state. If we perform an indepedent spin measurment along some axis $\mathbf{w}$ for both qubits, then outcome for the measurement $\mathbf{w}\cdot\sigma \;=\; \pm 1$.

Quantum experiment, for example with measurements of:

$$\begin{array}{ccccc} & \text{Alice} & |\psi\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}} & & \text{Bob} \\ P_Q: Z_1 & \longleftarrow & \text{source} & \longrightarrow & P_S: \frac{-Z_2 - X_2}{\sqrt{2}} \\ P_R: X_1 & & & & P_T: \frac{Z_2 - X_2}{\sqrt{2}} \end{array}$$

then one finds (after the computation of the expectation values):

$$\langle QS\rangle + \langle RS\rangle + \langle RT\rangle + \langle QT\rangle = 2\sqrt{2} => 2$$

In other words, Bell's inequality can be violated by an quantum mechanical experiment.

Nature: Suitable chosen experiments confirm QM and are in clear conflict with the classical expectations.

Consequences:

- ➢ At least one of the assumptions about Nature is wrong;

  either 'physical reality' of properties is wrong, i.e. the assumption that the properties P_Q, ..., P_T exist independently from the observation or
- ➢ the 'locality' of events, i.e. that causal independent events cannot influence each other.
- ➢ Apparently, the (quantum) world is not local-realistic.
- ➢ (Quantum-mechanical) Entanglement and nonlocality is an additional resource of quantum mechanics that is provided by quantum mechanics and which we do not have in the classical world. Indeed, there are many applications of these resources in QIP.

Many people belief that the 'physical reality' of properties does not exist independent of the observations.

3.9.e. Bipartite systems and the Bell basis

A bipartite system consists of two subsystems, for example, if Alice and Bob have each one member of an entangled pair of particles. The Hilbert space of the composite system is $H_A \otimes H_B$, and a basis for this systems is found by taking the tensor products $|a_i\rangle \otimes |b_j\rangle \equiv |a_i b_j\rangle$. Moreover, if the basis for Alice and Bob are both orthonormal, we have

$$\begin{aligned} \langle a_i b_j \,|\, a_k b_l\rangle &= \delta_{ik}\,\delta_{jl} \\ \Pr(a_i b_j) &= |\,\langle a_i b_j \,|\, \psi\rangle\,|^2 \\ A &= \sum_{ijkl} \langle a_i b_j|\, \langle a_i b_j\,|A|\, a_k b_l\rangle\, |a_k b_l\rangle \end{aligned}$$

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

A frequently considered alternative is the Bell basis which is formed by the four Bell states

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

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

The Bell states can be written more compactly in the form

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

where $\bar{y}$ is 'not"y; x is also called the phase bit and y the parity bit.

Blackboard example ($Z \otimes Z \; |\beta_{xy}\rangle$):

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

3.9.f. 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

$$\rho = P_{ij} \, \sigma_i \otimes \sigma_j \qquad \text{Pauli representation with generalized Stokes parameters}$$

$$\rho = \sum_{ij} c_{ij} \, |\beta_{ij}\rangle\langle\beta_{ij}|$$

$$= c_{00} \, |\beta_{00}\rangle\langle\beta_{00}| + c_{01} \, |\beta_{01}\rangle\langle\beta_{01}| + c_{10} \, |\beta_{10}\rangle\langle\beta_{10}| + c_{11} \, |\beta_{11}\rangle\langle\beta_{11}| \, .$$

The outer products in this expansion can be expressed also in terms of the Pauli matrices

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

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

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

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

When expressible in this form, a density operator ρ is separable if and only if

$$c_{00} \leq \frac{1}{2} \, .$$

4. Multi-qubit applications in quantum information processing (QIP)

4.1. Information & physics. Non-cloning theorem

Information is part of physics (Landauer): ... (Blackboard)

No-cloning theorem: It is impossible to produce two copies of an unknown quantum state $|\psi\rangle$, that is $(|\psi\rangle\,,\,|\psi\rangle)$, because of the linearity of quantum mechanics.

Proof: Suppose we have $|\psi\rangle = \alpha\,|0\rangle\,+\,\beta\,|1\rangle$ and a unitary (cloning) operator $U:\ U\,|\psi'\rangle = |\psi'\rangle\,|\psi'\rangle$. Then, we have:

$$U\,|0\rangle = |00\rangle\,,\quad U\,|1\rangle = |11\rangle\ ,$$

and this gives rise to:

$$U\,|\psi\rangle = \alpha\,|00\rangle\,+\,\beta\,|11\rangle\ .$$

On the other hand, we also find:

$$U\,|\psi\rangle = |\psi\rangle\,|\psi\rangle = \alpha^2\,|00\rangle\,+\,\alpha\beta\,|01\rangle\,+\,\beta\alpha\,|10\rangle\,+\,\beta^2\,|11\rangle$$

the same still hold if we use anchillary systems.

Of course, it is possible to make imperfect copies. How can one quantify this imperfection ? How close can the copies come to original copies to be cloned ?

No-cloning is a powerful concept in QIP:

- ➢ In QM we can always have only a limited knowledge about an unknown state of a system. Otherwise, we could produce an unlimited number of copies and make experiments on them. In classical physics, measurements do not destroy the state of the system; they are noninvasive.
- ➢ Supports secure transmission of information (quantum cryptography); it enables one to transmit information due to the "security of nature's laws" (laws of quantum mechanics).
- ➢ No instantaneous communication via quantum entanglement is possible.
- ➢ Does not allow to use classical error correction techniques

➢ If we choose a certain known basis $\{|\phi\rangle_a\}$, we can always design a transformation that clones these basis states. But then, the operation acts as

$$U_{AB}\,|\psi\rangle_A\,|0\rangle_B \;\Rightarrow\; c_1\,|\phi_1\rangle_A\,|\phi_1\rangle_B + c_2\,|\phi_2\rangle_A\,|\phi_2\rangle_B$$

i.e. it copies only the individual components; this provide a tool to create strongly entangled states.

4.2. Quantum cloning (quantum copier)

Although we are not able to copy quantum states exactly, one may ask how accurate can we copy an arbitrary quantum state of a (given) system 1:

$$|\phi\rangle_1 \;=\; \alpha\,|0\rangle_1 + \beta\,|1\rangle_1$$

in the computational basis. Our aim is to transfer this state as faithfully as possible to the system 2, for which we also need a third system (3), called the anchilla. As usual, we have $|a\rangle_1\,|b\rangle_2\,|c\rangle_3 = |abc\rangle$.

Let us consider the following transformation:

$$|0\rangle_1\,|0\rangle_2\,|0\rangle_3 \;\Rightarrow\; \sqrt{\frac{2}{3}}\,|000\rangle - \frac{1}{\sqrt{6}}\,(|011\rangle + |101\rangle)$$

$$|1\rangle_1\,|0\rangle_2\,|0\rangle_3 \;\Rightarrow\; -\sqrt{\frac{2}{3}}\,|111\rangle + \frac{1}{\sqrt{6}}\,(|010\rangle + |100\rangle)$$

This transformation maps orthogonal states upon orthogonal ones and can be realized by unitary transformations; as seen from this map, we choose the systems 2 and 3 initially in the state $|0\rangle_2\,|0\rangle_3$.

The application of this transformation gives rise to:

$$|\Psi\rangle_{123} \;=\; \sqrt{\frac{2}{3}}\,(\alpha\,|000\rangle - \beta\,|111\rangle) - \frac{\alpha}{\sqrt{6}}\,(|011\rangle + |101\rangle)$$
$$+\,\frac{\beta}{\sqrt{6}}\,(|010\rangle + |100\rangle)\,.$$

To understand, how well the transformation works, we need to analyze the reduced density matrices

$$\rho_1 \;=\; \mathrm{Tr}_{23}\,(\rho) \qquad \rho_2 \;=\; \mathrm{Tr}_{13}\,(\rho)\,.$$

These traces can be written in the form

$$\rho_1 = \rho_2 = \rho_{\text{out}} = \frac{1}{6}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{2}{3}\begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix} = \frac{1}{6}\mathbf{1} + \frac{2}{3}\rho_{\text{in}}\,,$$

and it turns out that they are equal for the subsystems 1 and 2. I.e. both systems 1 and 2 retain the same information about the original state.

The expectation value of the projector $|\phi\rangle\langle\phi|$ is

$$\langle\phi\,|\rho_{\text{out}}|\,\phi\rangle = \frac{5}{6}\,,$$

independent of $|\phi\rangle$. We have therefore obtained a procedure that retains the original state with the probability of 83 %, and this holds for both subsystems 1 and 2. The expectation value above between the input and output state is called the fidelity of the copying process. It can be shown that this is the optimal value for a symmetric copying of a unknown state Buzek-Hillary quantum copying machine (QCM).

4.3. Quantum cryptography

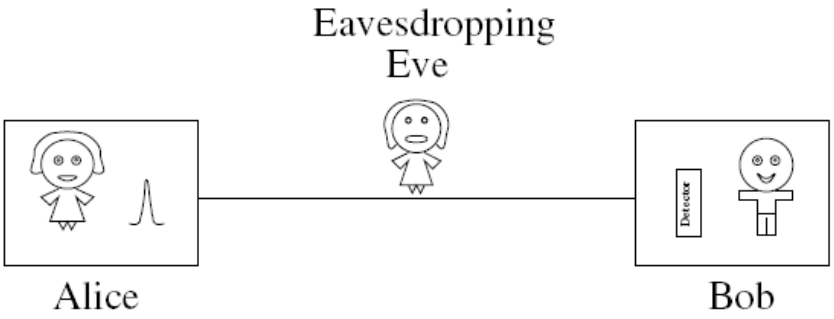


Figure 4.1.: Alice and Bob are trying to communicate secretly but there is an eavesdropper called Eve who is attempting to listen in on their communications (from: ...).

Quantum cryptography:

- ➢ A process by which two parties, Alice and Bob, can communicate secretly.
- ➢ 'No cloning' is an important ingredient for quantum cryptography since it prevents an eavesdropper from copying information.
- ➢ Main issue: to establish a secret key between Alice and Bob; i.e. a string of zeros and ones that can be used to encode information.
- ➢ There have been several protocols suggested in the literature; many of them requiring the entanglement of states.

BB84 quantum key exchange protocol: ... (Blackboard)

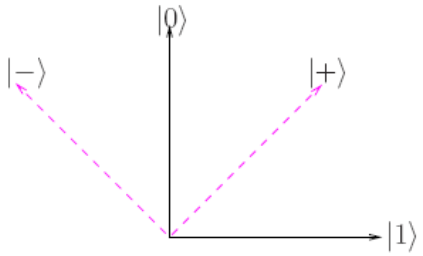


Figure 4.2.: Alice can store the bit either in the rectilinear basis or in the diagonal basis.

4.4. (Super-) dense coding

Entanglement ... (Blackboard)

Pure-state entanglement and Pauli operators:

Let us consider the four orthogonal entangled states

$$\left|\Phi^{\pm}\right\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle \pm |11\rangle\right), \qquad \left|\Psi^{\pm}\right\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle \pm |10\rangle\right)$$

and the Pauli operators

$$\begin{aligned}
\sigma_x &\equiv X = |1\rangle\langle 0| + |0\rangle\langle 1| \\
\sigma_y &\equiv Y = i\,|1\rangle\langle 0| - i\,|0\rangle\langle 1| \\
\sigma_z &\equiv Z = |0\rangle\langle 0| - |1\rangle\langle 1|
\end{aligned}$$

Alice (or Bob) can apply one or more of the Pauli operators locally to change between any of the Bell states

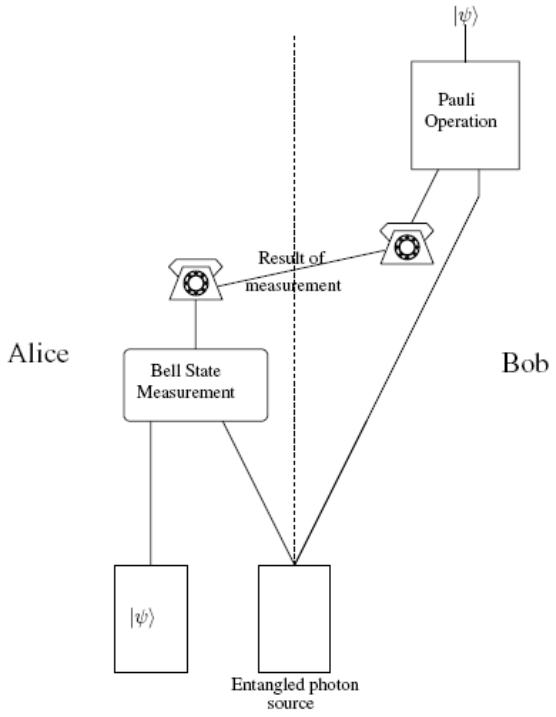
$$\begin{aligned}
(\sigma_x \otimes I)\left|\Phi^{\pm}\right\rangle &= \left|\Psi^{\pm}\right\rangle \\
(\sigma_x \otimes I)\left|\Psi^{\pm}\right\rangle &= \left|\Phi^{\pm}\right\rangle \\
(\sigma_z \otimes I)\left|\Phi^{\pm}\right\rangle &= \left|\Phi^{\mp}\right\rangle \\
(\sigma_z \otimes I)\left|\Psi^{\pm}\right\rangle &= \left|\Psi^{\mp}\right\rangle
\end{aligned}$$

and similar for $\sigma_y \sim \sigma_x\sigma_z$.

Dense coding ... (Blackboard)

4.5. Teleportation

Teleportation is a process by which Alice can send Bob one qubit in an unknown state $|\psi\rangle$ by sending Bob two classical bits if Alice and Bob initially share an entangled Bell state.



Alice's measurement	Bob's state	Bob's operation
$\|\Phi^+\rangle$	$\alpha\|0\rangle + \beta\|1\rangle$	I
$\|\Phi^-\rangle$	$\alpha\|0\rangle - \beta\|1\rangle$	σ_3
$\|\Psi^+\rangle$	$\alpha\|1\rangle + \beta\|0\rangle$	σ_1
$\|\Psi^-\rangle$	$\alpha\|1\rangle - \beta\|0\rangle$	$\sigma_1\sigma_3$

Figure 4.3.: Left: An unknown quantum state $|\psi\rangle$ is teleported from Alice to Bob. Initially, Alice has the unknown state $|\psi\rangle$ and one half of an entangled pair of photons. Right: Bob's operations afterwards.

When classical bits are sent over a classical channel, it is possible for Alice to retain a copy. However, the no-cloning theorem says that it is impossible for Alice to copy the unknown state $|\psi\rangle$. When she sends $|\psi\rangle$ to Bob, she retains no information about the state of $|\psi\rangle$ — it is simply 'moved' from Alice to Bob and, hence, the name: teleportation.

Teleportation protocol: ... (Blackboard)

4.6. Entanglement swapping

Can systems that have never interacted become entangled ? The answer is, very surprisingly, yes: and entanglement swapping is the method.

- ➢ Entanglement swapping is an example of a tripartite communication protocol. If Alice and Bob share entanglement, and Bob and Charlie share entanglement, entanglement swapping can be used to entangle Alice and Charlie.
- ➢ The purpose of entanglement swapping is to induce entanglement between systems that hitherto have shared no entanglement. An entanglement resource is required for entanglement swapping to occur; indeed, the nomenclature 'entanglement swapping' describes the transfer of entanglement from a priori entangled systems to a priori separable systems.

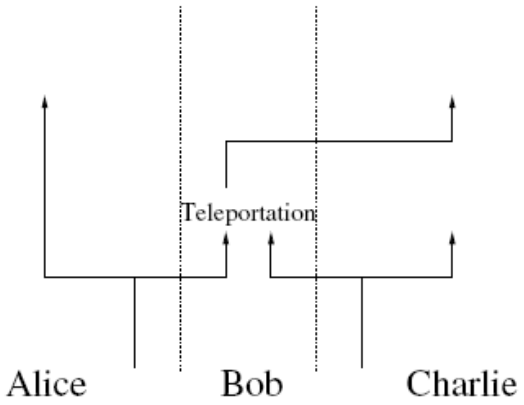


Figure 4.4.: Entanglement swapping. Initially, entangled pairs are shared between Alice and Bob, and between Bob and Charlie. There is no entanglement between Alice and Charlie. However, Bob can use his entanglement with Charlie to teleport his entanglement with Alice to Charlie. Thus Alice and Charlie become entangled even though they have never directly communicated.

Swapping protocol: ... (Blackboard)

4.7. No instantaneous transfer of information

Remarks: ... (Blackboard)

4.8. Di'Vincenzo's criteria on physical requirements

In an important article in 2000, Di'Vincenzo proposed five criteria that any physical system should satisify in order to represent a viable quantum computer. The discussion in this section here follows closely some work by Salomaa and Nakahara (conference contribution, World Scientific Publishing, 2005).

Five (+ two) criteria for a successful realization of a quantum computer: ... (Blackboard)

There are numerous physical systems proposed as a possible candidate for a viable quantum computer; they include

Physical realizations: ... (Blackboard)

ARDA QIST roadmap evaluates each of these realizations; see "A Quantum Information Science and Technology (QIST) Roadmap, Part 1: Quantum Computation" compiled by Advanced Research and Development Activity (ARDA), Los Alamos, USA. This article is updated annually.

4.9. Different models: A short overview

There are many models of quantum computation. Historically, the first was the quantum Turing machine, based on classical Turing machines. A more convenient model is the quantum circuit model.

Promising models for quantum computing ... (Blackboard)

4.10. Circuit model of quantum computations

Further reading (Circuit model of quantum computations):

➢ Read the section 3.2 The circuit model of quantum computations from the book of Benenti, Casati & Strini, Volume I (2004), pages 105-130.

4.10.a. Single-qubit operations

Properties: ... (Blackboard)

Problem (Single-qubit gates):

a) Prove that an arbitrary single-qubit unitary operation can be written in the form

$$U \;=\; \exp(i\alpha) R_{\mathbf{n}}(\theta)$$

where α and θ are real parameters, and $\mathbf{n}$ is a real three-dimensional unit vector.

b) Find the values of α, θ and $\mathbf{n}$ for the following gates:

$$\sigma_x \;=\; \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad H \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad S \;=\; \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}.$$

4.10.b. Conditional quantum operations

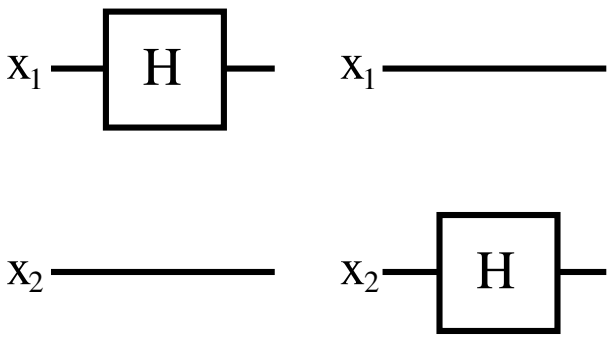


Figure 4.5.: Examples of two-qubit quantum circuits.

Blackboard example (Matrix representation of multi-qubit gates):

Problem (CNOT constructed from a controlled-Z gate): Construct a CNOT gate from a controlled-Z gate

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

and two Hadamard gates. Specify the control and target qubits.

Problem (Gate identities): Prove that $H\,\sigma_z\,H = \sigma_x$ and make use of this result to show that $H\,T\,H = R_x(\pi/4)$, up to a global phase, if $T = \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\pi/4) \end{pmatrix}$ and $R_x(\theta) = \exp\left(-i\theta\frac{X}{2}\right)$.

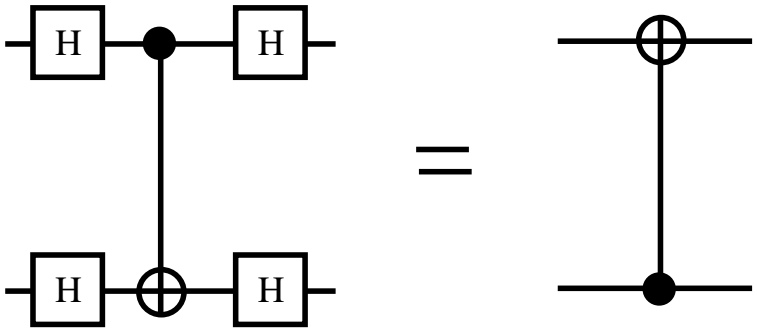


Figure 4.6.: Equivalence of simple circuits.

Example (CNOT basis transformation): Prove the equivalence of Figure 4.10.b.

The left-hand side is:

$$\begin{aligned}
&(H_1 \otimes H_2) \cdot \mathrm{CNOT} \cdot (H_1 \otimes H_2) \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}
\end{aligned}$$

Obviously, this transforms the basis states according to the rules:

$$U\,|00\rangle \;=\; U\begin{pmatrix}1\\0\\0\\0\end{pmatrix} \;=\; \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \;=\; |00\rangle$$

and, similarly,

$$U\,|10\rangle \;=\; |10\rangle\,, \qquad U\,|01\rangle \;=\; |11\rangle\,, \qquad U\,|11\rangle \;=\; |01\rangle\,.$$

This is apparently the transformation of a CNOT gate where the first qubit is the target and the second is the control-qubit.

4.10.c. Universal quantum gates

Blackboard example (Determine circuit from given gate):

Problem (Design of small circuits):

a) Construct a two-qubit gate that realizes the transformation

$$|a,b\rangle \;\longrightarrow\; |b,a\rangle \qquad \forall\, a,b, = |0\rangle\,,|1\rangle\;,$$

by using only the CNOT and Hadamard gates.

b) Prove that $U \;=\; \begin{pmatrix}1 & 0\\ 0 & e^{i\alpha}\end{pmatrix}$ can be written in the form $U \;=\; e^{i\theta}\,A\,\sigma_x\,B\,\sigma_x\,C$ where $\theta \;=\; \alpha/2$, $A \;=\; R_z(\alpha)$, $B \;=\; C \;=\; R_z(-\alpha/2)$ such that $A\,B\,C \;=\; I$.

4.11. Adiabatic model of quantum computations

Further reading (Adiabatic Evolution):

➢ Read the paper "Quantum Computation by Adiabatic Evolution" by E. Farhi *et al.*, quant-ph/0001106.

4.12. One-way or cluster state computations

Further reading (Measurement-based quantum compuations):

➢ Read the Letter "A One-Way Quantum Computer" by R. Raussendorf and H. J. Briegel, Phys. Rev. Lett. 86 (2002) 5188.

➢ Read the chapter 15. Cluster-state computing from the book of D. McMahon, Quantum Computing Explained (2008), pages 315-327.

4.13. Holonomic quantum computations

Further reading (Holonomic computations):

➢ Read the article by E. Sjöquist: "A new phase in quantum computations", Physics 1, 35 (2008).

4.14. Beyond the Di'Vincenzo's criteria

Remember the 5+2 criteria: ... (Blackboard)

Remarks:

➢ Some conditions can be relaxed; for example, in one-way quantum computing one make use of irreversible non-unitary gates.

➢ There has been a wide discussion of whether Di'Vincenzo's criteria are sufficient; these questions refer to topics such as:

+ Implementation of decoherence-free subsystems/subspaces.
+ Implementation of quantum error correction.
+ Fault-tolerant quantum computing.
+ Topologically protected qubits.

➢ Fault-tolerant quantum computing requires (Gottesman):

(1) Low gate error rates.
(2) Ability to perform operations in parallel.
(3) A way of remaining in, or returning to, the computational Hilbert space.
(4) A source of fresh initialized qubits during the computation.
(5) Proper error scaling: error rates that do not increase as the computer gets larger, and no large-scale correlated errors.

Many of the above conditions are necessary for quantum error corrections to work reasonably well.

5. Angular momentum in quantum physics

5.1. Angular momentum operators

Commutation relation & eigenfunctions:

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

The eigenfunctions Y_{lm} are called the spherical harmonics, and $\hbar$ is often omitted (if all angular momenta are taken in units of $\hbar$).

5.1.a. Algebraic definition of angular momentum

Definition by commutator: ... (Blackboard)

Problem (Commutation relations of AM operators): Derive the commutation relations

$$
\begin{aligned}
[j_i,\,\mathbf{j}^2] &= 0 \quad (i=1,2,3), & [j_+,\,j_-] &= 2\,\hbar\,j_z, \\
[j_z,\,j_\pm] &= \pm\hbar\,j_\pm, & [j_\pm,\,\mathbf{j}^2] &= 0
\end{aligned}
$$

from

$$
[j_i,\,j_j] = i\hbar\,\epsilon_{ijk}\,j_k\ ,
$$

5.1.b. Matrix representation of angular momentum operators

We wish to construct a matrix representation of the cartesian components j_x, j_y and j_z of the angular momentum operator $\mathbf{j} = j_x\,\mathbf{e}_x + j_y\,\mathbf{e}_y + j_z\,\mathbf{e}_z$.
We can form the matrix elements:

$$
\begin{aligned}
\langle u_{jm}\,|\,\mathbf{j}^2\,u_{jm'}\rangle &= \hbar^2\,j(j+1)\,\delta_{mm'} \\
\langle u_{jm}\,|\,j_z\,u_{jm'}\rangle &= \hbar\,\delta_{mm'} \\
\langle u_{jm}\,|\,j_\pm\,u_{jm'}\rangle &= \hbar\,\sqrt{j(j+1)\,-\,m(m\pm1)}\,\delta_{m,m'\pm1}
\end{aligned}
$$

and with $j_\pm = j_x \pm i\, j_y$

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

Example (Spin-1/2 systems): For spin-1/2 systems, we have $m = \pm 1/2$ and this gives rise to the matrix representations

$$j_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad j_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad j_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

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

Blackboard example (Spin-1 systems):

5.1.c. Algebra of Pauli matrices

Because of the significance of spin-1/2 particles and systems, the matrix representation of the angular momentum operators (apart from the factor $\hbar/2$) are known also as Pauli matrices, and together with σ_o :

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_o = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

These Pauli matrices obey several important relations:

$$\begin{aligned}
\sigma_x^2 &= \sigma_y^2 = \sigma_z^2 = \sigma_o \\
[\sigma_i, \sigma_j] &= 2i\, \epsilon_{ijk}\, \sigma_k \\
\{\sigma_i, \sigma_j\} &= 2\delta_{ij}\, \sigma_o \\
\sigma_i \sigma_j &= \delta_{ij}\, \sigma_o + i\, \epsilon_{ijk}\, \sigma_k
\end{aligned}$$

Linear independence of the Pauli matrices:

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

only holds iff $a_o = a_1 = a_2 = a_3 = 0$. This completeness of the Pauli matrices means that they form a basis for arbitrary 2×2 matrices:

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

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

$$(\mathbf{a}\cdot\boldsymbol{\sigma})\,(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b} + i\,\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})\,, \qquad (\mathbf{a}\cdot\boldsymbol{\sigma})^2 = a^2\,.$$

5.2. Coupling of angular momenta

5.2.a. Example: Angular momentum of electrons (spin-1/2 particles)

Let us consider an electron (spin-1/2 particle) with spatial coordinate $\mathbf{r}$ and spin projection $m_s = \pm 1/2$.

Hilbert space: Product of the position space $\mathbf{r}$ and the spin space

$$|\mathbf{r},\pm\rangle = |\mathbf{r}\rangle \otimes |\uparrow,\downarrow\rangle$$

Rotation operator: still given by $\exp\left(\frac{-i\,\mathbf{j}\cdot\mathbf{n}\,\vartheta}{\hbar}\right)$ with

$$\mathbf{j} = \mathbf{l}\otimes\mathbf{1} + \mathbf{1}\otimes\mathbf{s} = \mathbf{l} + \mathbf{s} \qquad \text{and}$$

$$[l_i,\,l_j] = i\hbar\,\epsilon_{ijk}\,l_k\,, \qquad [s_i,\,s_j] = i\hbar\,\epsilon_{ijk}\,s_k\,, \qquad [l_i,\,s_j] = 0\,,$$

and where $\mathbf{n}$ is a unit vector along the rotation axis. This gives rise to the rotation operator in the product space

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

Wave functions in product space: Superposition of two spin components

$$\psi(\mathbf{r},\sigma) = \begin{pmatrix} \psi_\uparrow(\mathbf{r}) \\ \psi_\downarrow(\mathbf{r}) \end{pmatrix} = \psi_\uparrow(\mathbf{r})\,|\uparrow\rangle + \psi_\downarrow(\mathbf{r})\,|\downarrow\rangle\,.$$

Operators and product states of composite system: $\{\mathbf{l}^2, l_z, \mathbf{s}^2, s_z\}$

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

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

$$l_z\,|\ell, m_\ell\rangle = m_\ell\,\hbar\,|\ell, m_\ell\rangle$$

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

$$s_z\,|s, m_s\rangle = m_s\,\hbar\,|s, m_s\rangle$$

5.2.b. Coupling of two angular momenta

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

Useful bases: ... (Blackboard)

Clebsch-Gordan expansion: The functions of the uncoupled and coupled bases can be easily transformed into each other:

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

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

These expansions coefficients are called the Clebsch-Gordan coefficients

$$\langle j_1, m_1, j_2, m_2 \,|\, j_1, j_2, j, m_j\rangle \equiv \langle j_1, m_1, j_2, m_2 \,|\, j, m_j\rangle \; ;$$

these coefficients freqently appear in the description of multi-qubit and quantum many-particle systems and elsewhere.

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

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

Clebsch-Gordan ... (Blackboard)

Problem (Clebsch-Gordan coefficients): Show the that Clebsch-Gordan coefficients are *zero* unless $m = m_1 + m_2$.

5.2.d. Calculation of Clebsch-Gordan coefficients

Recursion relations, etc. ... (Blackboard)

5.3. Wigner n–j symbols

5.3.a. Wigner 3–j symbols

Instead of the Clebsch-Gordan coefficients, one often uses the (so-called) Wigner n–j symbols which obey a higher symmetry. To this end, let us introduce the Δ symbol by

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

Then, the numerical value of a Wigner 3–j symbol is calculated by the expression due to Racah from 1942:

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

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

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

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

Moreover, an analogue phase factor occurs for

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

Recursion relations for the Wigner3–j symbols: are listed by Rotenberg *et al.* (1959), eqs. (1.45)–(1.48). If we assume $J = j_1 + j_2 + j_3$ in this subsection, we find for example:

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

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

From Louck (1958) is the following 1/2-step recursion relation [Louck]:

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

5.3.b. Wigner 6–j and 9–j symbols

Apart from the Wigner 3–j symbols, one can define Wigner 6–j and 9–j symbols, which also obey high symmetries. For example, the 9–j symbols with given numeric arguments can be calculated by means of a known sum rule over three Wigner 6–j symbols

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

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

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

The Wigner n–j symbols obey a very large number of sum rules which can be utilized to enourmoulsy simplify the spin-angular integration in the treatment of most quantum many-particle systems with some kind of rotational symmetry. An extensive list of such sum rules are provided in the monograph of Varshalovich *et al.* (1988) to which we here refer just for a few examples.

Sum rules for one 3–j symbol

Varshalovich *et al.* (1988), eq. (12.1.2) give one sum rule with one 3–j symbol.

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

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

Sum rules for one 6–j symbol

Rotenberg *et al.* (1959), eqs. (2.9–10) give sum rules with one 6–j symbol. A more general form is given by Varshalovich *et al.* (1988), eqs. (12.2.3–4).

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

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

Sum rules for two 3–j symbols

Two orthogonality relations for 3–j symbols are given by Rotenberg *et al.* (1959), eqs. (1.13–14). The same rules are given by Varshalovich *et al.* (1988), eqs. (12.1.3–4).

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

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

Sum rules for two 3–j symbols and one 6–j symbol

One such rule is given by Rotenberg *et al.* (1959), eq. (2.19). The same rule is shown by Varshalovich *et al.* (1988), eq. (12.1.5).

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

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

Sum rules for three 6–j symbols

There is a sum rule for three 6–j symbols from Biedenharn and Elliot [see Rotenberg *et al.* (1959), eq. (2.8)]. The same rule is given by Varshalovich *et al.* (1988), eq. (12.2.18).

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

$$= \begin{Bmatrix} p & q & r \\ e & a & d \end{Bmatrix} \begin{Bmatrix} p & q & r \\ f & b & c \end{Bmatrix}$$

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

Figure 5.1.: Structure of a Racah expression, i.e. typical expressions which appear in Racah's algebra.

$$\text{Racahexpr} := \sum_{j_1, j_2, l_1, \ldots} (-1)^{2j_1 - j_2 + \ldots} \; j_1^{3/2} \; [j_2] \ldots \begin{pmatrix} \cdot & \cdot & j_1 \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} j_1 & j_2 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{Bmatrix} \cdot & j_3 & \cdot \\ j_1 & \cdot & \cdot \\ J & \cdot & j_2 \end{Bmatrix} \ldots$$
$$\times \int d\Omega_1 \, Y_{l_1 m_1}(\Omega_1) \, Y_{l_2 m_2}(\Omega_2) \int d\beta \; d^{j_3}_{p_3 q_3}(\beta) \; d^{j_4}_{p_4 q_4}(\beta') \; \ldots$$

Sum rules for one 6–j symbol and three 9–j symbols

Varshalovich *et al.* (1988), eq. (12.2.44) gives a sum rule for one 6–j symbol and three 9–j symbols.

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

5.4. The RACAH program in Maple

In atomic and nuclear structure theory, the evaluation and spin-angular integration of many-particle matrix elements is typically based on standard quantities like the matrix elements of the unit tensor, the (reduced) coefficients of fractional parentage as well as a number of other reduced matrix elements concerning various products of creation and annihilation operators. These quantities arise very frequently both in configuration interaction approaches and the derivation of perturbation expansions for many-particle systems using symmetry-adapted configuration state functions.

In the framework of the RACAH program (Fritzsche 1997; Fritzsche *et al.* 1998), we provide a set of procedures for the manipulation and computation of such standard quantities in atomic theory. This (so-called) RACAH program is designed for interactive work and appropriate for almost any complexity of expressions from Racah algebra. In Figure 5.4, we display the typical structure of such expressions to which we refer as *Racah expressions*.

5.4.a. Presently supported symbols and functions in the RACAH program

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

Symbol	Designation	RACAH program
$\begin{pmatrix} a & b & c \\ m_a & m_b & m_c \end{pmatrix}$	Wigner 3–j symbol	Racah_w3j()
$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix}$	Wigner 6–j symbol	Racah_w6j()
$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}$	Wigner 9–j symbol	Racah_w9j()
$\langle a\ m_a,\ b\ m_b \mid c\ m_c \rangle$	Clebsch–Gordan coefficient	Racah_ClebschGordan()
$W(abcd;ef)$	Racah's W coefficient	Racah_Wcoefficient()
$d^j_{mm'}(\beta)$	Wigner $d^j_{mm'}(\beta)$ rotation matrix	Racah_dmatrix()
$D^j_{mm'}(\alpha,\beta,\gamma)$	Wigner's $D-$function	Racah_Dmatrix()
$U^j_{mm'}(\omega;\Theta,\Phi)$	Rotation matrix $U(\omega)$	Racah_Umatrix()
$Y_{lm}(\vartheta,\varphi)$	Spherical harmonic	Racah_Ylm()
$\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\cdot\cdot\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\}_{LM}$	Bipolar spherical harmonic	Racah_bipolarY()
$\left\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\cdot\cdot\{\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\cdot\cdot\mathbf{Y}_{l_3}(\vartheta_3,\varphi_3)\}_{l_{23}}\right\}_{LM}$	Tripolar spherical harmonic	Racah_tripolarY()
$\mathbf{Y}^l_{jm}(\vartheta,\varphi)$	Vector spherical harmonic	Racah_vectorY()
$\Omega^l_{jm}(\vartheta,\varphi)$	Spinor spherical harmonic	Racah_spinorY()
$Y^{ls}_{jm}(\vartheta,\varphi)$	Tensor spherical harmonic	Racah_tensorY()
$\langle l_a m_a \,\vert l_b m_b\vert\, l_c m_c\rangle$	Gaunt coefficient	Racah_Gaunt()
$C^k(l_a,m_a;l_b,m_b)$	Condon–Shortley coefficient	Racah_CondonShortley()
$\mathbf{H}_{l,\{\mu\}}$ †	Hyperspherical spherical harmonic	Racah_hypersphericalY()
$\left(\gamma\ \alpha Q\Gamma \,\vert\vert\vert\, a^{(q\gamma)} \,\vert\vert\vert\, \gamma\ \alpha' Q'\Gamma'\right)$	Reduced coefficient of fractional parentage	Racah_cfp()
...		

Spherical harmonics: The $Y_{lm}(\theta,\phi)$ functions form a complete and orthonormal set on the unit sphere, and are therefore widely used in classical and quantum physics; the spherical harmonics frequently appear in the representation of wave functions for a wide range of

physical systems, in the evaluation of the corresponding (quantum) matrix elements, and at many places elsewhere.

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

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

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

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

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

$$\begin{aligned}&\Big\{\mathbf{Y}_{l_1}(\vartheta_1,\varphi_1)\otimes\{\mathbf{Y}_{l_2}(\vartheta_2,\varphi_2)\otimes\mathbf{Y}_{l_3}(\vartheta_3,\varphi_3)\}_{l_{23}}\Big\}_{LM}\\ &\quad=\sum_{m_1,m_2,m_3,m_{23}}\langle l_1 m_1,\, l_{23} m_{23}\,|\,LM\rangle\;\langle l_2 m_2,\, l_3 m_3\,|\,l_{23} m_{23}\rangle\\ &\qquad\qquad Y_{l_1 m_1}(\vartheta_1,\varphi_1)\,Y_{l_2 m_2}(\vartheta_2,\varphi_2)\,Y_{l_2 m_2}(\vartheta_3,\varphi_3)\;.\end{aligned}$$

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

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

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

so that a irreducible tensor of rank j is obtained. While the l quantum number always occurs as a (nonnegative) integer, the indices j and s are both either integers or half-integers. For given j and s, the (orbital) angular momentum l can take the values $|j-s|,\;|j-s|+1,\;\ldots,\;j+s$; the allowed values of m are $-j,\;-j+1,\;\ldots,\;j$. Similar to the spherical harmonics, which form a complete set of functions on the unit sphere, the tensor spherical harmonics $Y^{ls}_{jm}(\vartheta,\varphi)$ form a complete and orthonormal set of functions for the expansion of rank s spinors with the domain of arguments $0\le\vartheta\le\pi$, $0\le\varphi\le 2\pi$.

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

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

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

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

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

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

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