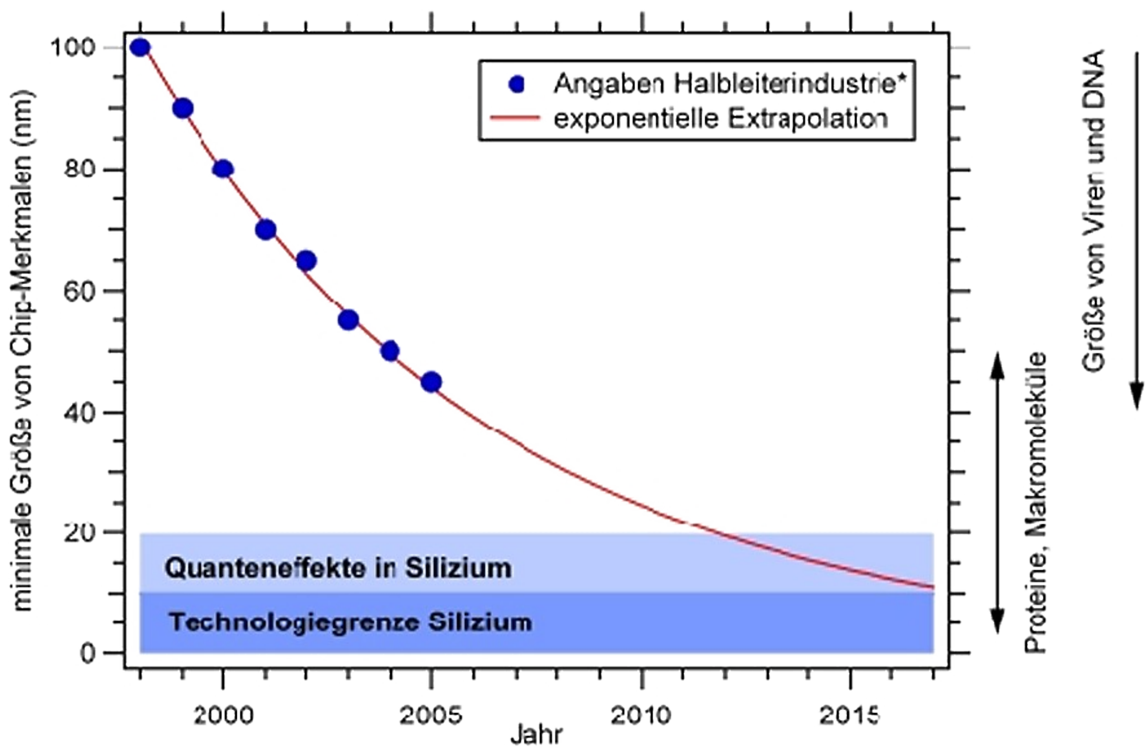
Computer algebra: A „classical“ path to explore decoherence and entanglement phenomena in quantum information theory

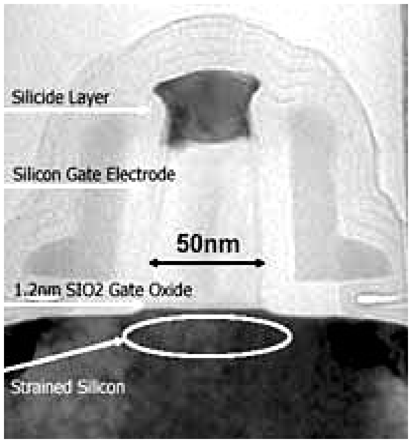
S. Fritzsche
GSI Darmstadt and MPIK Heidelberg
Bonn, 17th September 2007

Classical (electronic) computers will reach fundamental limits quite soon …



*Quelle: 'International Technology Roadmap for Semiconductors 2001'

60 .. 90nm generation transistor in current processors…



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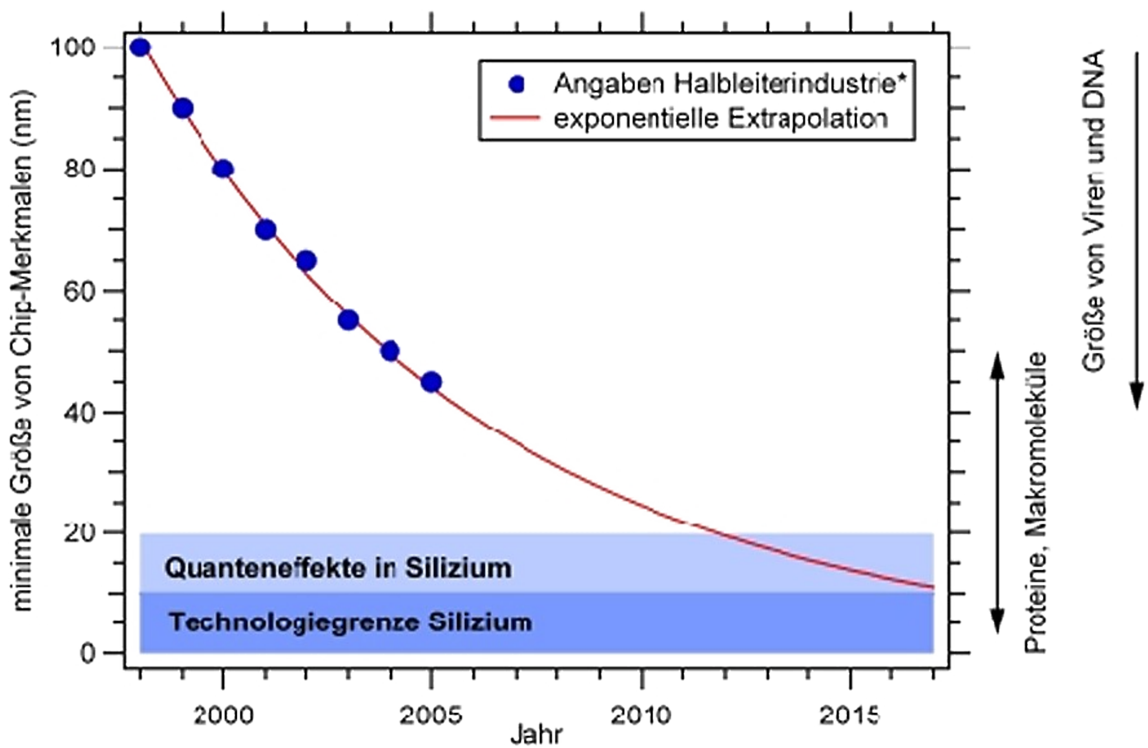

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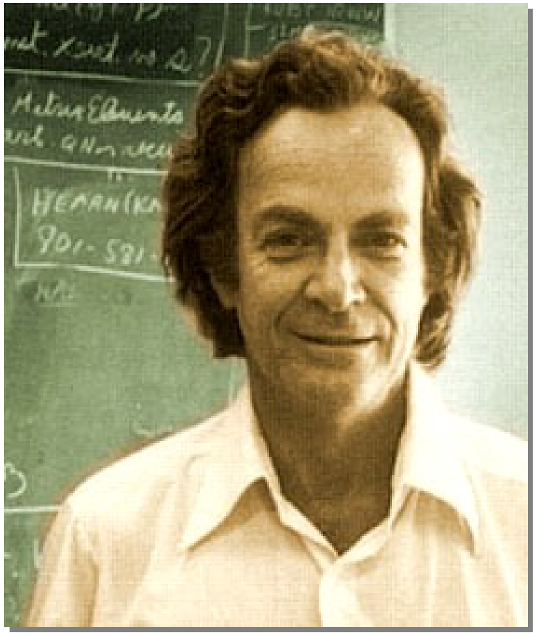
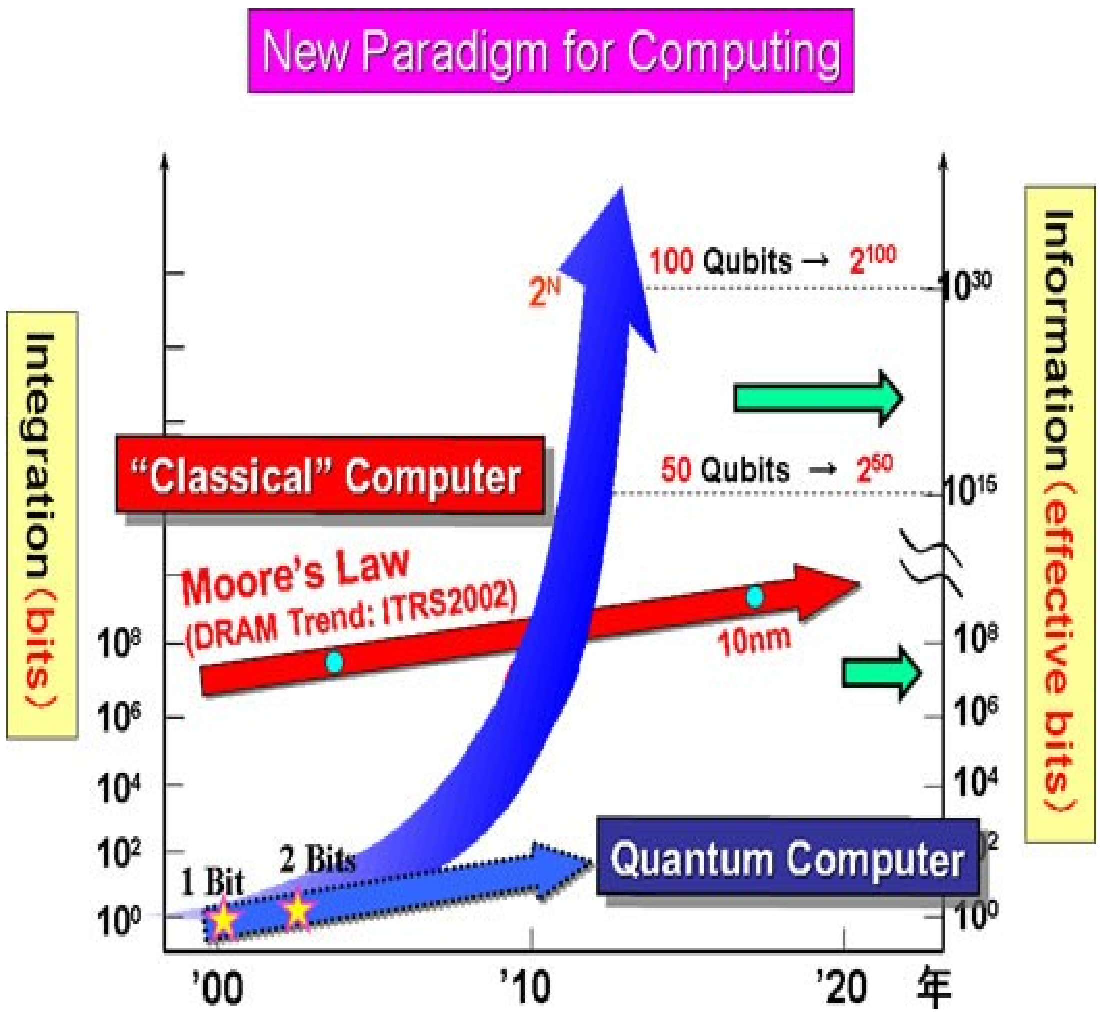
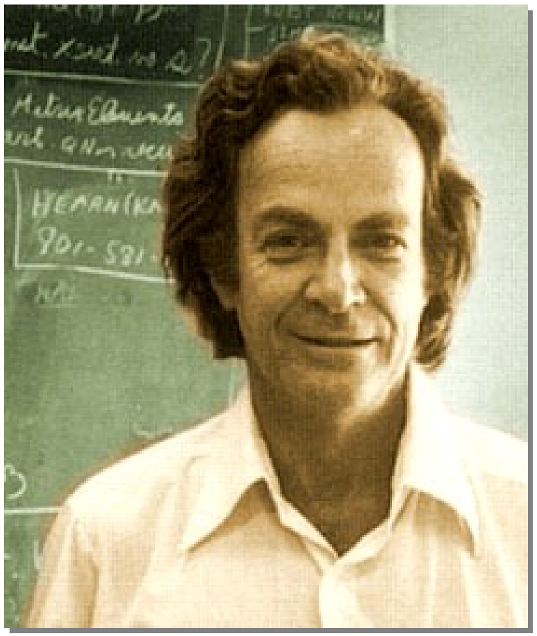


R.P. Feynman
Int. J. Theoret. Phys., 21 (1982) 467

“Quantum Mechanics cannot be simulated efficiently on a classical PC !“

Computer algebra: A „classical“ path to explore decoherence and entanglement phenomena in quantum information theory





Quantum properties such as superposition, entanglement, uncertainty, and interference have led to new brand of theory, where computational and communication processes are based on fundamental physics.

Computer algebra: A „classical“ path to explore decoherence and entanglement phenomena in quantum information theory

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Outline of this talk:

i) Short reminder: qubits and quantum registers

ii) Resources of quantum computing

iii) The FEYNMAN program: Quantum measures and noise models

iv) Quantum entanglement in atomic photoionization processes

v) Two-photon decay: Photon pairs with tailor-made entanglement

Qubits and N-qubit quantum registers

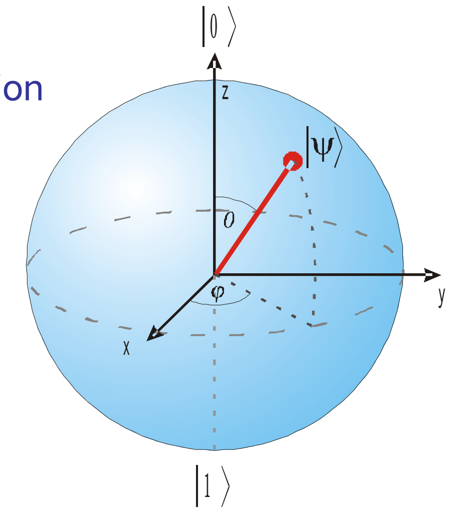
-- rapid growth in effort and complexity

Qubits:

$$|\Psi> = \alpha|0> + \beta|1> = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$|\alpha|^2 + |\beta|^2 = 1$$

Bloch sphere visualization



$$|0> = |\uparrow> = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1> = |\downarrow> = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Computational basis

Qubits and N-qubit quantum registers

-- rapid growth in effort and complexity

Qubits:

$$|\Psi> = \alpha|0> + \beta|1> = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

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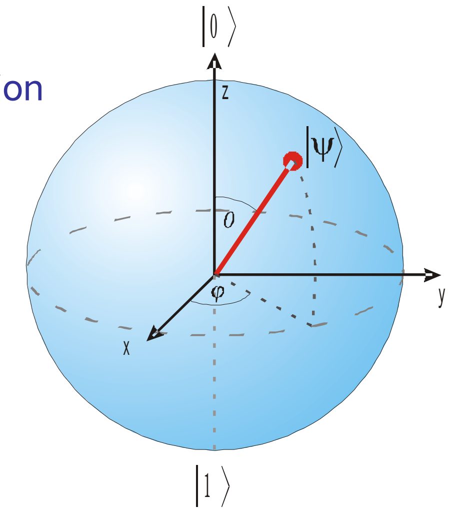
Computational basis

Bloch sphere visualization



$$H_N = H_1 \otimes H_2 \otimes \ldots \otimes H_n$$

$$|\Psi_3> = \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} \otimes \begin{bmatrix} \alpha_2 \\ \beta_2 \end{bmatrix} \otimes \begin{bmatrix} \alpha_3 \\ \beta_3 \end{bmatrix} = \begin{bmatrix} \alpha_1\alpha_2\alpha_3 \\ \alpha_1\alpha_2\beta_3 \\ \cdot \\ \cdot \\ \cdot \\ \beta_1\beta_2\beta_3 \end{bmatrix}$$

3 qubits

$2^3 = 8$ complex amplitudes

Basis states of product Hilbert space = classical binary combinations

$$= \alpha_1\alpha_2\alpha_3|000> + \alpha_1\alpha_2\beta_3|001> + \ldots + \beta_1\beta_2\beta_3|111>$$

N-qubit quantum registers

-- rapid growth in effort and complexity

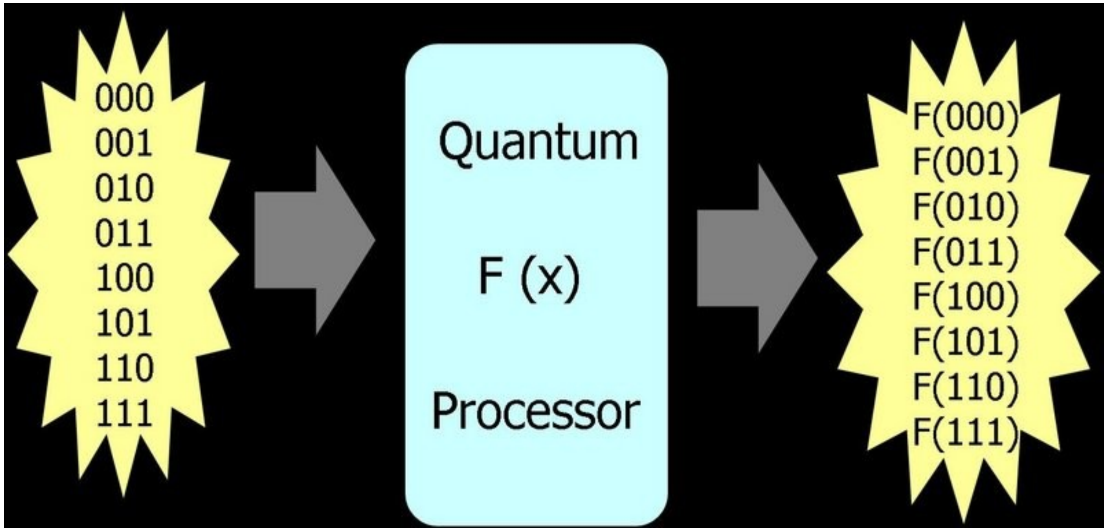
From: www.labs.nec.co.jp/ Eng/innovative/E3/03.html

Quantum algorithms and „quantum parallelism“

-- The great promise of quantum computations ...

In quantum systems, an exponential increase in parallelism requires only a linear increase in the amount of space needed.

→ Promise to solve efficiently most difficult problems in computational sciences such as simulation of quantum systems, integer factorization, or database searching.



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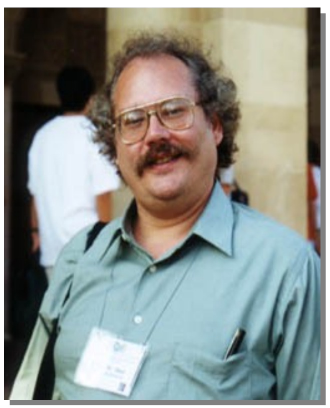
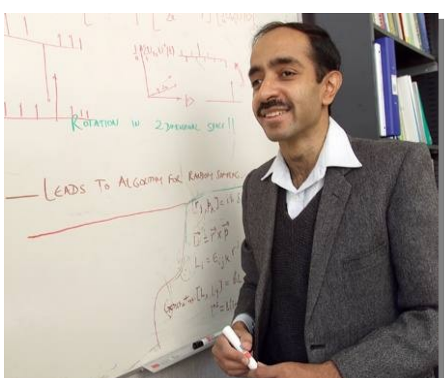


Shor‘s factorization algorithm for prime numbers

SIAM J. Sci. Statist. Comput. 26, 1484 (1997)

Factorizes large numbers into prime numbers **exponentially** faster than the best known classical algorithm

→ Some classical (asymmetric) cryptography can be broken by this !



Grover‘s database search algorithm

Phys. Rev. Lett. 79, 325 (1997)

Quadratic speedup compared to a classical search algorithm

→ Many problems can be translated into search problems !

N-qubit quantum registers

-- representation and time evolution

„real physics“

$$i\hbar \frac{d|\Psi>}{dt} = H|\Psi> \;\rightarrow\; |\Psi'> = U|\Psi> \;\rightarrow\; U(\Delta t) = \mathrm{e}^{-iH\Delta t/\hbar}$$

Abstract logical operator

Formal requirements for dealing with quantum registers:

- stable representation of basis states |0> and |1>
- reliable preparation of initial states
- perform a universal set of unitary transformations (including the creation of entanglement!)
- measurement of output results
- scalability (we need at least 20 ... 50 qubits)
- ...

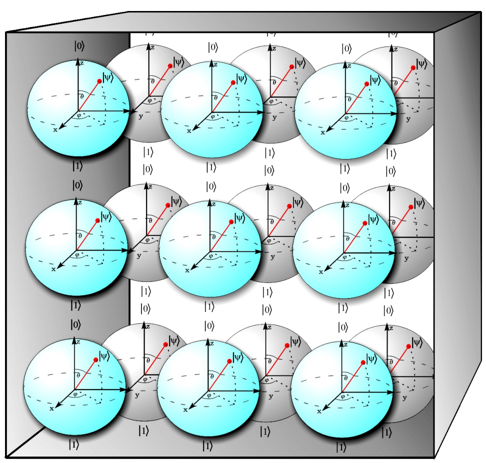
N-qubit quantum registers

-- representation and time evolution

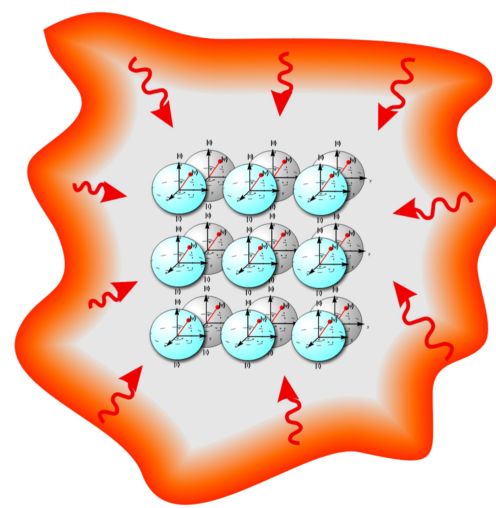
„real physics“

$$i\hbar \frac{d|\Psi>}{dt} = H|\Psi> \rightarrow |\Psi'> = U|\Psi> \rightarrow U(\Delta t) = e^{-iH\Delta t/\hbar}$$

Abstract logical operator



Closed system



Open system

$$\mathcal{E}(\rho) = \mathrm{Tr}_{env}\left[U(\rho \otimes \rho_{env})U^{\dagger}\right]$$

Partial trace and reduced density matrix

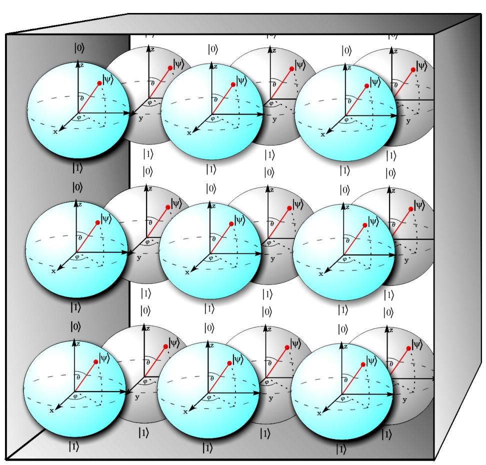
N-qubit quantum registers

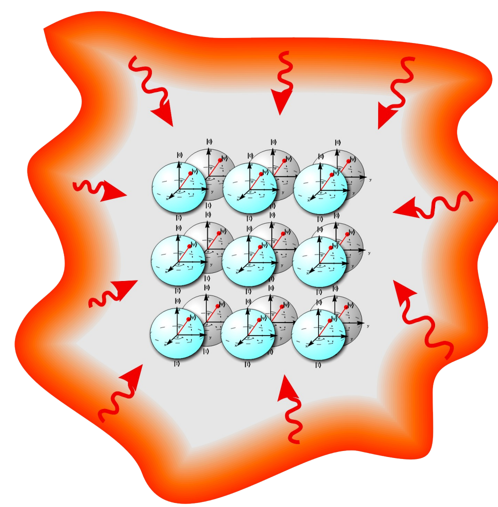
-- representation and time evolution

„real physics“

$$i\hbar \frac{d|\Psi>}{dt} = H|\Psi> \rightarrow |\Psi'> = U|\Psi> \rightarrow U(\Delta t) = e^{-iH\Delta t/\hbar}$$

Abstract logical operator





Open system

The unitary evolution preserves the state‘s purity

by tracing over the environment degrees of freedom the principal system will become mixed

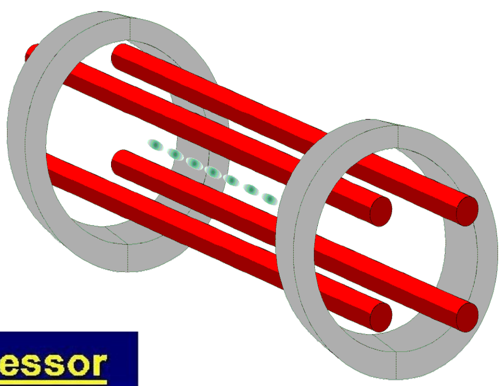
Realization and simulation of quantum computers

$$\mathcal{E}(\rho) = \mathrm{Tr}_{env}\left[U(\rho \otimes \rho_{env})U^{\dagger}\right]$$

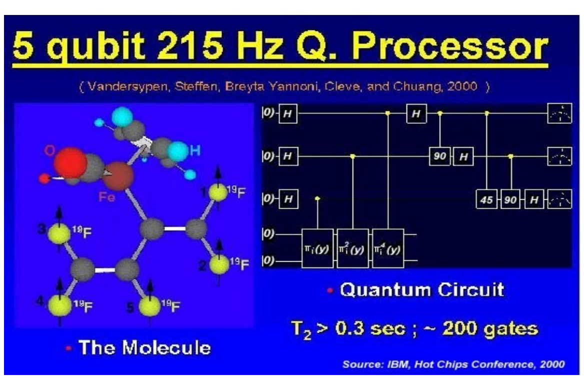
Experiment

Different schemes have been suggested in the past.

Ion traps



NMR computers

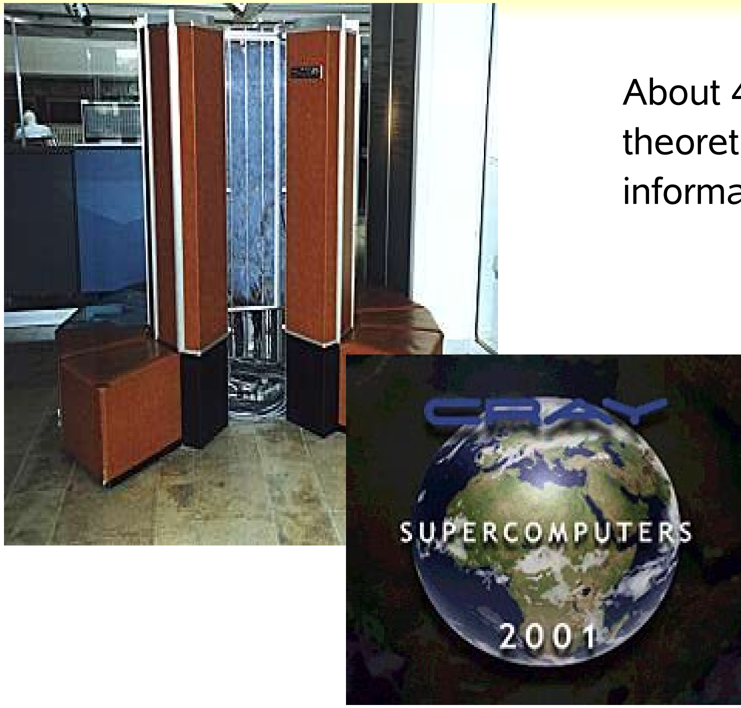


Theory

Use of classical computers to simulate parts of quantum computers including quantum measurements, design of algorithms, or the coupling to the environment.

„Numerical studies“

-- An accepted route in theoretical physics ?



About 40 years ago, (pure) numerical studies became an accepted instrument in theoretical physics; they -- in fact -- often provide the only route to obtain sufficient information about many systems.

Matrix diagonalization:

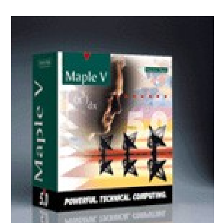
$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$10^{4 \ldots 7}$ (today's dimensions)

Numerical libraries: LU decomposition, Davidson algorithm, ...

Symbolic manipulations:

- automatic search for symmetries and appropriate coordinates
- simplification of expressions, operators and/or matrix elements
- classification of (many-particle) quantum states
- manipulation of spin chains
- ...



maple, mathematica, derive, ...
(included in present-day curricula)

Applications of CAS in many-particle physics and quantum computing

Experience: Implementation and computations often require the dominant effort in studying (quantum-) many-particle systems.

- Advanced calculus for „hydrogenic systems“
- Angular momentum in physics (Racah's algebra)
- Point-group symmetries
- Dynamics of spin chains
- Manipulation of quantum registers and quantum circuits
- Classification and control of decoherence
- ...

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Advantages of using CAS in theoretical physics

- Knowledge of the mathematical rules.
- Facilitates tedious derivations; often used if the basic transformations of some theory are well understood.
- Fast, reliable and easily reproducible.
- Help examine different approximations.
- Stepwise manipulation of expressions.

Requirements for studying quantum many-particle systems

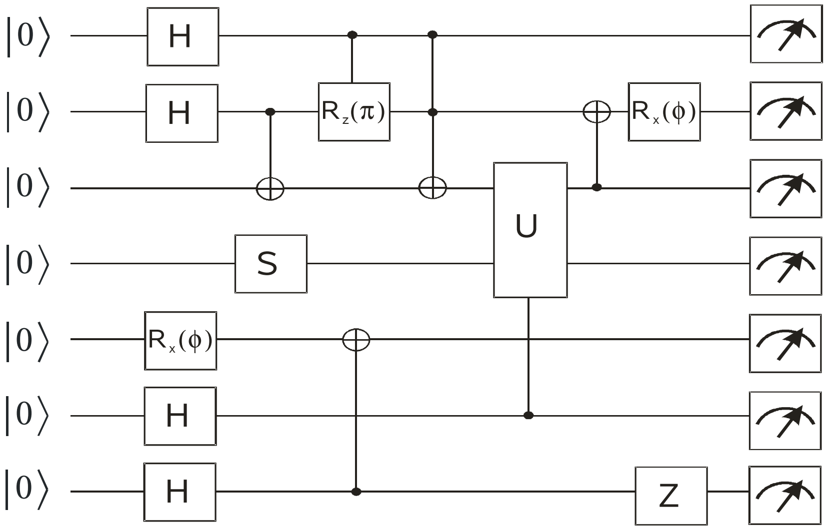
-- in addition to the use of CAS in other fields

- The "language", which is used in the design, must be adjusted to the community (e.g. group theory in atomic physics, physical chemistry, or crystallography).
- Simplicity and user-friendliness as these tools may provide only 'intermediate results'.
- Prepared and easily extentable data structures as well as support for changing the data types.
- Scalable algorithms which can be followed *step by step*.
- Tools for error tracing.
- Simple and instructive test cases; they often decide whether the tools and methods are accepted by the community.
- For quantitative predictions about many-particle systems, the interplay of algebraic and numerical methods must be improved.

Simulation of quantum computers

-- computational requests

$$H_N = H_1 \otimes H_2 \otimes \ldots \otimes H_n$$



Simulation of N-qubit systems

- Large state vectors and density matrices
- Graphical representation of qubit states
- Application of unitary and non-unitary operations
- Construction of quantum gates and circuits
- Partial trace operations
- Classification of decoherence
- ...

Aim in the manipulation of quantum registers

Efficient set-up and treatment of quantum registers as a necessary requirement in order to describe and to follow up the time evolution of model systems and real physical implementations.

FEYNMAN program

-- Simple applications of the toolbox

PhD work of Thomas Radtke

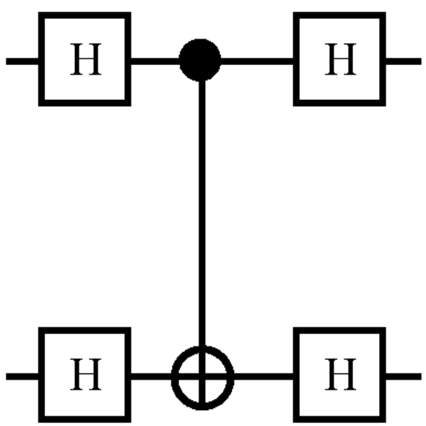
T. Radtke and S. Fritzsche, CPC 173 (2005) 91; CPC 175 (2006) 145

The FEYNMAN program

-- a quantum simulator using Maple

- Set of Maple procedures to deal with qubits, quantum registers, operators
- Provides data structures which are flexible for most applications.
- Modular structure: with(Feynman);
- ...

Show the identity of quantum circuits:



$$\leftrightarrow \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

The FEYNMAN program

-- a simple example

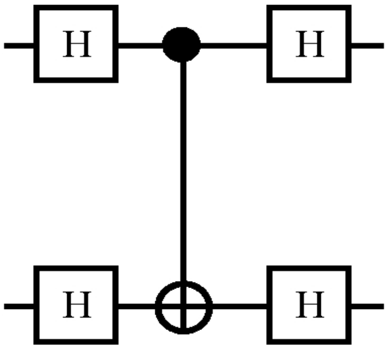
```
> with(Feynman):
```

Welcome to Feynman (May 2005) !

--- The Swiss Army Knife for Quantum Computation ---

```
> H1 := Feynman_quantum_operator(2, "H", [1]);
```

$$H1 := \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix}$$



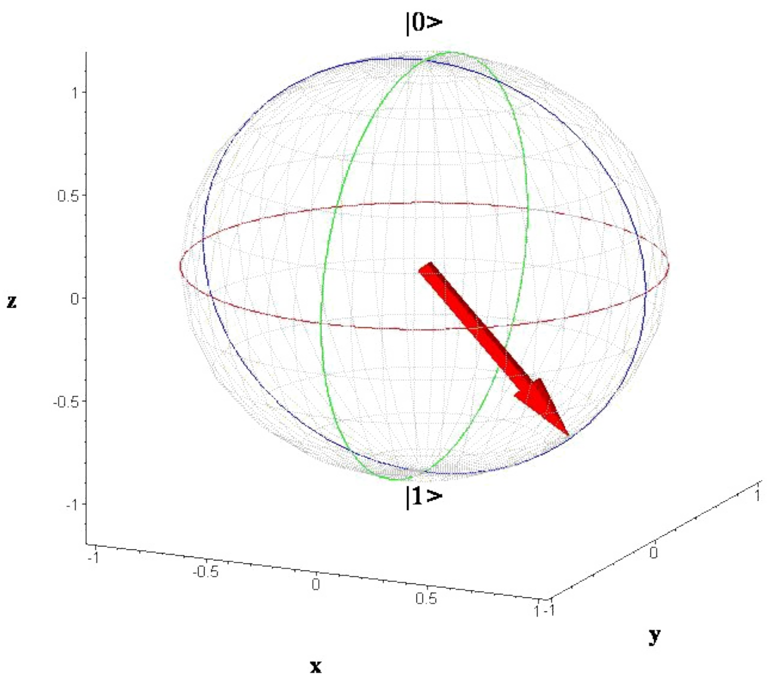

```
> H2 := Feynman_quantum_operator(2, "H", [2]):
> CN := Feynman_quantum_operator("cnot"):
> H1.H2.CN.H1.H2;
```

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \longleftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Spontaneous decay of single-qubit state

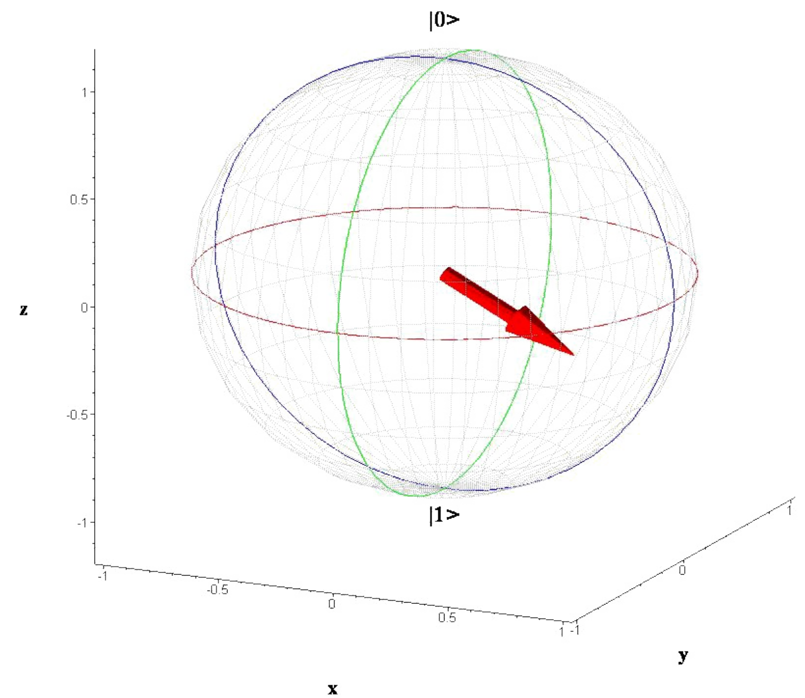
-- amplitude damping of single-qubit density matrix

Example: decay to ground state with a given probability p = 0.25



initial state

$$\rho = E(\rho)$$



final state

General questions:

- How close are input and output state ?
- How much „mixedness“ (i.e. entropy) will be created ?
- How well is entanglement preserved ?

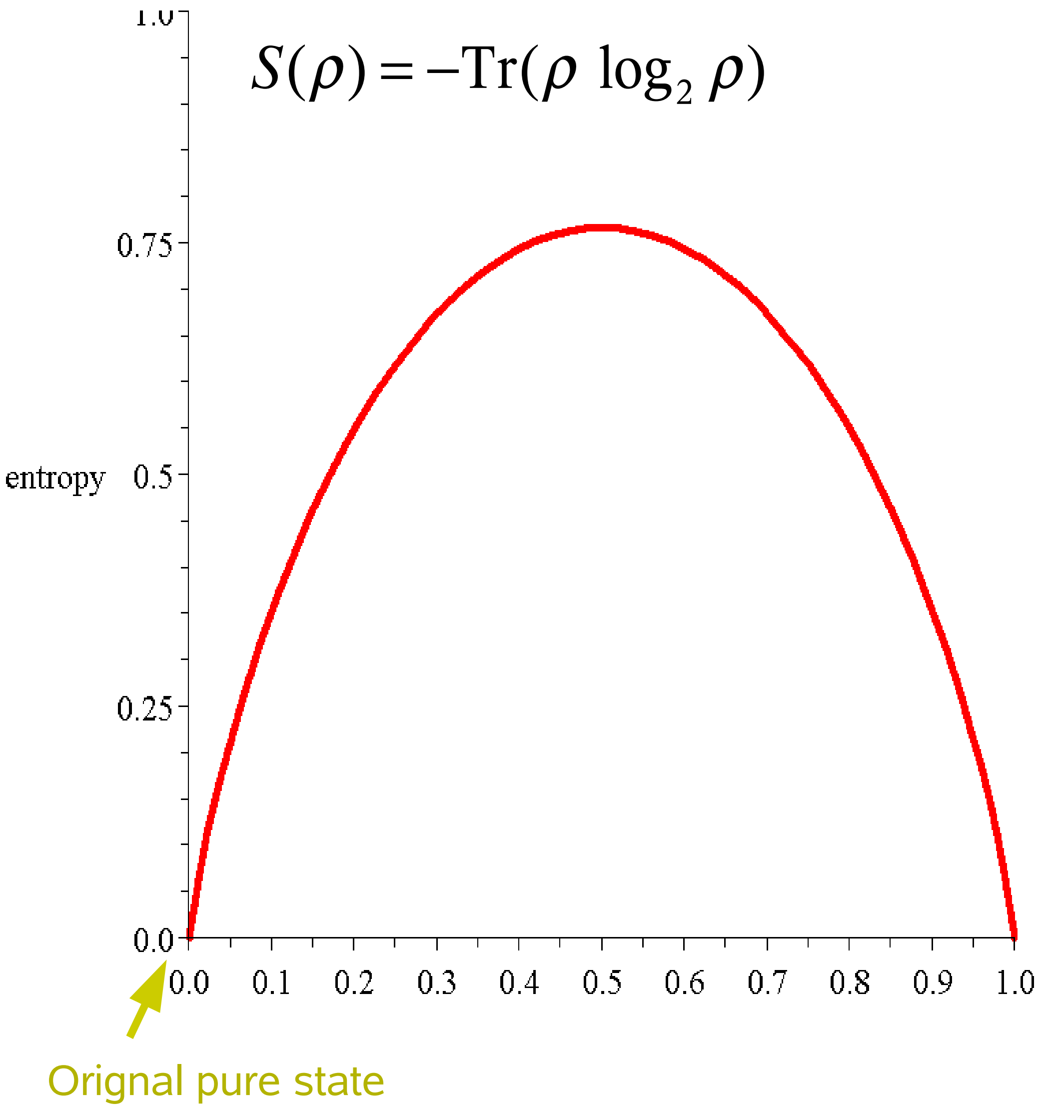
$$E_0 = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{bmatrix}, \quad E_1 = \begin{bmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{bmatrix}$$

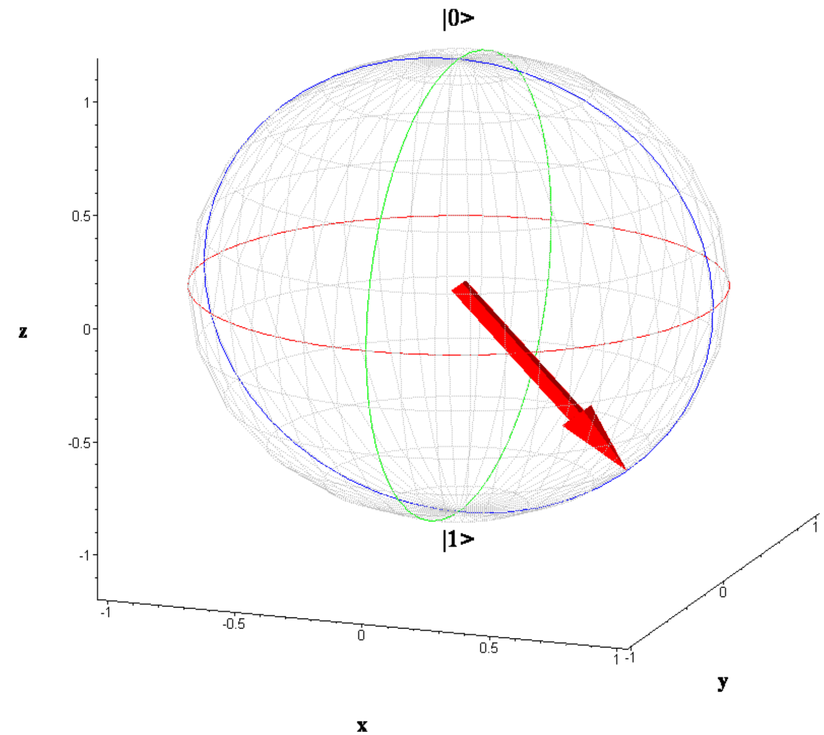
Spontaneous decay of single-qubit state

-- amplitude damping of single-qubit density matrix

Entropy of single-qubit state:

$$S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho)$$





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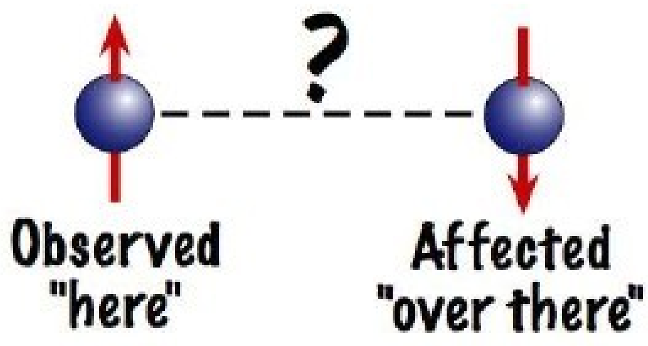
Entanglement in quantum systems

-- nonlocal correlations between two or more subsystems

Quantum entanglement occurs when two or more particles interact in a way that causes their fates to become linked. ... Collectively they constitute a single quantum state.



„...spooky action at a distance..." *(Einstein)*

Quantification of entanglement remains in general unsolved; already the decision for density matrix about being separable or entangled is NP-hard.

Applications of entanglement:

- superdense coding
- quantum state teleportation
- quantum cryptography (key distribution)
- efficient quantum algorithms

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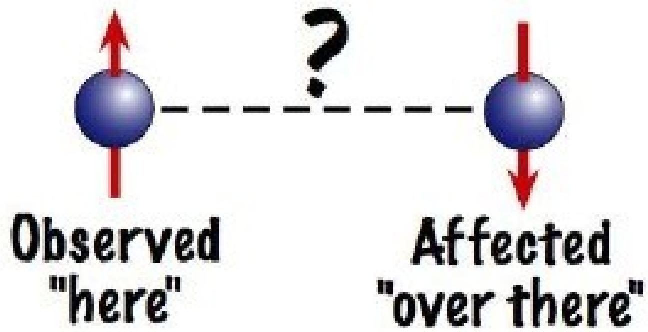

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Later in this talk.

Search for physical processes where entanglement can be observed and manipulated !

Quantum entanglement

-- A key ingredient of quantum information protocols

A physical resource, like energy, associated with the peculiar nonclassical correlations that are possible between separated quantum systems.

$$\left|\Phi^+\right\rangle = \frac{\left|00\right\rangle + \left|11\right\rangle}{\sqrt{2}} \neq \left|a\right\rangle \otimes \left|b\right\rangle \quad \forall\ \left|a\right\rangle \in \mathrm{H}_A, \left|b\right\rangle \in \mathrm{H}_B$$

Wotter`s Concurrence

-- entanglement measure for an arbitrary two-qubit density matrix $0 \leqslant C(\rho) \leqslant 1$

$C = max(0,\ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$ are eigenvalues of $\rho\bar{\rho} = \rho(\sigma_y^A \otimes \sigma_y^B)\rho^*(\sigma_y^A \otimes \sigma_y^B)$

Examples:

Bell state $|\Psi^+> = \frac{|01> + |10>}{\sqrt{2}}$ ⟶ $C(\Psi^+) = 1$

Product state $|\Psi> = |00>$ ⟶ $C(\Psi) = 0$

W.K. Wotters, Phys. Rev. Lett. 80 (1998) 2245.

Entanglement of a pure two-qubit state

-- to be recognized by means of a Schmidt decomposition

$$|\psi_{AB}\rangle \;=\; \sum_{i=1}^{r} \sqrt{\lambda_i}\, |a_i\rangle\, |b_i\rangle$$

<u>Example:</u>

$$|\psi_{AB}\rangle \;=\; \frac{1+\sqrt{6}}{2\sqrt{6}}|00\rangle + \frac{1-\sqrt{6}}{2\sqrt{6}}|01\rangle + \frac{\sqrt{2}-\sqrt{3}}{2\sqrt{6}}|10\rangle + \frac{\sqrt{2}+\sqrt{3}}{2\sqrt{6}}|11\rangle$$

$$\sum_{i=1}^{r} \lambda_i \;=\; 1$$

```
> psi_AB := Feynman_set_qregister((1 + sqrt(6))/(2*sqrt(6))*cbs("00")
            + (1 - sqrt(6))/(2*sqrt(6))*cbs("01")
            + (sqrt(2) - sqrt(3))/(2*sqrt(6))*cbs("10")
            + (sqrt(2) + sqrt(3))/(2*sqrt(6))*cbs("11")):
```

$$[[\sqrt{\lambda_1}, [|a_1\rangle, |b_1\rangle]], [\sqrt{\lambda_2}, [|a_2\rangle, |b_2\rangle]]]$$

$$\left[\left[\frac{\sqrt{3}}{2}, \begin{bmatrix} \frac{\;}{3} \\ -\frac{\sqrt{3}}{3} \end{bmatrix}, \begin{bmatrix} \frac{\;}{2} \\ -\frac{\sqrt{2}}{2} \end{bmatrix}\right], \left[\frac{1}{2}, \begin{bmatrix} \frac{\;}{3} \\ \frac{\sqrt{6}}{3} \end{bmatrix}, \begin{bmatrix} \frac{\;}{2} \\ \frac{\sqrt{2}}{2} \end{bmatrix}\right]\right]$$

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$$\sum_{i=1}^{r} \lambda_i = 1$$

```
> psi_AB := Feynman_set_qregister((1 + sqrt(6))/(2*sqrt(6))*cbs("00")
          + (1 - sqrt(6))/(2*sqrt(6))*cbs("01")
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          + (sqrt(2) + sqrt(3))/(2*sqrt(6))*cbs("11")):
```

$$[[\sqrt{\lambda_1}, [|a_1\rangle, |b_1\rangle]], [\sqrt{\lambda_2}, [|a_2\rangle, |b_2\rangle]]]$$

$$\left[\left[\frac{\sqrt{3}}{2}, \left[\begin{matrix} \frac{[illegible]}{3} \\ -\frac{\sqrt{3}}{3} \end{matrix}\right], \left[\begin{matrix} \frac{[illegible]}{2} \\ -\frac{\sqrt{2}}{2} \end{matrix}\right]\right], \left[\frac{1}{2}, \left[\begin{matrix} \frac{[illegible]}{3} \\ \frac{\sqrt{6}}{3} \end{matrix}\right], \left[\begin{matrix} \frac{[illegible]}{2} \\ \frac{\sqrt{2}}{2} \end{matrix}\right]\right]\right]$$

Entropy of entanglement:

$$E_E(|\psi_{AB}\rangle) = S(\rho_A) = S(\rho_B)$$

```
> evalf(Feynman_measures("entropy of entanglement", psi_AB, [1],[2]));
```

0.8112781242

Argument option	Explanation
i) Fidelity and distance measures	
("fidelity", ...)	fidelity $F(\rho,\sigma) = [\mathrm{Tr}(\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}})]^2$
("trace distance", ...)	trace distance $D_{\mathrm{Tr}}(\rho,\sigma) = \frac{1}{2}\|\rho-\sigma\|_{\mathrm{Tr}} = \frac{1}{2}\mathrm{Tr}\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}$
("Hilbert-Schmidt distance", ...)	Hilbert-Schmidt distance $D_{\mathrm{HS}}(\rho,\sigma) = \|\rho-\sigma\|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}[(\rho-\sigma)^\dagger(\rho-\sigma)]}$
("Bures distance", ...)	Bures distance $D_{\mathrm{B}}(\rho,\sigma) = \sqrt{2-2\,\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}}$
ii) Entropy measures and related quantities	
("entropy", ...)	von Neumann entropy $S(\rho) = -\mathrm{Tr}(\rho\log_2\rho)$
("linear entropy", ...)	linearized version of the von Neumann entropy, $S_l(\rho) = \frac{d}{d-1}\,(1-\mathrm{Tr}(\rho^2))$
("participation ratio", ...)	participation ratio $R(\rho) = 1/\mathrm{Tr}(\rho^2)$ of a given state. It can be interpreted as the effective number of pure states that enter the mixture.
("relative entropy", ...)	relative entropy $S(\rho\,\|\,\sigma) = -S(\rho) - \mathrm{Tr}(\rho\log_2\sigma)$
("conditional entropy", ...)	(von Neumann) conditional entropy $S(A\|B) = S(\rho_{AB}) - S(\rho_B)$
("mutual information", ...)	mutual information $S(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$
iii) Bipartite entanglement	
("entropy of entanglement", ...)	entropy of entanglement $E_E(\|\psi_{AB}\rangle) = S(\rho_A) = S(\rho_B)$
("negativity", ...)	neg
("logarithmic negativity", ...)	logarithmic negativity $E_N(\rho) = \log_2\|\rho^{T_A}\|_{\mathrm{Tr}}$

Using the command Feynman_measures(...)

Entanglement decay through amplitude damping

-- decay of a single qubit of a Bell state

$$|\Psi^- > = \frac{|01> - |10>}{\sqrt{2}}$$

```
> input_state := Feynman_set_qregister("Bell","Psi-"):
> assume(p>=0, p<=1);
  noisy_channel := qoperation(2, "amplitude damping", p, [2]);
```

noisy_channel := qoperation(2, "amplitude damping", p~, [2])

Entanglement decay through amplitude damping

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```
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> assume(p>=0, p<=1);
  noisy_channel := qoperation(2, "amplitude damping", p, [2]);
```

$$noisy\_channel := qoperation(2, \text{"amplitude damping"}, p\sim, [2])$$

```
> output_state := Feynman_apply(noisy_channel, input_state);
```

$$output\_state := qregister\left(\text{"Psi-"}, 2, \begin{bmatrix} \frac{p\sim}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} - \frac{p\sim}{2} & -\frac{\sqrt{1-p\sim}}{2} & 0 \\ 0 & -\frac{\sqrt{1-p\sim}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\right)$$

Entanglement decay through amplitude damping

-- decay of a single qubit of a Bell state

Input state:

$$|\Psi^- > = \frac{|01> - |10>}{\sqrt{2}}$$

$$\text{output\_state} := \text{qregister}\left(\text{"Psi-"}, 2, \begin{bmatrix} \frac{p\sim}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} - \frac{p\sim}{2} & -\frac{\sqrt{1-p\sim}}{2} & 0 \\ 0 & -\frac{\sqrt{1-p\sim}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \right)$$

```
> plot([Feynman_measures("concurrence", output_state),
        Feynman_measures("negativity",  output_state, [1],[2]),
        Feynman_measures("entropy", output_state)],            p=0..1);
```

Entanglement decay through amplitude damping

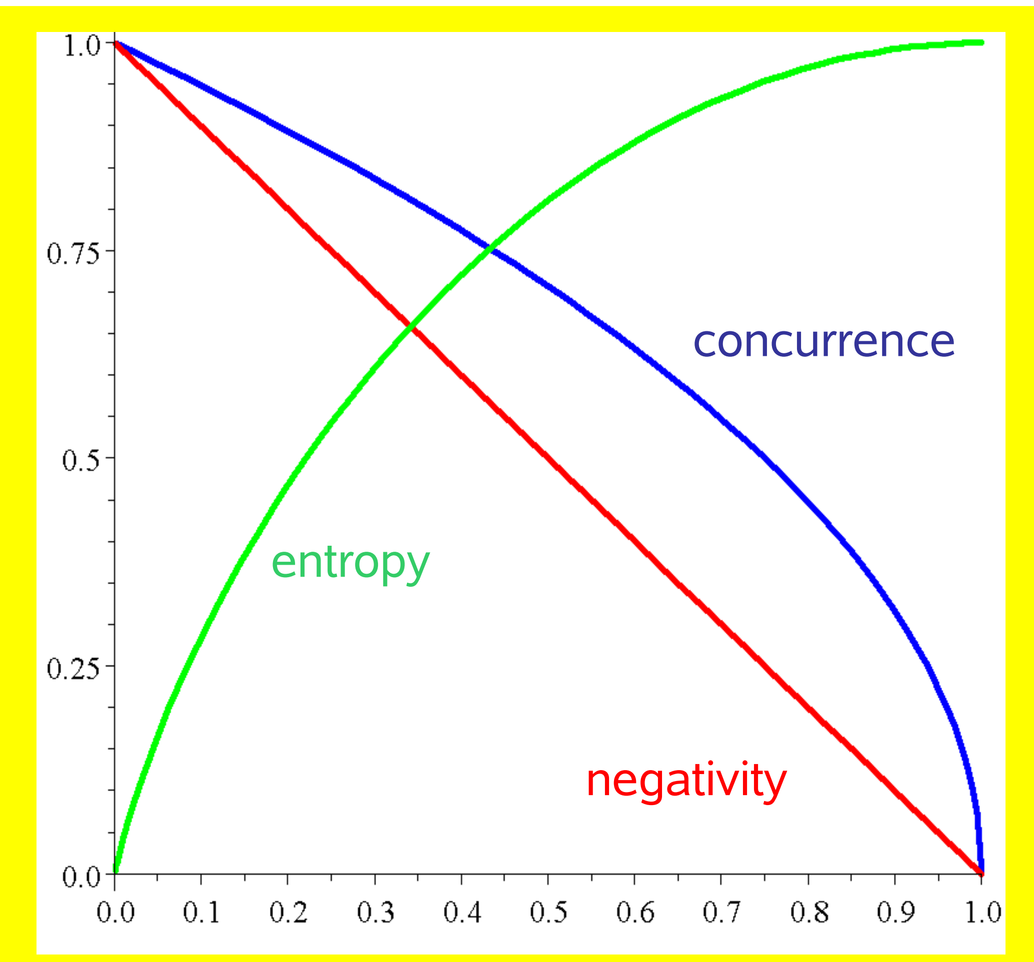
-- decay of a single qubit of a Bell state

Input state:

$$|\Psi^{-}> = \frac{|01> - |10>}{\sqrt{2}}$$

ter $\left(\text{"Psi-"}, 2, \begin{bmatrix} \frac{p\sim}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} - \frac{p\sim}{2} & -\frac{\sqrt{1-p\sim}}{2} & 0 \\ 0 & -\frac{\sqrt{1-p\sim}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \right)$

```
", output_state),
, output_state, [1],[2]),
utput_state)],                    p=0..1);
```



Finite-time disentanglement via spontaneous decay

-- amplitude damping of two entangled qubits

Consider two-qubit state:

$$\rho = \frac{1}{3}\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & z & 0 \\ 0 & z^* & c & 0 \\ 0 & 0 & 0 & d \end{pmatrix}$$

with $0 \le a \le 1,\ d = 1 - a \text{ and } b = c = z = 1$

```
> rho := 1/3*Matrix([[a,0,0,0],[0,1,1,0],[0,1,1,0],[0,0,0,1-a]]):
  input := qregister(id, 2, rho);
```

$$input := \mathrm{qregister}\left(id, 2, \begin{bmatrix} \frac{a}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} - \frac{a}{3} \end{bmatrix}\right)$$

Finite-time disentanglement via spontaneous decay

-- amplitude damping of two entangled qubits

Kraus operators:

$$E_1 = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix}$$

$$E_2 = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix}$$

$$E_3 = \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix} \otimes \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix}$$

$$E_4 = \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix}$$

Operator-sum or Kraus representation:

$$\rho' = \sum_{i=1}^{4} E_i \rho E_i^\dagger$$

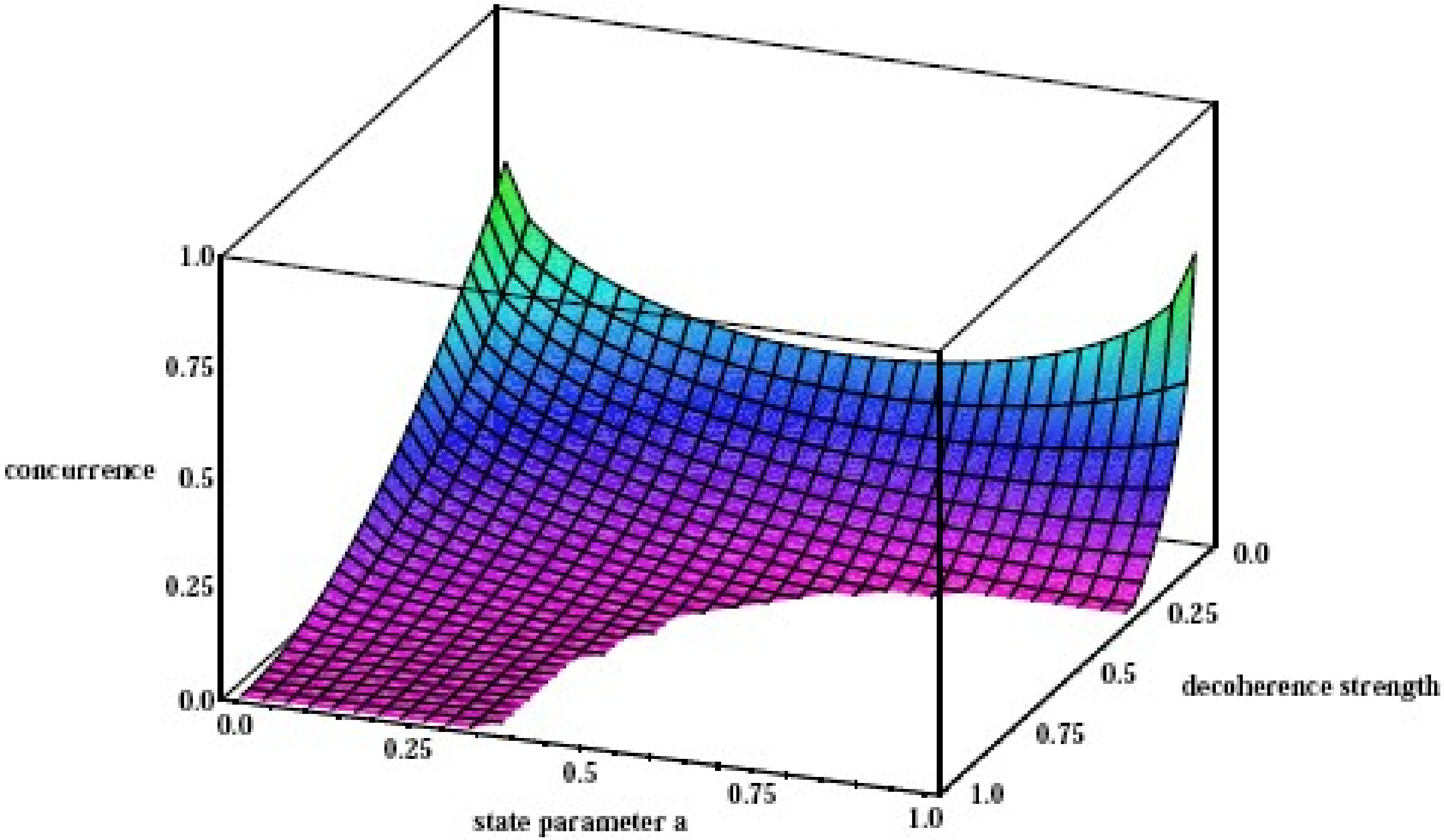
```
> E1 := Feynman_product("Kronecker", Matrix([[gamma,0],[0,1]]), Matrix([[gamma,0],[0,1]])):
  E2 := Feynman_product("Kronecker", Matrix([[gamma,0],[0,1]]), Matrix([[0,0],[omega,0]])):
  E3 := Feynman_product("Kronecker", Matrix([[0,0],[omega,0]]), Matrix([[gamma,0],[0,1]])):
  E4 := Feynman_product("Kronecker", Matrix([[0,0],[omega,0]]), Matrix([[0,0],[omega,0]])):
```

```
> assume(g>=0, g<=1):
  Kraus_ops := subs(omega=sqrt(1-gamma^2), [E1, E2, E3, E4]):
  Kraus_ops := simplify(subs(gamma=1-g, Kraus_ops)):
  output    := simplify(Feynman_apply(qoperation(Kraus_ops), input)):
```

T. Hu, J.H. Eberly, Phys. Rev. Lett. 93 (2004) 140404.

Finite-time disentanglement via spontaneous decay

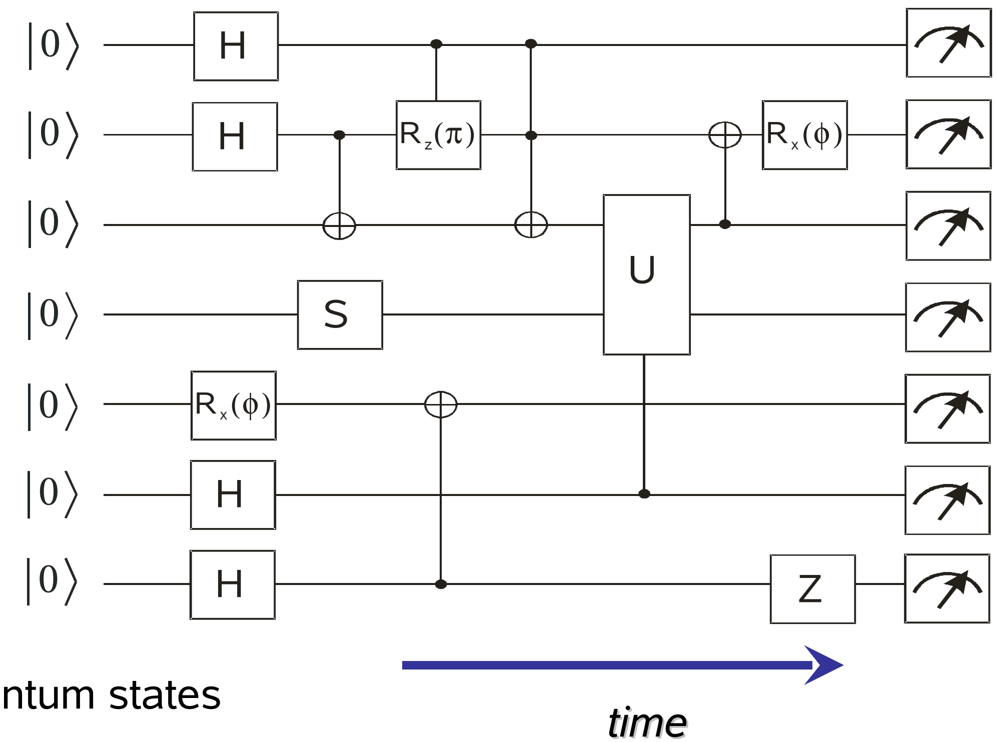
-- amplitude damping of two entangled qubits



In contrast to the purely exponential decay of the individual qubits, two entangled qubits may become completely disentangled within a finite time (for a > 1/3).

The FEYNMAN program

-- computations with quantum circuits and operations



Features of the FEYNMAN program

- Library of frequently required operators and quantum states
- Operator products of various types (inner, tensor, Hilbert-Schmidt,...)
- Type of operators
- Time evolution of pure states due to given Hamiltonian matrix
- Set of quantum operations and noisy channels
- Quantum measures (fidelity, entanglement, ...)
- Bloch-shpere representation of single-qubit states.
- ...

T. Radtke and S. Fritzsche, CPC 173 (2005) 91; CPC 175 (2006) 145.

The FEYNMAN program

-- a quantum simulator using Maple

- Set of Maple procedures to deal with qubits, quantum registers, operators
- Provides data structures which are flexible for most applications.
- Modular structure: with(Feynman);

Main commands of the FEYNMAN package

Feynman_apply()	Applies a given quantum operator to the state of a N-qubit q. Register.
Feynman_decompose()	Calculates the Schmidt as well as various matrix decompositions.
Feynman_measures()	Evaluates various distance and entanglement measures.
Feynman_operator_function()	Evaluates an operator function for a given matrix or qoperator() and returns its explicit matrix representation.
Feynman_operator_type()	Determines the properties of a given matrix or qoperator().
Feynman_plot_Bloch_vector()	Returns a 3D plot of the Bloch sphere representation.
Feynman_print()	Prints the state vector or density matrix of a quantum register
Feynman_product()	Carries out several types of operator products including the inner, outer, Kronecker and Hadamard product for two or more operators.
Feynman_qgate()	Carries out some pre-defined quantum gate on a sequence of qbit()'s.
Feynman_quantum_operator()	Evaluates the explicit matrix representation of various predefined and distributed one-, two-, three, or N-qubit quantum operators.
Feynman_trace()	Calculates the reduced density operator of a qregister(), i.e. the partial trace.

FEYNMAN program

-- Decay of entanglement under noise

The problem of `decoherence'

-- Convex-roof extensions of pure-state measures

Interaction with the environment ("decoherence") leads to mixed quantum states.

Often, an (entanglement) measure E for pure states can be extended to mixed states via an ensemble decomposition of the density matrix:

$$E(\rho) = \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \, E(|\psi_i\rangle)$$

PROBLEM: ensemble decomposition not unique!

$$\rho = \sum_i p_i \, |\psi_i\rangle \, \langle\psi_i| = \sum_i |\tilde{\psi_i}\rangle\langle\tilde{\psi_i}| \qquad |\tilde{\psi_i}\rangle = \sqrt{p_i} \, |\psi_i\rangle$$

unitarily equivalent decompostion:

$$\rho = \sum_{i=1}^{m} |\tilde{\phi_i}\rangle\langle\tilde{\phi_i}| \, , \quad |\tilde{\phi}\rangle_i = \sum_{j=1}^{m} U_{ij} |\tilde{\psi}\rangle_j \qquad m \leq \mathrm{Rank}(\rho)^2$$

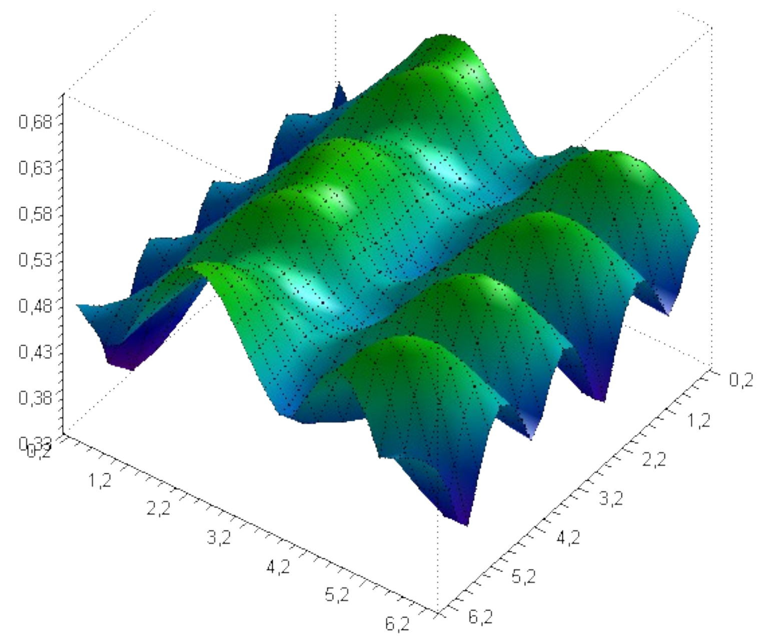
[Uhlmann, 1998]

optimization over all mxm unitaries required

The problem of `decoherence'

-- Optimization over the set of unitary matrices

Parametrization of nxn unitary matrix requires n^2-1 parameters
(e.g. generalized Euler angle parametrization [Tilma et al., 2002])



Random snapshot from a 2-dimensional subspace of the total parameter space when optimizing the convex-roof extendend "concurrence" of a two-qubit system.

High-dimensional global optimization problem

- Evolutionary algorithms
- Maple's Global Optimization Toolbox

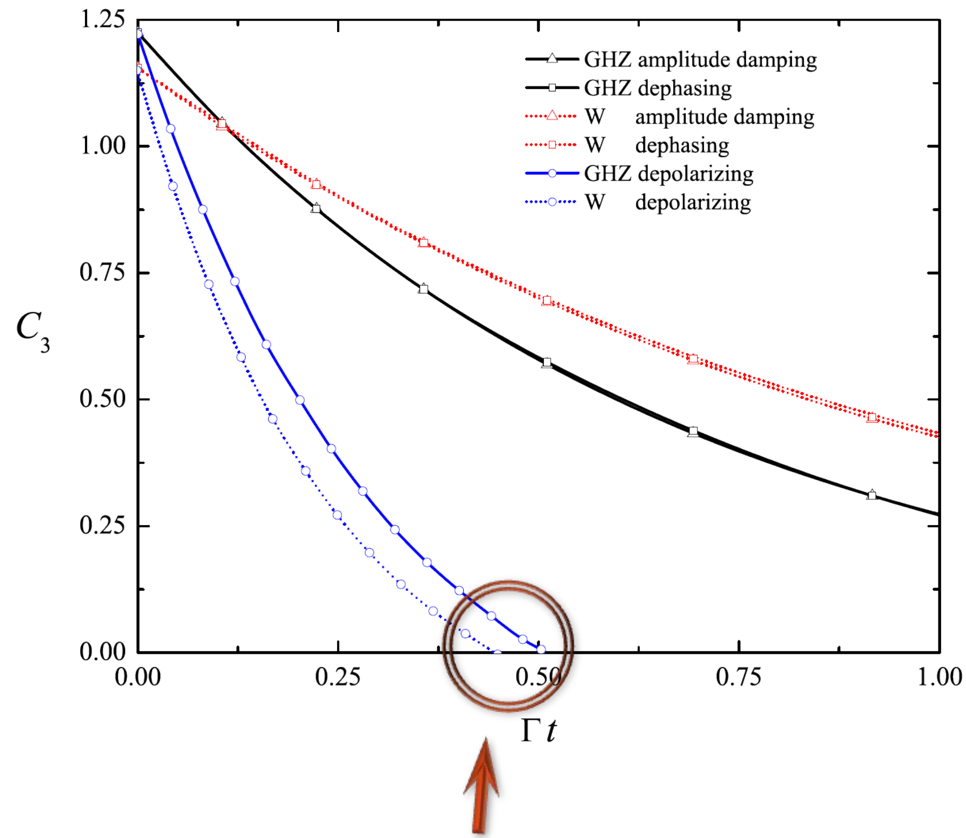
3-qubit states under local decoherence

-- Optimization over the set of unitary matrices

"N-concurrence" as measure of N-qubit multipartite entanglement

$$C_N(|\psi\rangle) = 2^{1-(N/2)} \sqrt{2^N - 2 - \sum_{\alpha} \mathrm{Tr}\,(\rho_\alpha^2)}$$

α = reduced density matrices which are obtained by tracing out n=1,...,N-1 different subsystems (qubits)



only depolarizing noise leads to complete disentanglement

Initially entangled states:

$$|GHZ\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes N} + |1\rangle^{\otimes N})$$

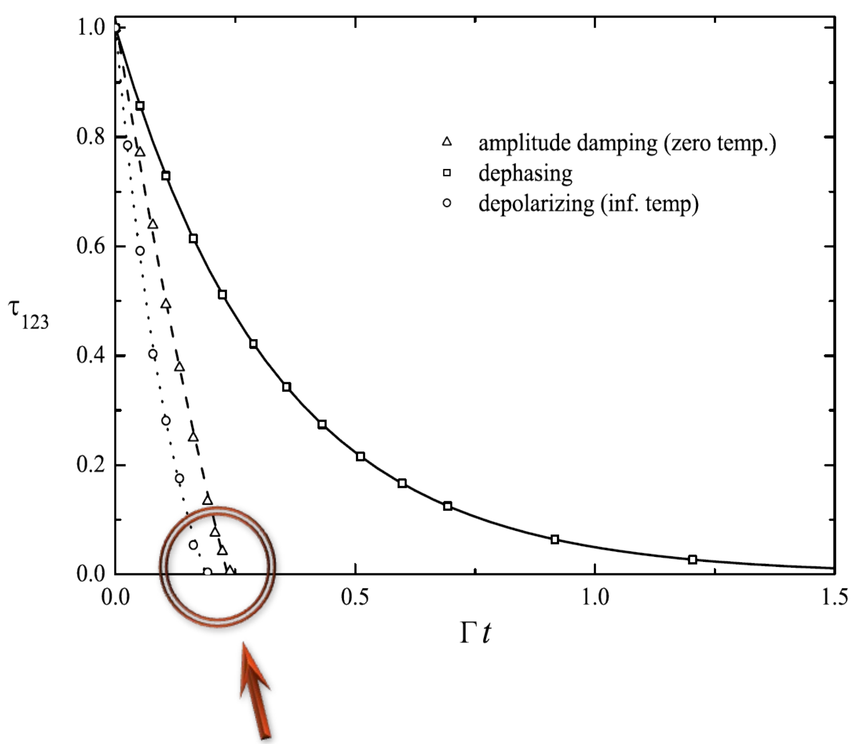
$$|W\rangle_N = \frac{1}{\sqrt{N}}(|00...01\rangle + |00...10\rangle + ... + |10...00\rangle)$$

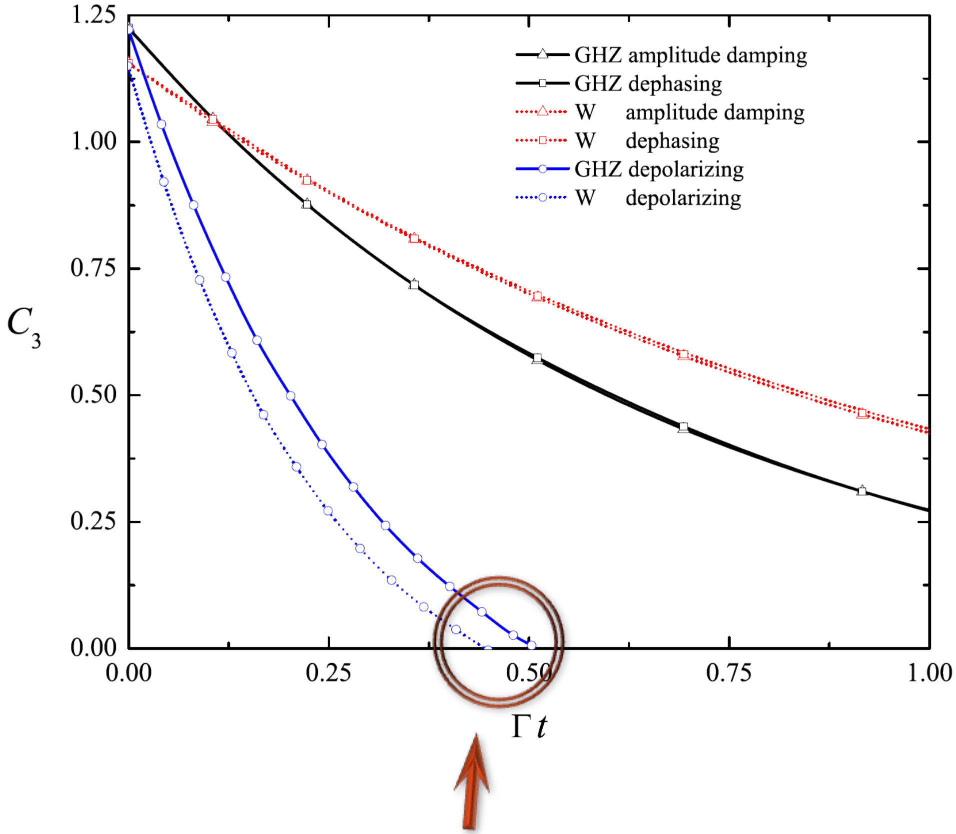
3-qubit states under local decoherence

-- Optimization over the set of unitary matrices

Decay of the genuine 3-qubit entanglement

measured by the so-called "residual entanglement"





now depolarizing and amplitude damping noise lead to complete disentanglement

only depolarizing noise leads to complete disentanglement

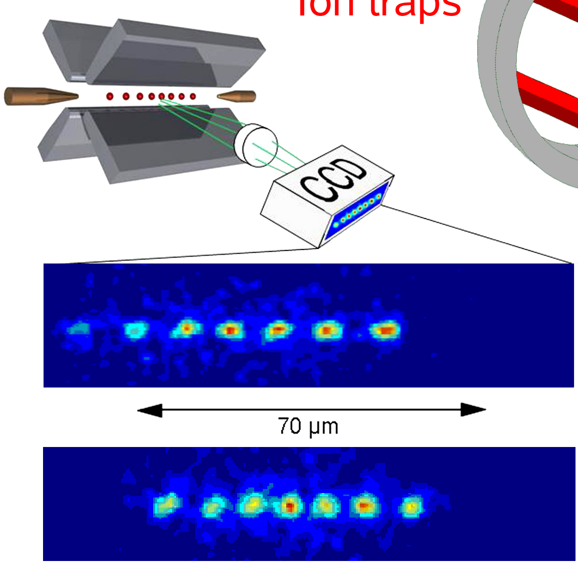
Realization and simulation of quantum computers

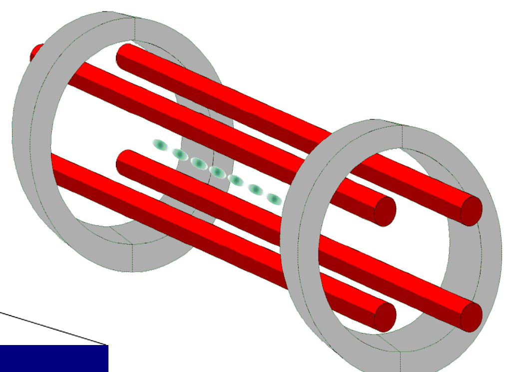
$$\mathcal{E}(\rho) = \mathrm{Tr}_{env}\left[U(\rho \otimes \rho_{env})U^{\dagger}\right]$$

Experiment

Different schemes have been suggested in the past.

Ion traps





From: www.europhysicsnews.com/. ../article5.html

Theory

Use of classical computers to simulate parts of quantum computers including quantum measurment, design of algorithms, or the coupling to the environment.

Quantum entanglement

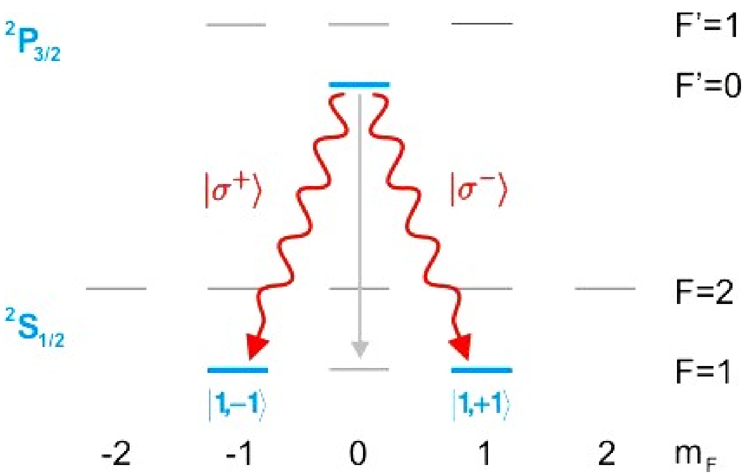
-- A key ingredient of quantum information protocols

A physical resource, like energy, associated with the peculiar nonclassical correlations that are possible between separated quantum systems.

$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \neq |a\rangle \otimes |b\rangle \quad \forall\ |a\rangle \in \mathrm{H}_A, |b\rangle \in \mathrm{H}_B$$

- Photon pairs were first successful candidates for nonlocality & entanglement experiments (Aspect 1982, Kleinpoppen 1984)
- Atom-photon entanglement (H. Weinfurter et al., Munich)

Example:
A Rb atom is excited to a state which has two selected decay channels.



$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|1,-1\rangle|\sigma^+\rangle + |1,+1\rangle|\sigma^-\rangle\right)$$

Entanglement between atom and emitted photon

Necessary for entanglement between atoms at remote locations.

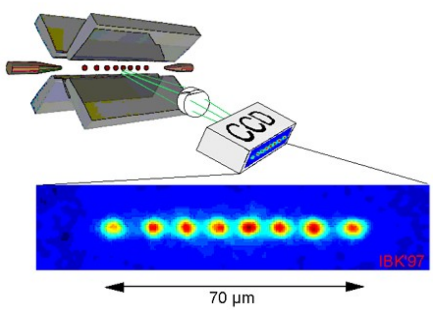
Quantum entanglement

-- A key ingredient of quantum information protocols

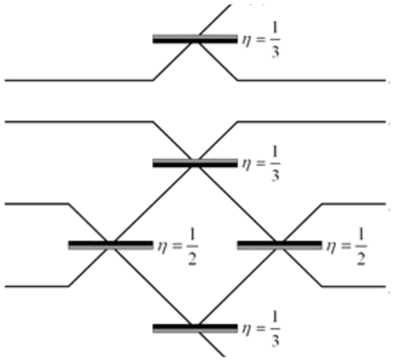
A physical resource, like energy, associated with the peculiar nonclassical correlations that are possible between separated quantum systems.

$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \neq |a\rangle \otimes |b\rangle \quad \forall \; |a\rangle \in \mathrm{H}_A, |b\rangle \in \mathrm{H}_B$$

Necessary for entanglement between atoms at remote locations.



From: www.europhysicsnews.com/. ../article5.html



Trapped atoms/ions are good candidates for a sufficiently stable ***quantum memory***

Photons are good candidates for a sufficiently stable ***quantum processor***

Link between processor and memory: Atom-photon entanglement

Pairs of photons with „well-defined degree of entanglement“

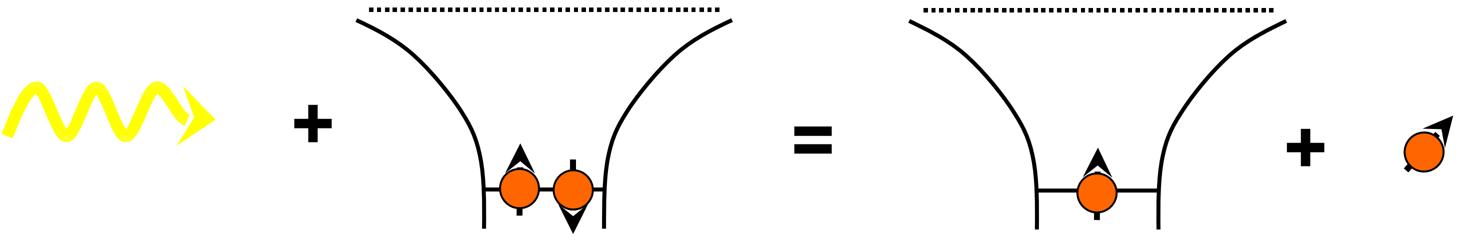
Atomic photoionization

-- Entanglement between electrons and ions

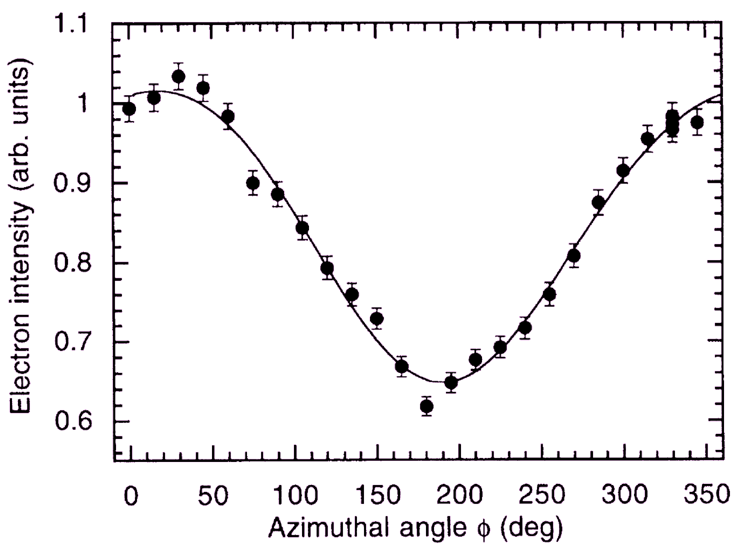
Search for physical processes where entanglement can be observed and manipulated !

Entanglement in atomic photoionization

-- one of the most intensively studied processes in Nature



photon	atomic (or ionic) bound state	residual ion	photoelectron in the continuum
$\lvert \mathbf{k}\lambda \rangle$	$\lvert \alpha_0 J_0 M_0 \rangle$	$\lvert \alpha_f J_f M_f \rangle$	$\lvert \mathbf{p} m_s \rangle$

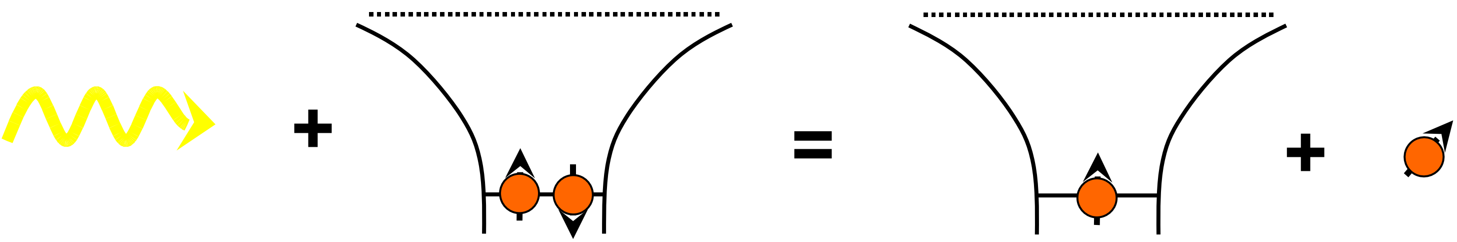


Studies on atomic photoionization

- (Total) cross section
- Angular distributions
- Spin-polarization

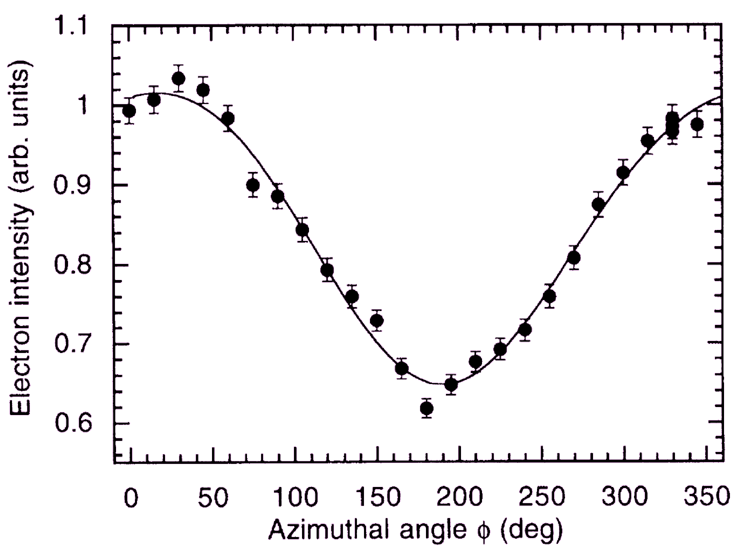
Entanglement in atomic photoionization

-- one of the most intensively studied processes in Nature



photon | *atomic (or ionic) bound state* = *residual ion* + *photoelectron in the continuum*

$|\mathbf{k}\lambda\rangle \quad + \quad |\alpha_0 J_0 M_0\rangle \quad = \quad |\alpha_f J_f M_f\rangle \quad + \quad |\mathbf{p} m_s\rangle$

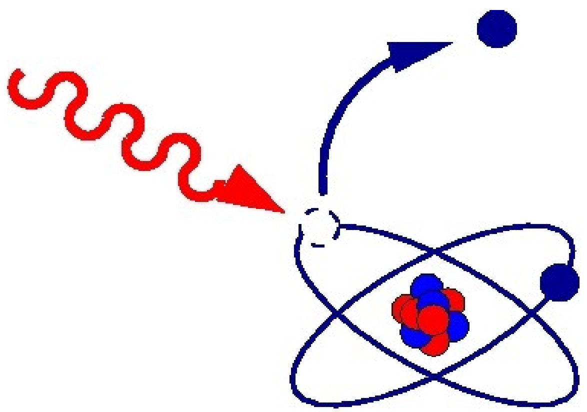


Studies on atomic photoionization

- (Total) cross section
- Angular distributions
- Spin-polarization
- Entanglement as additional resource

Change of entanglement in atomic photoionization

-- physics of photoionization

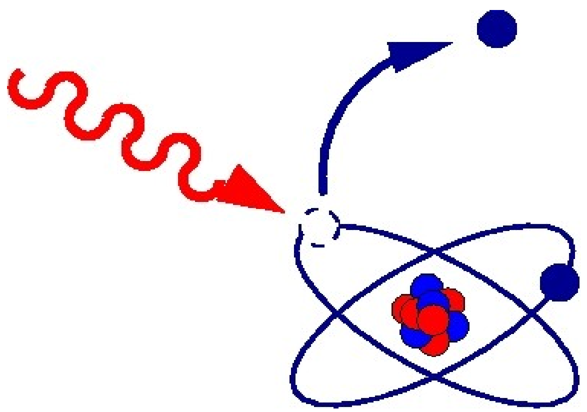


$$M_{fb} = \int \Psi_f^+(\boldsymbol{r}) \; \boldsymbol{\alpha}\,\boldsymbol{u}\,\mathrm{e}^{i\boldsymbol{k}\boldsymbol{r}} \; \Psi_b(\boldsymbol{r}) \; d\boldsymbol{r}$$

electron-photon interaction

Change of entanglement in atomic photoionization

-- physics of photoionization



$$M_{fb} = \int \Psi_f^+(\boldsymbol{r}) \; \boldsymbol{\alpha u} \, e^{i\boldsymbol{kr}} \; \Psi_b(\boldsymbol{r}) \; d\boldsymbol{r}$$

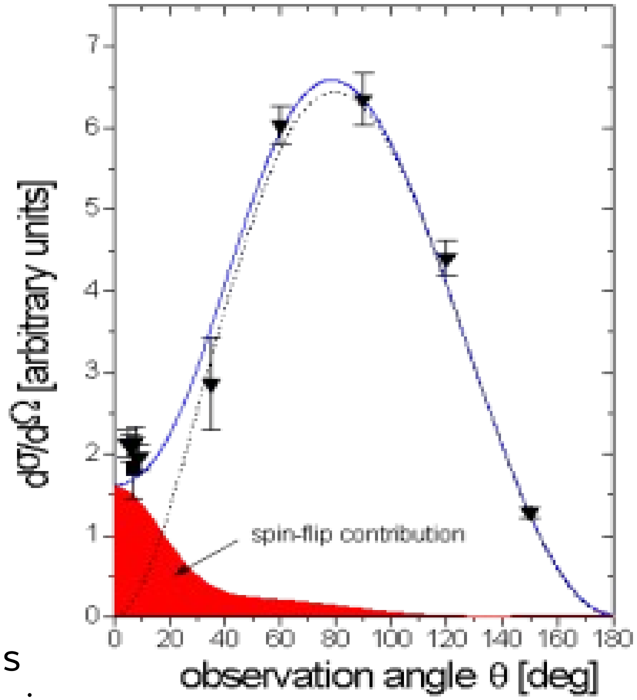
electron-photon interaction

multipole expansion of the photon field

$$\mathbf{u}_\lambda e^{i\mathbf{k}\cdot\mathbf{r}} = \sqrt{2\pi} \sum_{L=1}^{\infty} \sum_{M=-L}^{L} i^L \sqrt{2L+1} \; \mathcal{A}_{LM}^{(\lambda)} \; D_{M\lambda}^{L}(\hat{\mathbf{k}} \rightarrow \mathbf{e}_z)$$

photon multipole fields

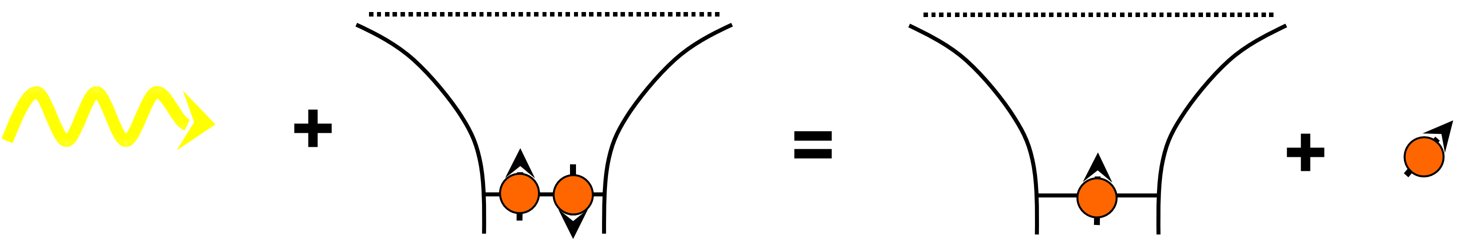
Wigner rotation matrices



angular distribution of photoelectrons following ionization of H-like uranium ion

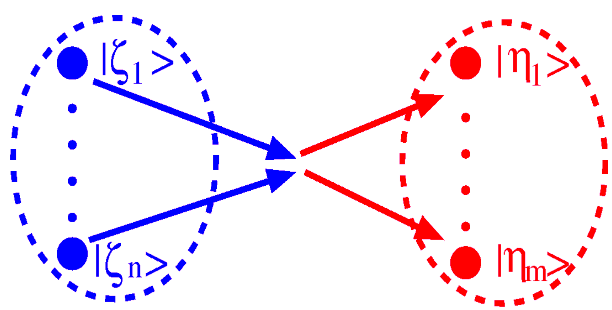
Entanglement in atomic photoionization

-- Theoretical framework



photon	atomic (or ionic) bound state	residual ion	photoelectron in the continuum
$\lvert \mathbf{k}\lambda \rangle$	$\lvert \alpha_0 J_0 M_0 \rangle$	$\lvert \alpha_f J_f M_f \rangle$	$\lvert \mathbf{p} m_s \rangle$

Initial state $(t \to -\infty)$ $\hat{\rho}_i$



Final state $(t \to +\infty)$ $\hat{\rho}_f$

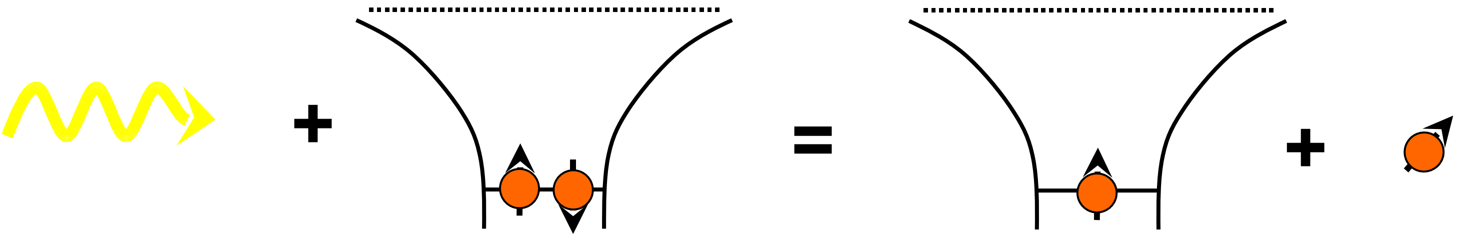
Use of the time-independent density matrix

$$\hat{\rho}_f = \hat{S}\,\hat{\rho}_i\,\hat{S}^+$$

$\hat{S}$ - scattering operator

Entanglement in atomic photoionization

-- Theoretical framework



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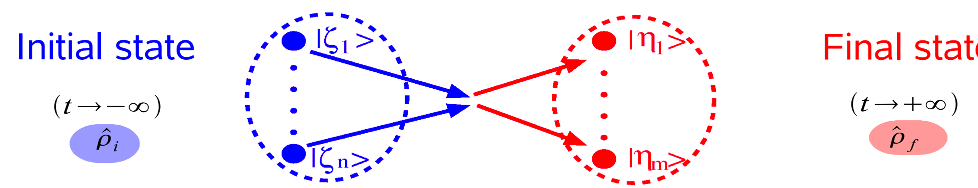


$$\hat{\rho}_f = \hat{S}\,\hat{\rho}_i\,\hat{S}^+$$

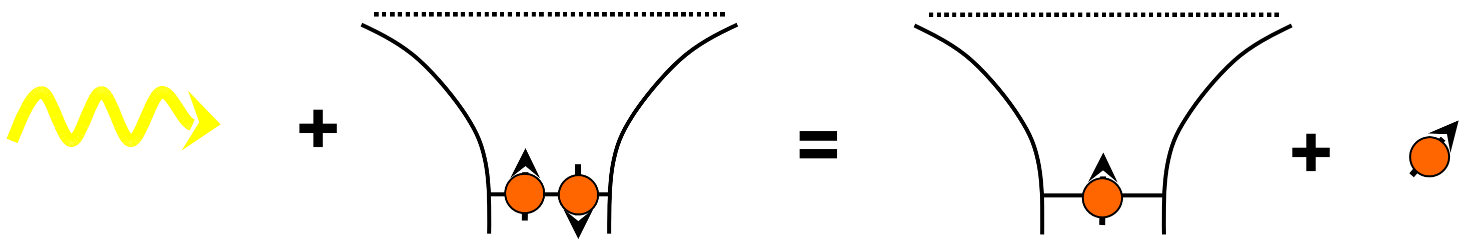
Measurement of physical properties:

- 'detector operator' describes the experimental setup: $\hat{P} = |\epsilon><\epsilon|$
- probability to get a 'click' at the detectors:

$$W = Tr\left(\hat{P}\,\hat{\rho}_f\right) = \sum_{\eta_1 \dots \eta_m} \langle \eta_1 \dots \eta_m | \hat{P}\,\hat{\rho}_f | \eta_1 \dots \eta_m \rangle$$

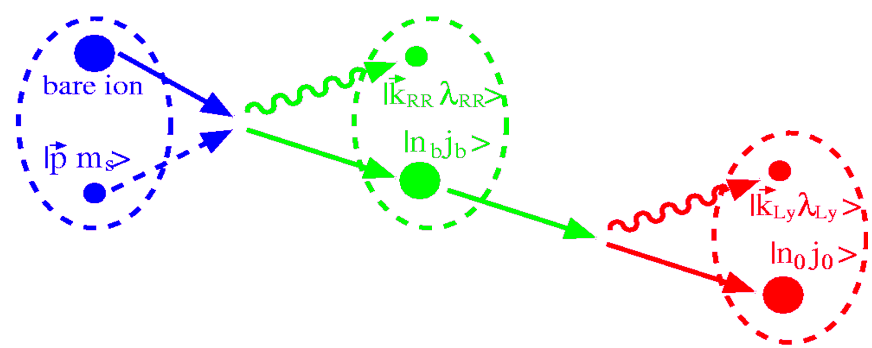
Entanglement in atomic photoionization

-- Theoretical framework



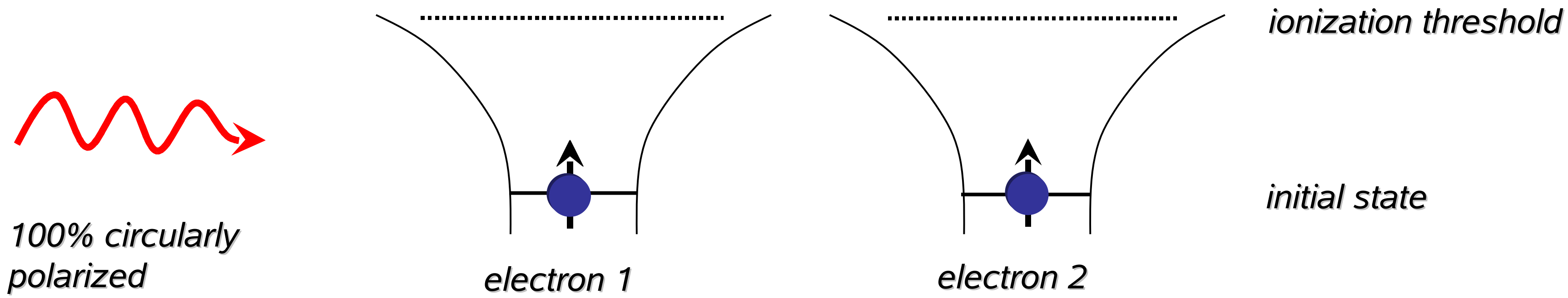
photon	atomic (or ionic) bound state	residual ion	photoelectron in the continuum
$\left\vert \mathbf{k}\lambda \right\rangle$	$\left\vert \alpha_0 J_0 M_0 \right\rangle$	$\left\vert \alpha_f J_f M_f \right\rangle$	$\left\vert \mathbf{p} m_s \right\rangle$

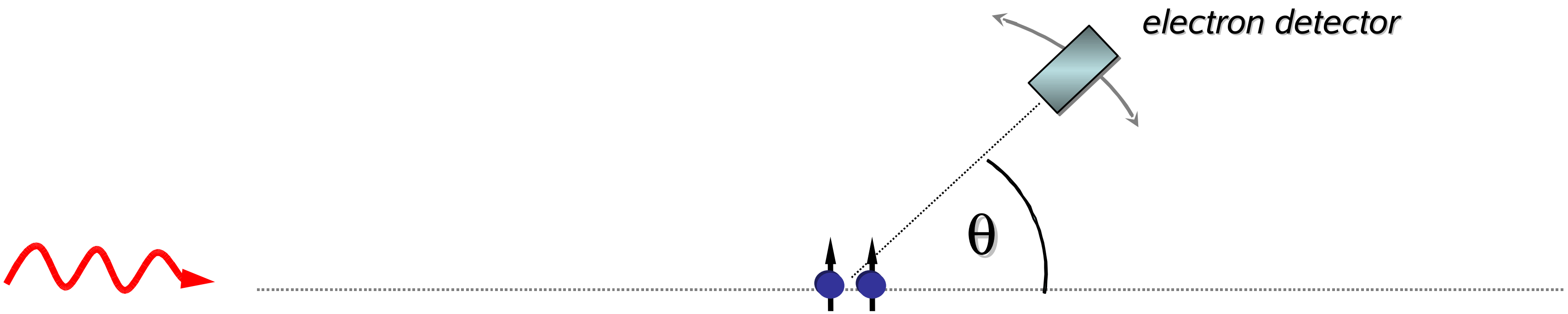
Great advantage !



Using the density matrix, the system can be accompanied through several steps of the interaction which may lead to the emission of photons, electrons, ...

Toy model: Two independent H-like ions in a trap





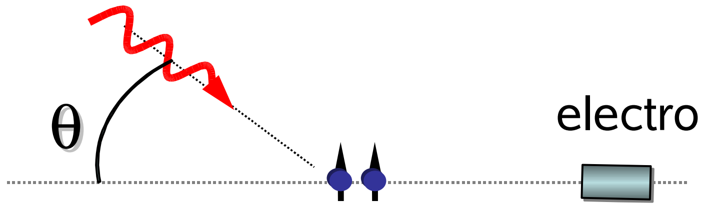
measure angular dependence of ejected electron spin polarization

- Two electrons are distinguishable & non-interacting !
- Nuclear spins neglected.

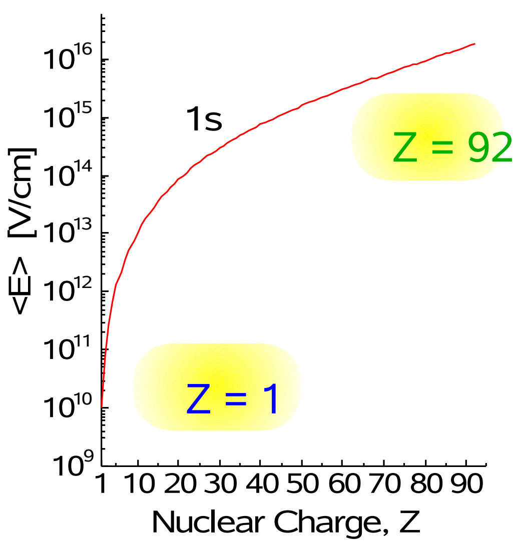
T. Radtke et al., Phys. Lett. A 347 (2005) 73.

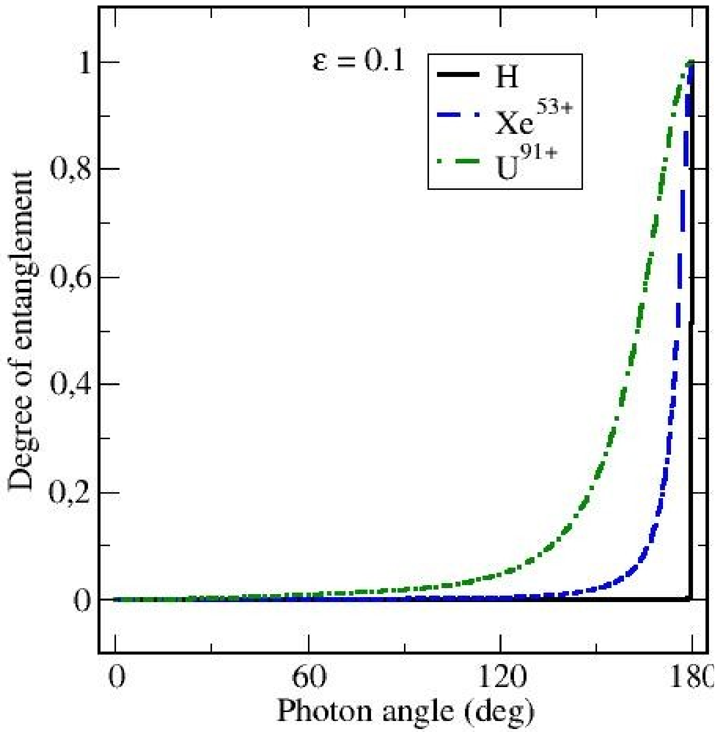
Change of entanglement in atomic photoionization

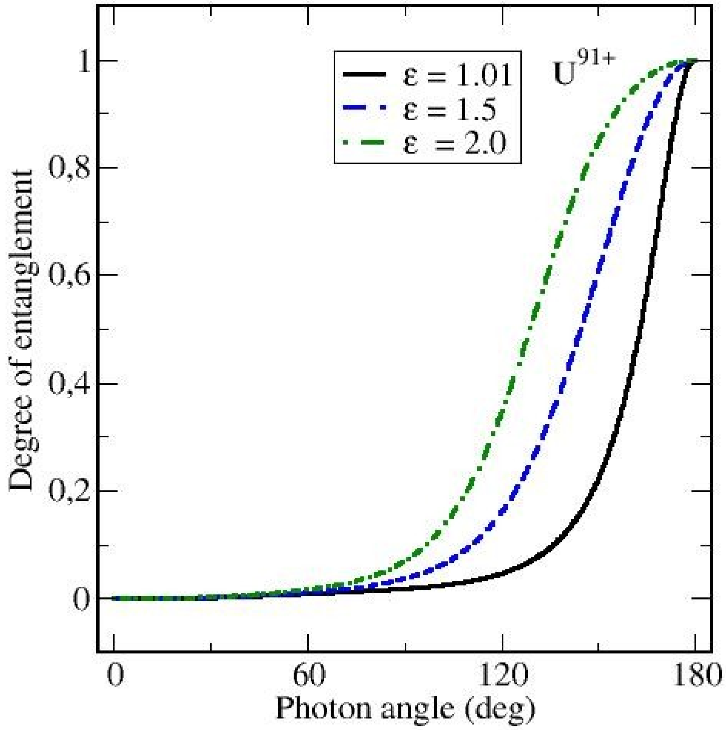
-- entanglement as function of the photon angle



Calculations are performed for the relative photon energy $\varepsilon = E_\gamma / E_{1s}$ where E_{1s} is the 1s ionization threshold.







Relativistic effects result in a change of entanglement !

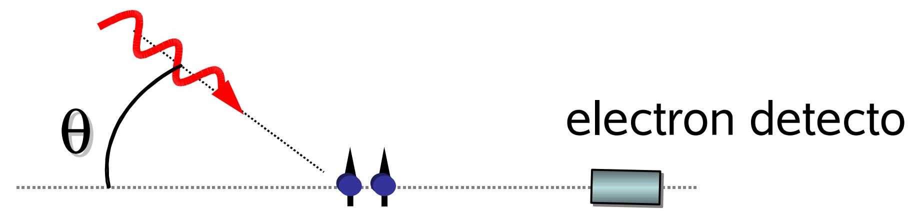
T. Radtke et al., Phys. Lett. A 347 (2005) 73.

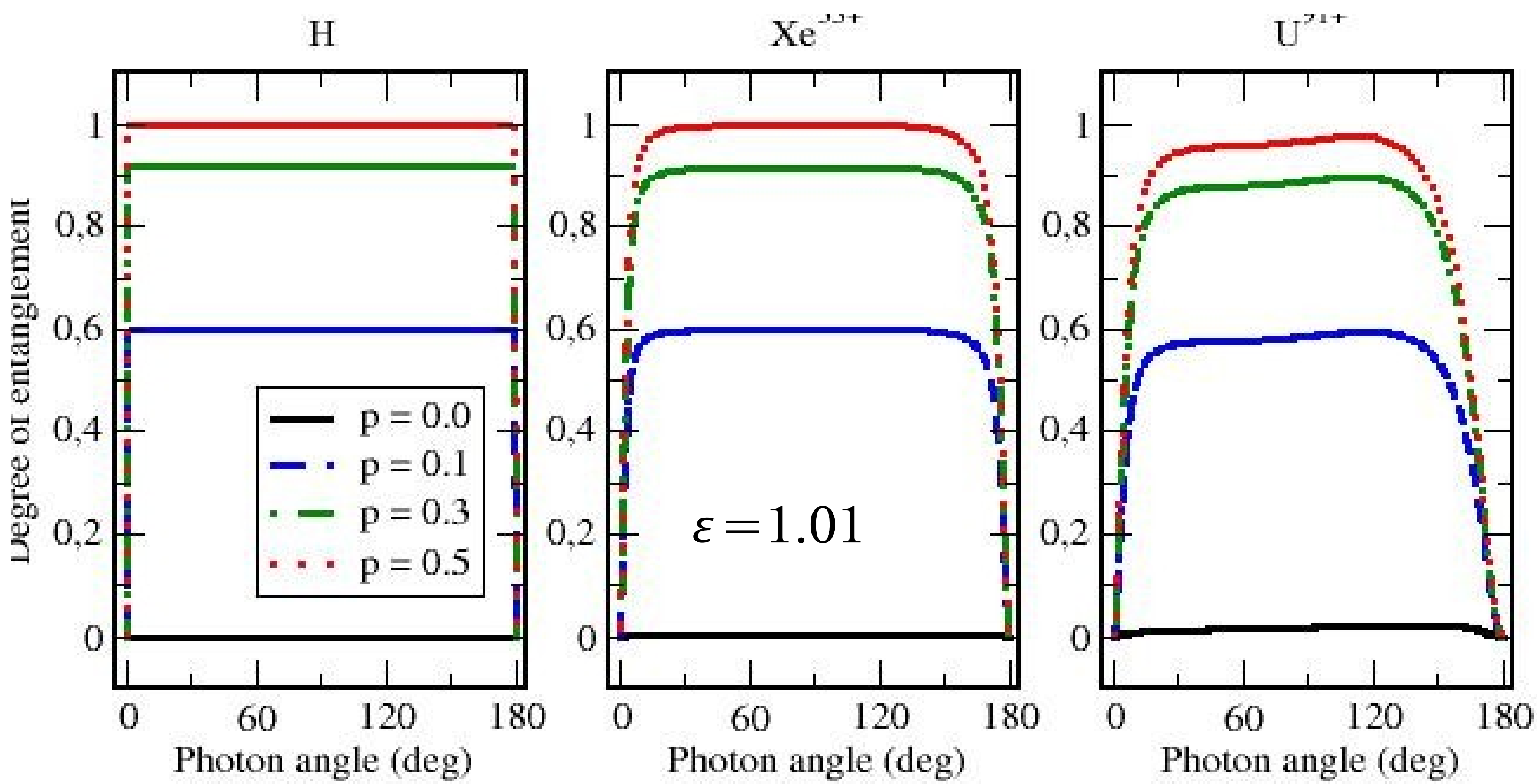
Toy model: Two independent H-like ions in a trap

-- entanglement as function of the initial 2-qubit state

Calculations are performed for the initial state:

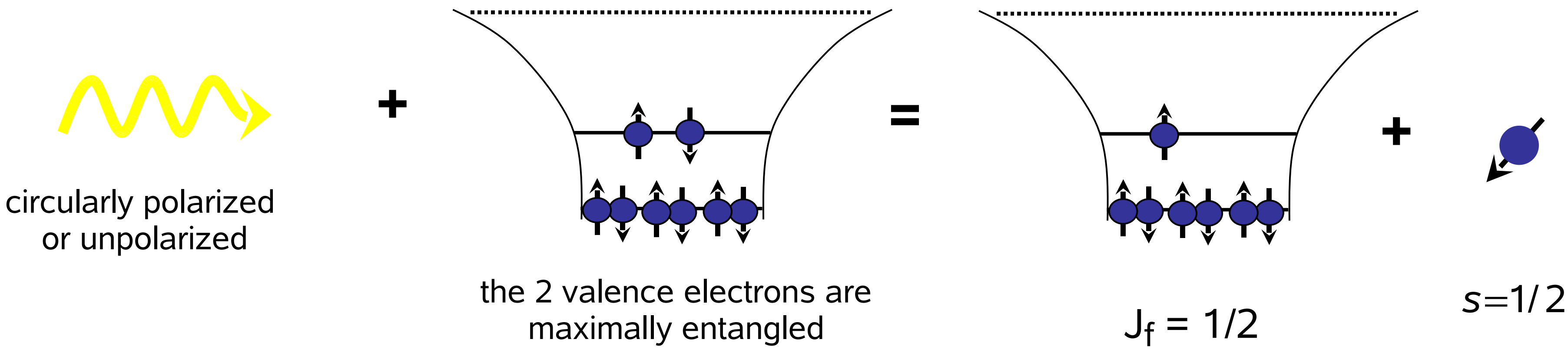
$$|\Psi> = \sqrt{p}\,|01> + \sqrt{1-p}\,|10>$$





5s photoionization of atomic strontium (Z=38)

$$\mathrm{Sr}\,(5s^2\ {}^1S_0) + h\upsilon \rightarrow \mathrm{Sr}^+\,(5s\ {}^2S_{1/2}) + e^-$$



composite system
of two qubits:
Photoion + electron

$$\left\langle \alpha_f J_f M_f, \mathbf{p} m_s \left| \rho_f \right| \alpha_f J_f M_f', \mathbf{p} m_s' \right\rangle \propto \sum W \left\langle (\alpha_f J_f, \varepsilon\kappa j)\, J_{tot} \left\| \boldsymbol{\alpha} \mathcal{A}_L^{(\lambda)} \right\| \alpha_0 J_0 \right\rangle$$

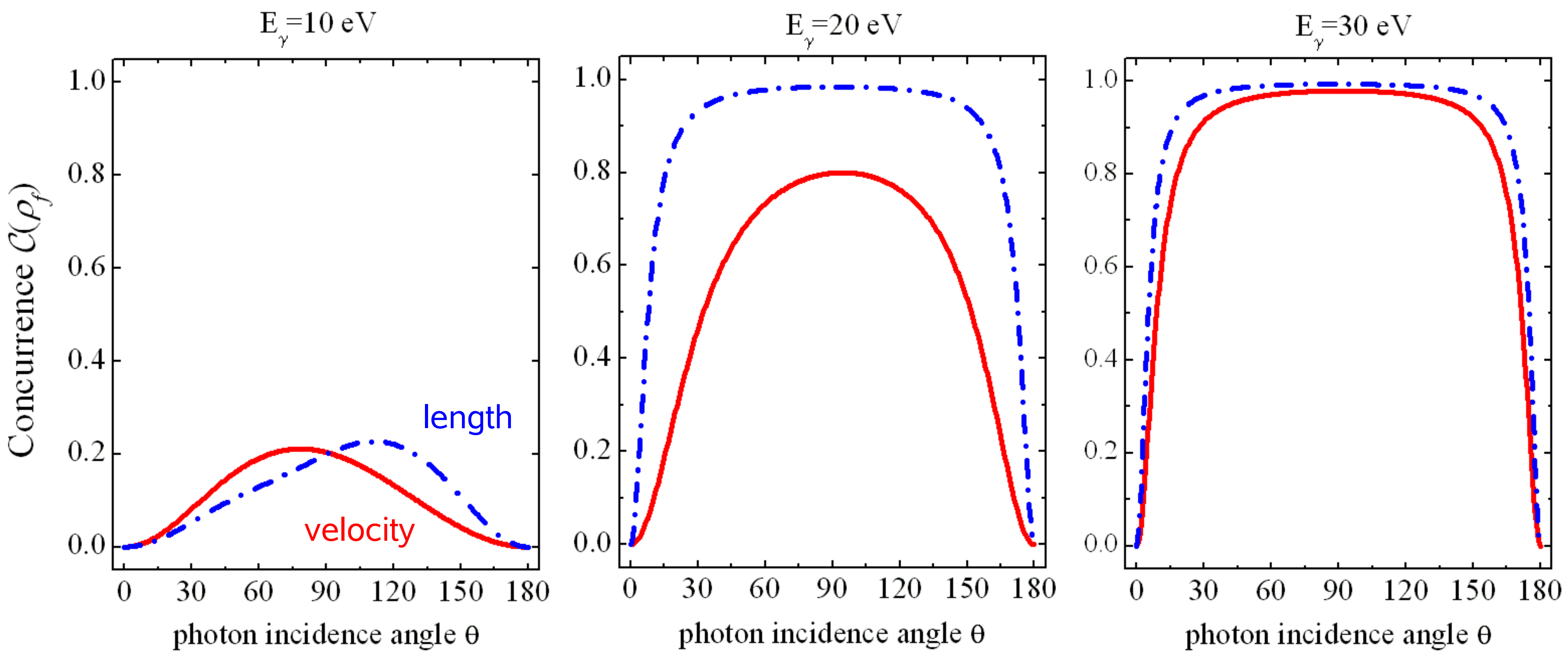
$$\times \left\langle (\alpha_f J_f, \varepsilon\kappa' j')\, J_{tot}' \left\| \boldsymbol{\alpha} \mathcal{A}_{L'}^{(\lambda)} \right\| \alpha_0 J_0 \right\rangle^*$$

lenghty geometric factor
(Clebsch-Gordans, D-matrix etc.)

T. Radtke et al., PRA 74 (2006) 032709.

Final-state entanglement as function of the photon angle

-- comparison of length and velocity gauge

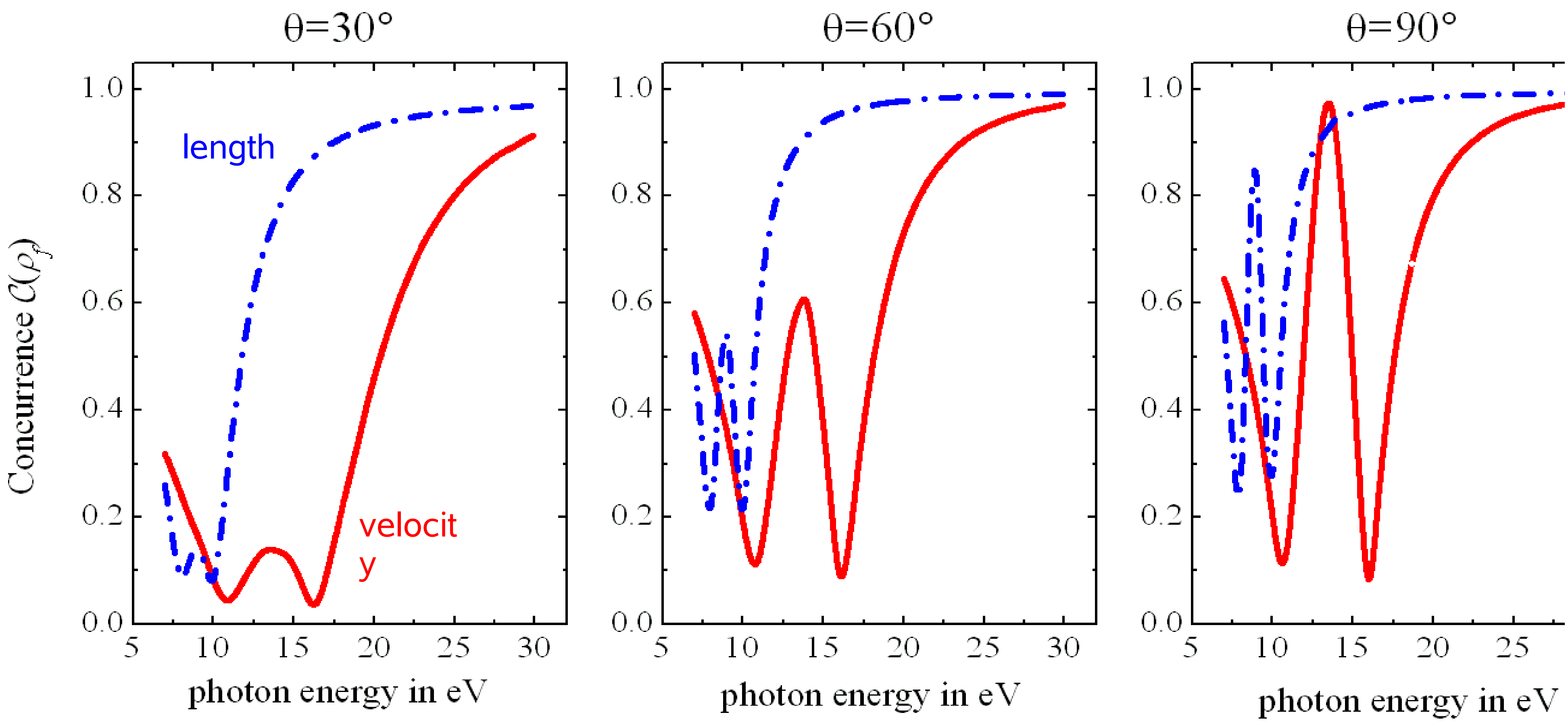


Angular distribution similar to IPM results, but much lower values near to the ionization threshold.

T. Radtke et al., PRA 74 (2006) 032709.

Final-state entanglement as function of the photon energy

-- with right-cicularly polarized light



Good agreement with IPM results for high photon energies.

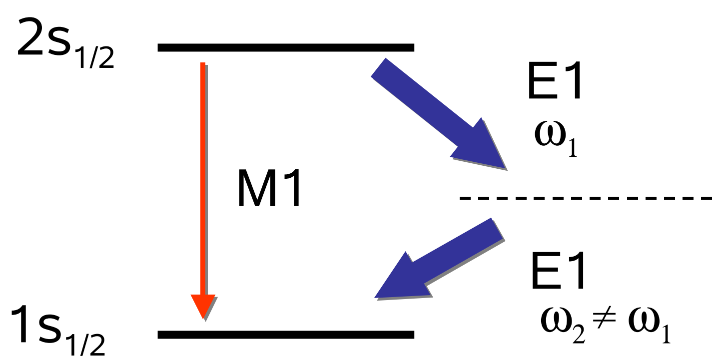
Entanglement can be observed and manipulated in atomic photoionization

- sensitive to relativistic/multipole effects
- strongly sensitive to many-particle effects

Two-photon decay

-- Entanglement between pairs of photons

Polarization entanglement in the two-photon decay of atomic hydrogen



$w(M1) = 2.496 \cdot 10^{-6}$ sec^{-1}

$w(E1E1) = 8.229$ sec^{-1}

The (E1E1) two-photon decay is the dominant decay channel of metastable hydrogen!

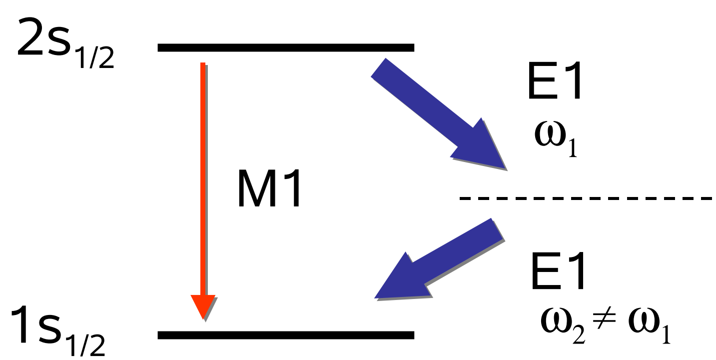
- Predicted by M. Göppert-Mayer (1931)
- First decay rate estimations by Breit and Teller (1940)
- First observed only in 1975 by O'Connell et al.
- Polarization correlation (for back-to-back geometry) measured and found to violate Bell inequality (Perrie et al.,1985)

$$\frac{dW}{dx} = Z^6 \frac{9\alpha^6}{2^{10}} \psi(x)$$

Multipole	Contribution (sec^{-1})	
	Z=1	Z=92
2E1	8.229	$3.826 \cdot 10^{12}$
E1M2	$2.537 \cdot 10^{-10}$	$9.139 \cdot 10^{9}$
2M1	$1.380 \cdot 10^{-11}$	$1.109 \cdot 10^{9}$
2E2	$4.907 \cdot 10^{-12}$	$1.786 \cdot 10^{8}$
2M2	$3.069 \cdot 10^{-22}$	$9.907 \cdot 10^{5}$

Santos et al., Eur. Phys. J. D **3**, 43 (1998)

Polarization entanglement in the two-photon decay of atomic hydrogen



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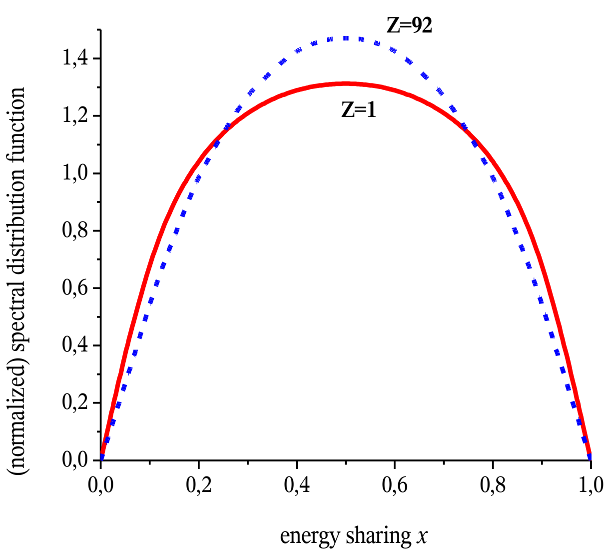
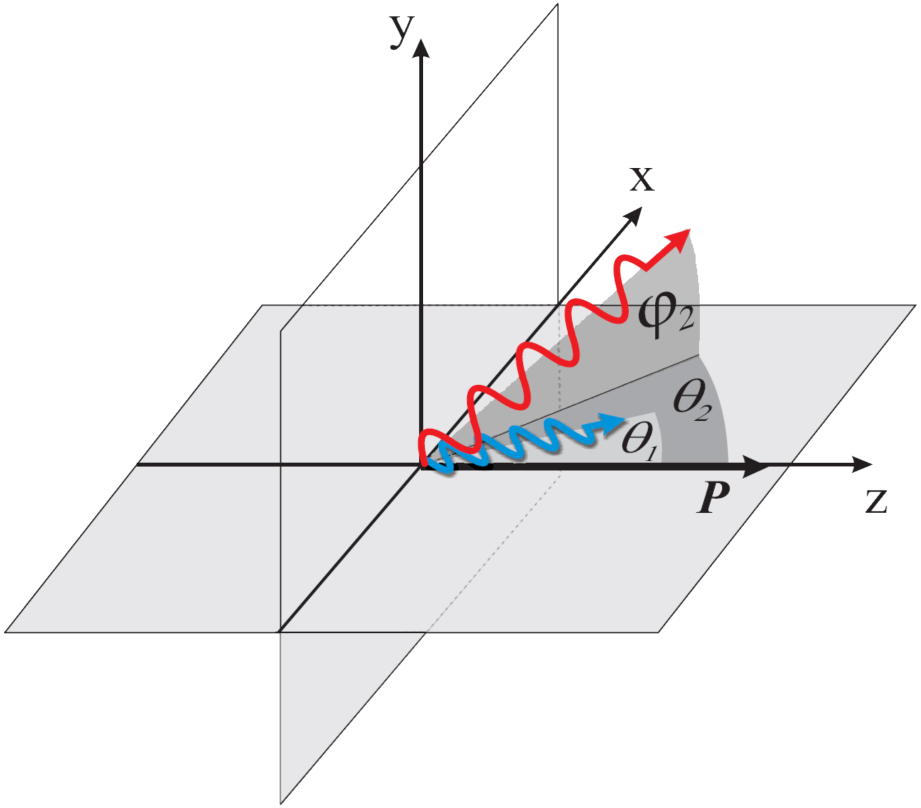


Polarization entanglement in the two-photon decay of atomic hydrogen

-- geometry and control parameters



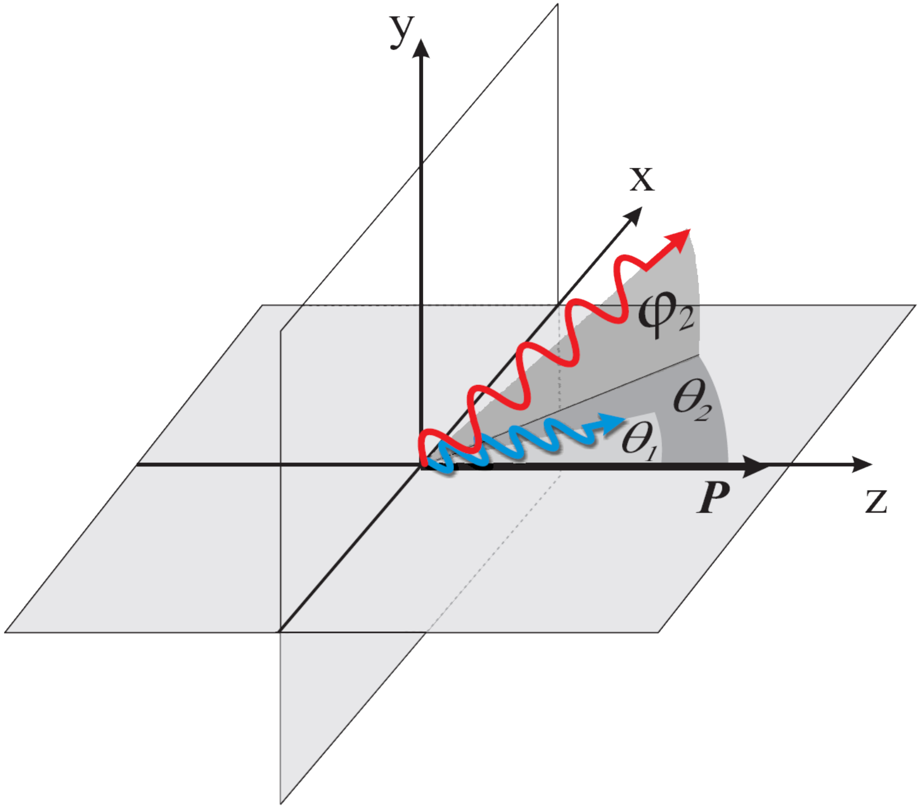
Parameters:

- 3 polar and azimuth angles
- energy ratio between the photons
- initial polarization state of the atom/ion
- Z-dependence (i.e. relativistic effects)

Search for tailor-made entanglement !

Polarization entanglement in the two-photon decay of atomic hydrogen

-- geometry and control parameters



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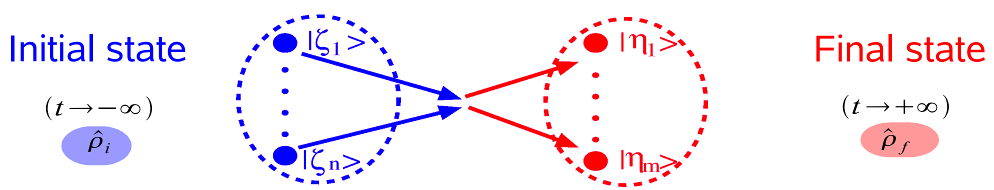


$$\hat{\boldsymbol{\rho}}_f = \hat{S}\,\hat{\rho}_i\,\hat{S}^{+}$$

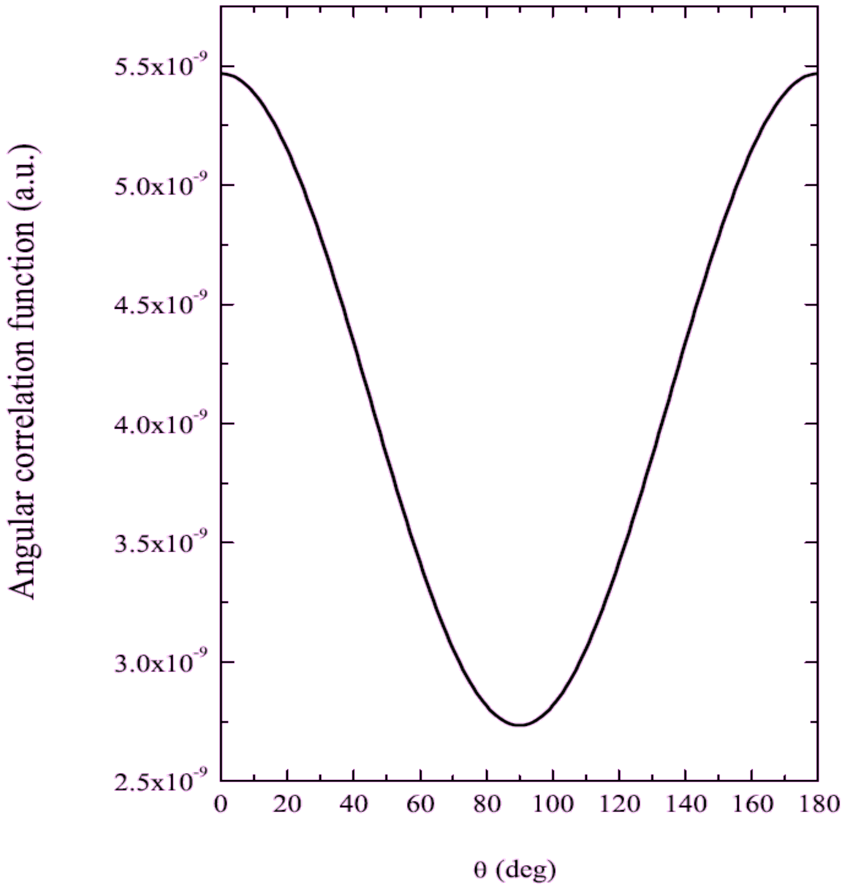
$$M_{fi}(\mu_f,\mu_i,\lambda_1,\lambda_2) = \sum\!\!\!\!\!\!\int_\nu \frac{\langle \psi_{n_f j_f \mu_f} | \boldsymbol{\alpha}\cdot\boldsymbol{u}^*_{\lambda_1} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} | \psi_\nu \rangle \langle \psi_\nu | \boldsymbol{\alpha}\cdot\boldsymbol{u}^*_{\lambda_2} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}} | \psi_{n_i j_i \mu_i} \rangle}{E_\nu - E_i + E_{\gamma 2}}$$

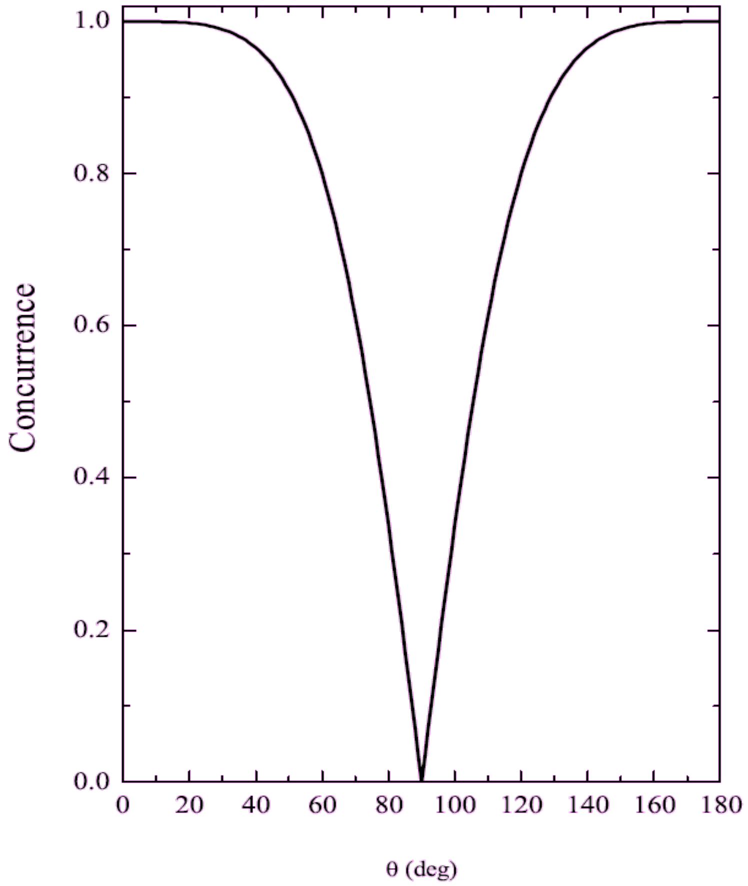
$$+ \sum\!\!\!\!\!\!\int_\nu \frac{\langle \psi_{n_f j_f \mu_f} | \boldsymbol{\alpha}\cdot\boldsymbol{u}^*_{\lambda_2} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}} | \psi_\nu \rangle \langle \psi_\nu | \boldsymbol{\alpha}\cdot\boldsymbol{u}^*_{\lambda_1} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} | \psi_{n_i j_i \mu_i} \rangle}{E_\nu - E_i + E_{\gamma 1}}$$

Polarization entanglement in the $2s_{1/2} \rightarrow 1s_{1/2}$ two-photon decay

-- unpolarized initial state

The opening angle between the photons is the only free parameter in this case.



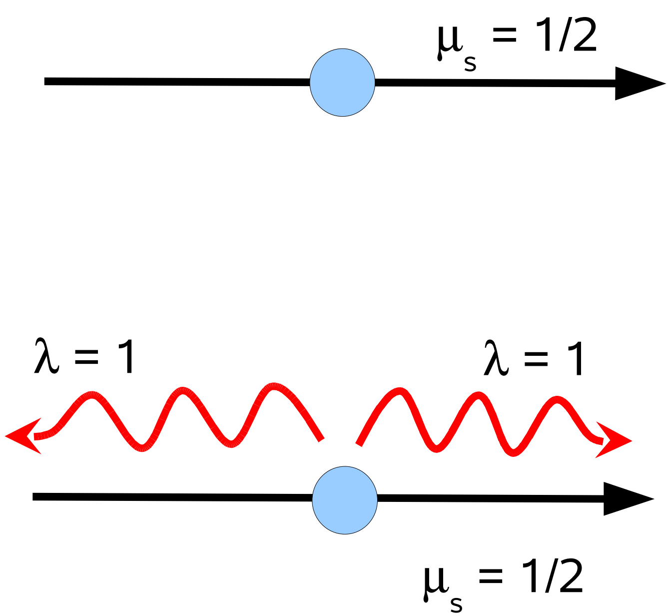


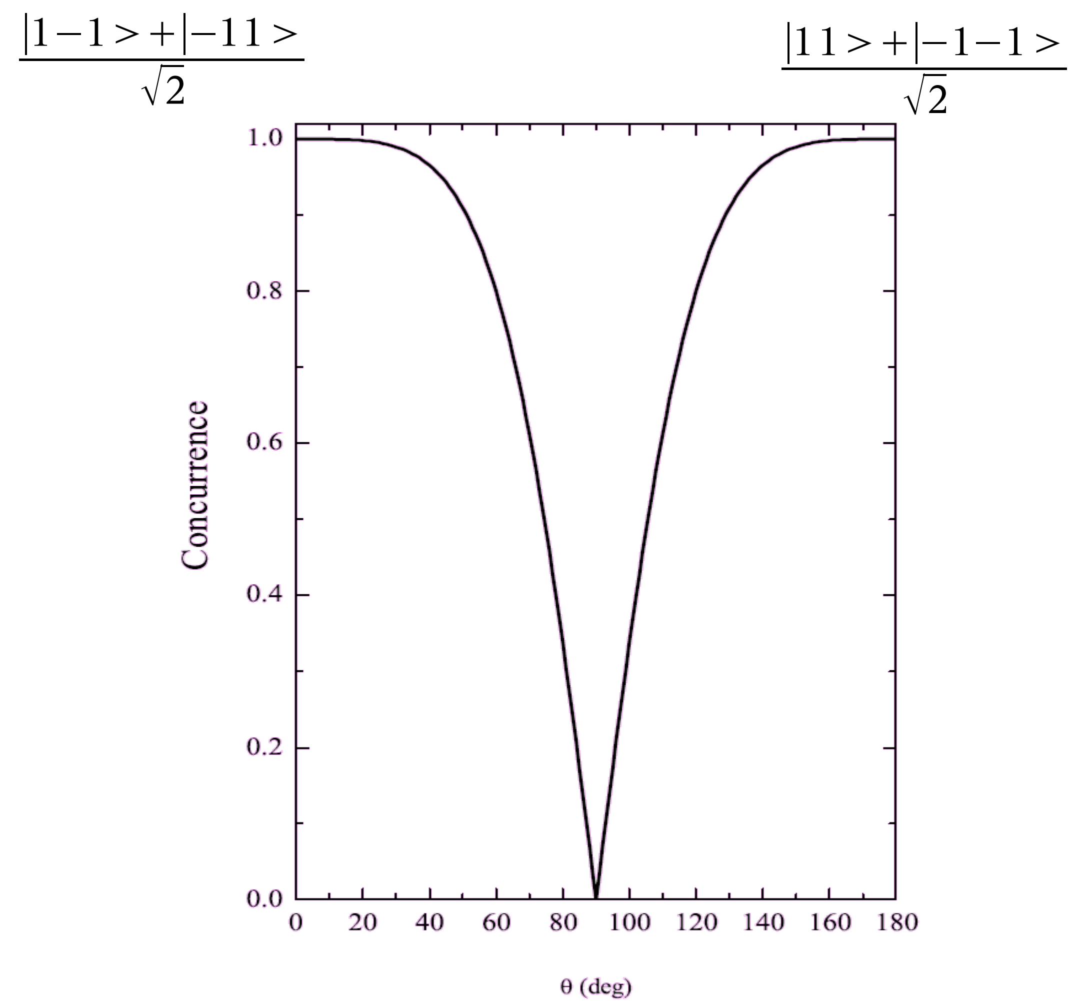
Independent from the energy sharing between the photons.

Polarization entanglement in the $2s_{1/2}$ → $1s_{1/2}$ two-photon decay

-- unpolarized initial state

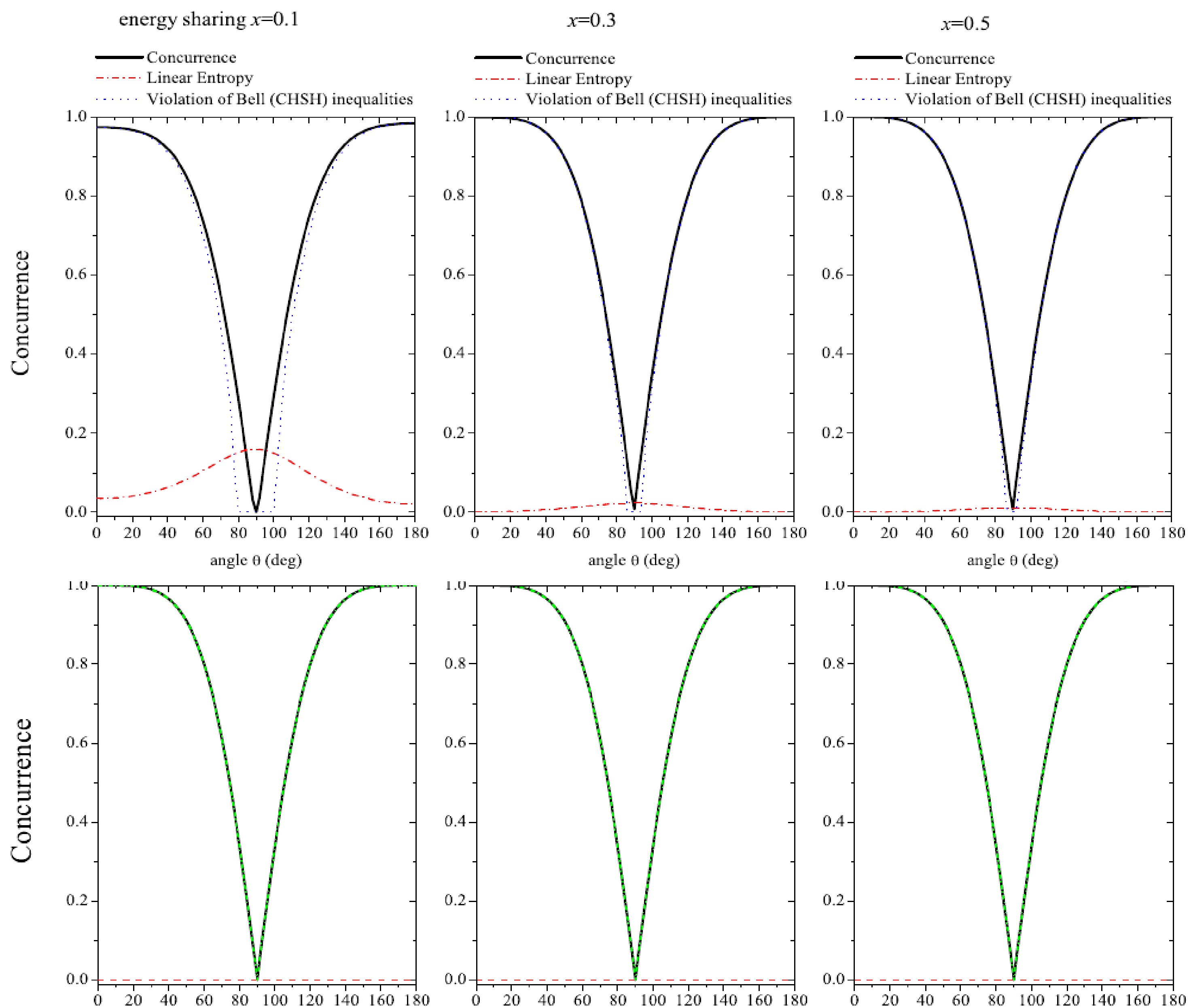
The opening angle between the photons is the only free parameter in this case.





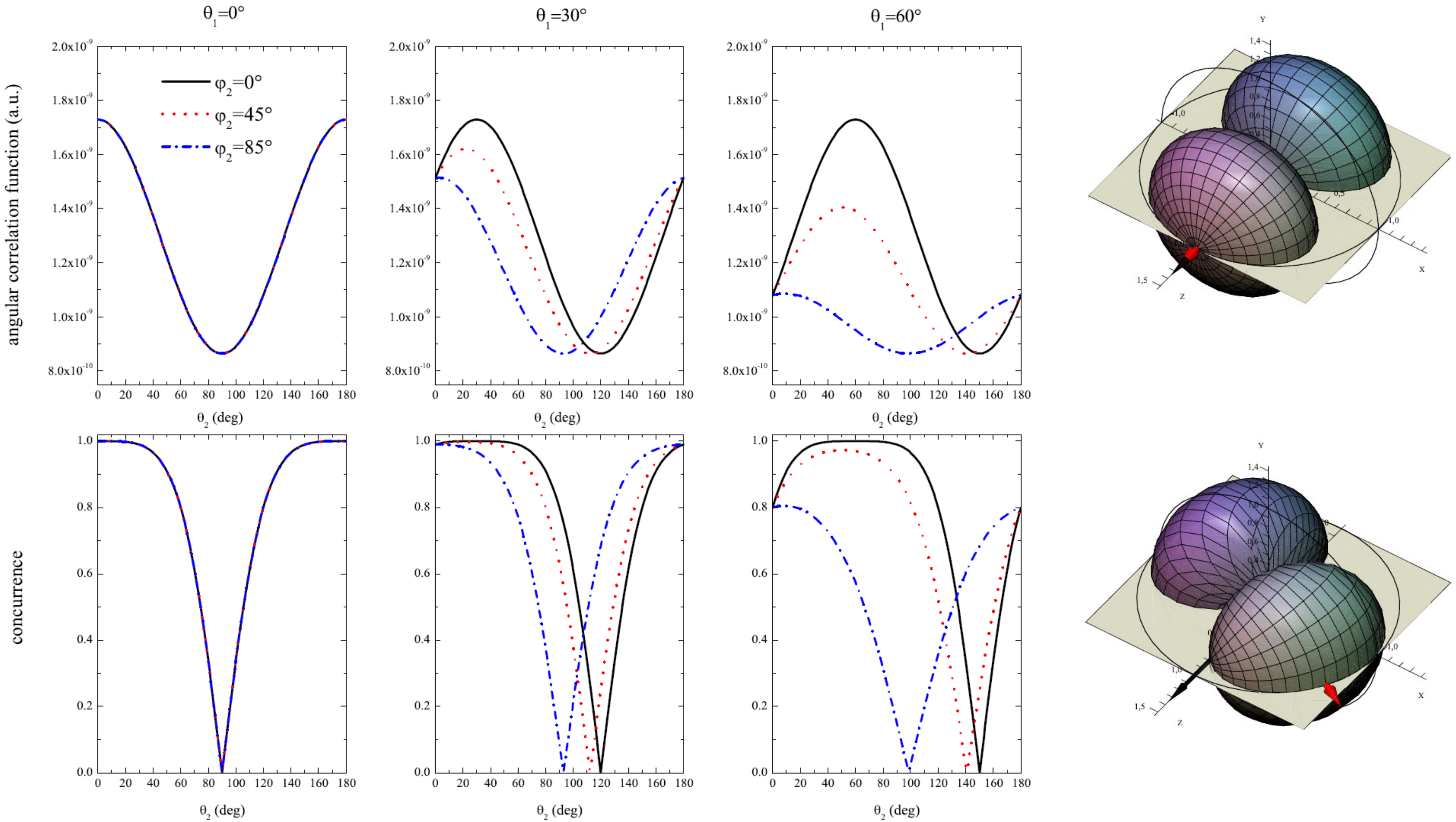
Polarization entanglement in the $2s_{1/2} \rightarrow 1s_{1/2}$ two-photon decay

-- relativistic increase



Polarization entanglement in the $2s_{1/2} \rightarrow 1s_{1/2}$ two-photon decay

-- initial polarization state $\mu_i = \pm 1/2$



Summary and outlook

- Quantum technologies promise a high efficiency far beyond the capacity of present-day equipment, both in computing and communications.

- However, in order to make use of these advantages, a great deal of simulations will be needed to understand the physics and elementary operations of quantum computers.

- Computer algebra offers here a powerful alternative to simulate the behaviour of N-qubit quantum registers, their internal evolution and the interplay with the physical world. → FEYNMAN program

- Quantum entanglement is a key resource and essential to the performance of QC; therefore, a large number of case studies have been carried out recently.

  → influence of decoherence on multi-partite entanglement

- Photoionization of trapped ions may support the control and modification of entanglement in coupled spin systems.

Happy birthday and all the best to you,

Vladimir Gerdt

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