Quantum Computing with Para-hydrogen

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S S E

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Entanglement in two qubit mixed states

Entanglement: Pure States

Separable $|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\chi\rangle_B$

$$|0\rangle \otimes |0\rangle = |00\rangle$$

$$|0\rangle \otimes (|0\rangle + |1\rangle)/\sqrt{2} = (|00\rangle + |01\rangle)/\sqrt{2}$$

$$(|0\rangle + |1\rangle)/\sqrt{2} \otimes (|0\rangle + i|1\rangle)/\sqrt{2} = (|00\rangle + i|01\rangle + |10\rangle + i|11\rangle)/2$$

Entangled $|\psi\rangle_{AB} \neq |\phi\rangle_A \otimes |\chi\rangle_B$

$$|\varphi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$$

$$|\varphi^-\rangle = (|00\rangle - |11\rangle)/\sqrt{2}$$

$$|\psi^+\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$$

$$|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$$

Bell or EPR States

Entanglement and Density Matrices 1

Density matrix ρ

$$\rho_{AB} = \sum_k \lambda_k |\psi\rangle_{AB} \langle\psi|_{AB}$$

Pure and mixed states

Density matrices of the Bell States

$$(|00\rangle + |11\rangle)/\sqrt{2} \longrightarrow \rho = \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}$$

$$(|01\rangle - |10\rangle)/\sqrt{2} \longrightarrow \rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & -1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Entanglement and Density Matrices 2

Maximally mixed state

$$\rho = \begin{pmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix} = (|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11|)/4$$

$$= (|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |0\rangle\langle 0| \otimes |1\rangle\langle 1| + |1\rangle\langle 1| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|)/4$$

Another mixed state

$$\rho = \begin{pmatrix} 3/4 & 1/4 & 0 & 0 \\ 1/4 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = (\overline{|0\rangle\langle 0|} \otimes \overline{|0\rangle\langle 0|} + \overline{|0\rangle\langle 0|} \otimes \overline{(|0\rangle + |1\rangle)(\langle 0| + \langle 1|)/2})/2$$

Entanglement and Density Matrices 3

Separable density matrix

$$\rho_{AB} = \sum_k \eta_k (\rho_A \otimes \rho_B)_k$$

Convex sum of direct product states

Entangled density matrix

$$\rho_{AB} \neq \sum_k \eta_k (\rho_A \otimes \rho_B)_k$$

Detecting and Quantifying Entanglement 1

Can we find a separable decomposition of ρ ?

$$\rho = \frac{1}{18}\begin{pmatrix} 5 & 0 & 0 & 1 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 1 & 0 & 0 & 5 \end{pmatrix}$$

Ensemble fallacy

$$\rho = \begin{pmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix} = (|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11|)/4$$

$$= (|\varphi^+\rangle\langle\varphi^+| + |\varphi^-\rangle\langle\varphi^-| + |\psi^+\rangle\langle\psi^+| + |\psi^-\rangle\langle\psi^-|)/4$$

D. T. Pegg, J. Jeffers J. Mod. Opt. **52**, 1835 (2005)

Detecting and Quantifying Entanglement 2

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = (|01\rangle\langle 01| + |10\rangle\langle 10|)/2$$

$$= (|\psi^+\rangle\langle\psi^+| + |\psi^-\rangle\langle\psi^-|)/2$$

Test for Separability

PPT Test $|\psi^+\rangle = 1/\sqrt{2}(|00\rangle + |11\rangle)$

$$\rho = |\psi^+\rangle\langle\psi^+| = \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}$$

$$\rho^T = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 1/2 \end{pmatrix}$$

Eigenvalues of ρ^T are {1/2,1/2,1/2,-1/2}.

ρ is non-separable or entangled.

A. Peres Phys. Rev. Lett. **77**, 1413 (1996)

Separability of the Werner State

Werner or *pseudo*pure state

$$\rho = (1-\varepsilon)\mathbf{1}/4 + \varepsilon\,|\psi^-\rangle\langle\psi^-|$$

$$= \begin{pmatrix} \frac{1-\varepsilon}{4} & 0 & 0 & 0 \\ 0 & \frac{1+\varepsilon}{4} & -\frac{\varepsilon}{2} & 0 \\ 0 & -\frac{\varepsilon}{2} & \frac{1+\varepsilon}{4} & 0 \\ 0 & 0 & 0 & \frac{1-\varepsilon}{4} \end{pmatrix}$$

$$\rho^T = \begin{pmatrix} \frac{1-\varepsilon}{4} & 0 & 0 & -\frac{\varepsilon}{2} \\ 0 & \frac{1+\varepsilon}{4} & 0 & 0 \\ 0 & 0 & \frac{1+\varepsilon}{4} & 0 \\ -\frac{\varepsilon}{2} & 0 & 0 & \frac{1-\varepsilon}{4} \end{pmatrix}$$

- Eigenvalues of PPT of ρ are {1/4(1-3ε),1/4(1+ ε), 1/4(1+ ε), 1/4(1+ ε)}. ρ is non-separable or entangled only if **ε > 1/3**.

The problem of initialization

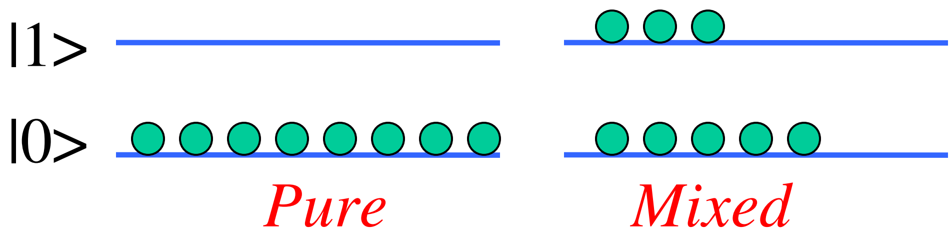
Requirements for Practical QC

- Existence of Qubits
- Initialization
- Universal Quantum Networks
- Read-out or Measure
- Decoherence

D.P. DiVincenzo quant-ph/0002077 (2000)

Initialization 1

NMR states are highly mixed.

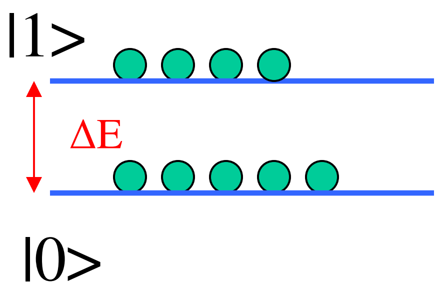


Ideal initial state

$$\rho = |0\rangle\langle 0| \otimes |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Initialization 2

Thermal equilibrium state



ρ_{eq}= exp(-βH)/Z where β=ħ/(k_BT)

ΔE = γħB_z = ħω =2.8 × 10^{-25} J

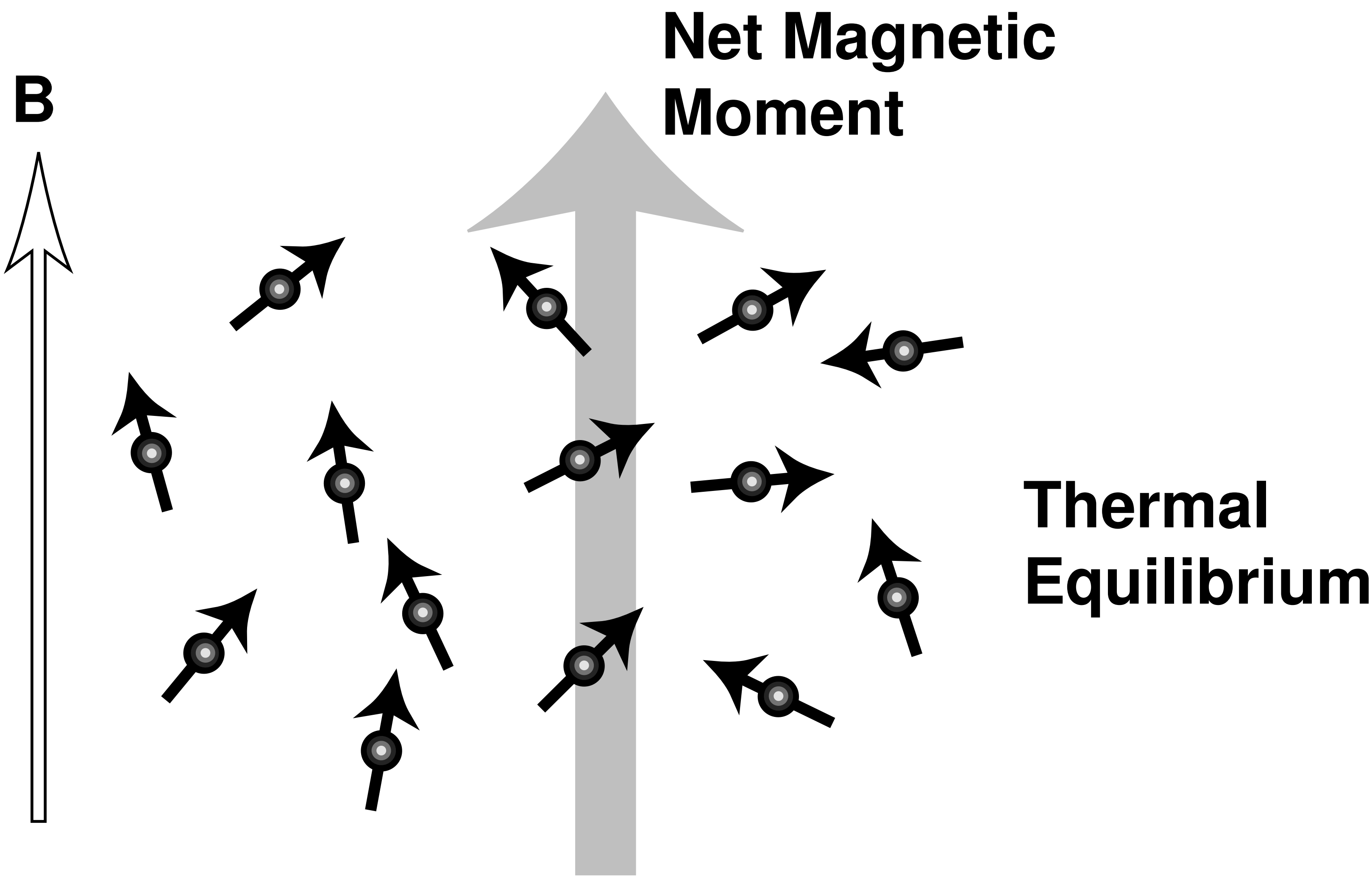
k_BT=4 × 10^{-21}J at 10T, 300K

Population difference only ~10^{-4} **k_BT >> ΔE**

$$\rho = \begin{pmatrix} 0.25001 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0.24999 \end{pmatrix}$$

={{1/4+*B*,1/4,1/4,1/4-*B*}}=1/4+*B*/4(I_z+S_z) where *B* = ħω / kT.

Initialization 3



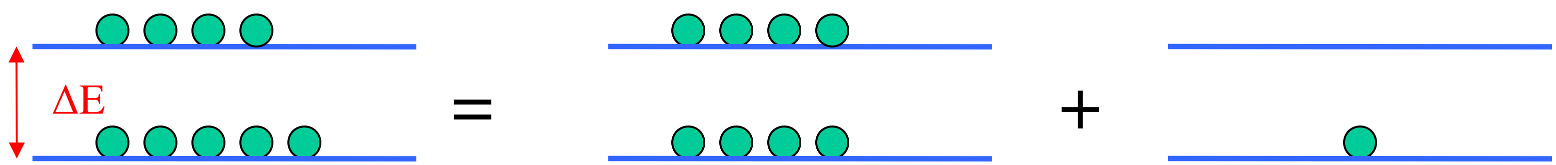
Pseudopure States

$$\begin{pmatrix} 0.25001 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0.24999 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Thermal equilibrium state

Ideal initial state

Pseudopure state $\rho_{ps} = (1-\varepsilon)\mathbf{1/4} + \varepsilon\, |\psi\rangle\langle\psi|$ ε is polarization.

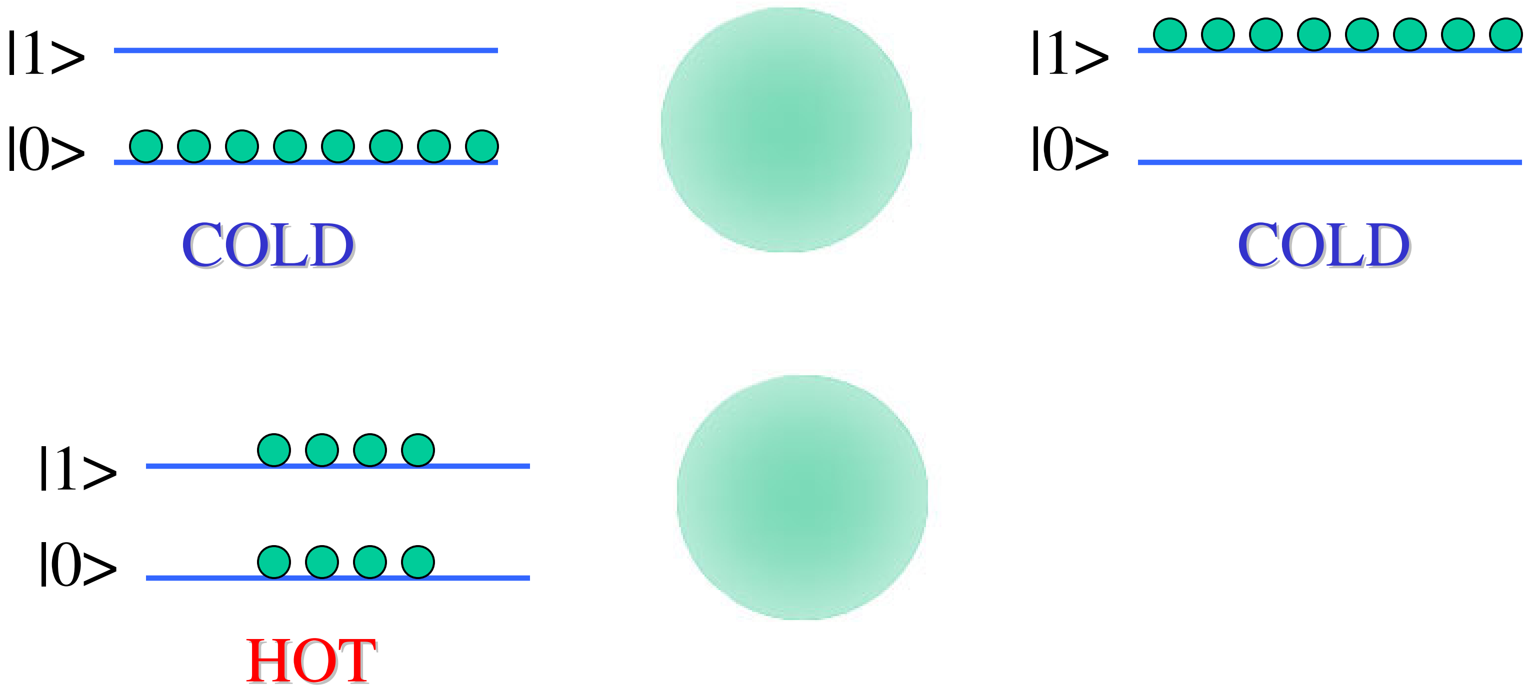


Thermal, mixed

Maximally mixed

Pure

Spin Temperature



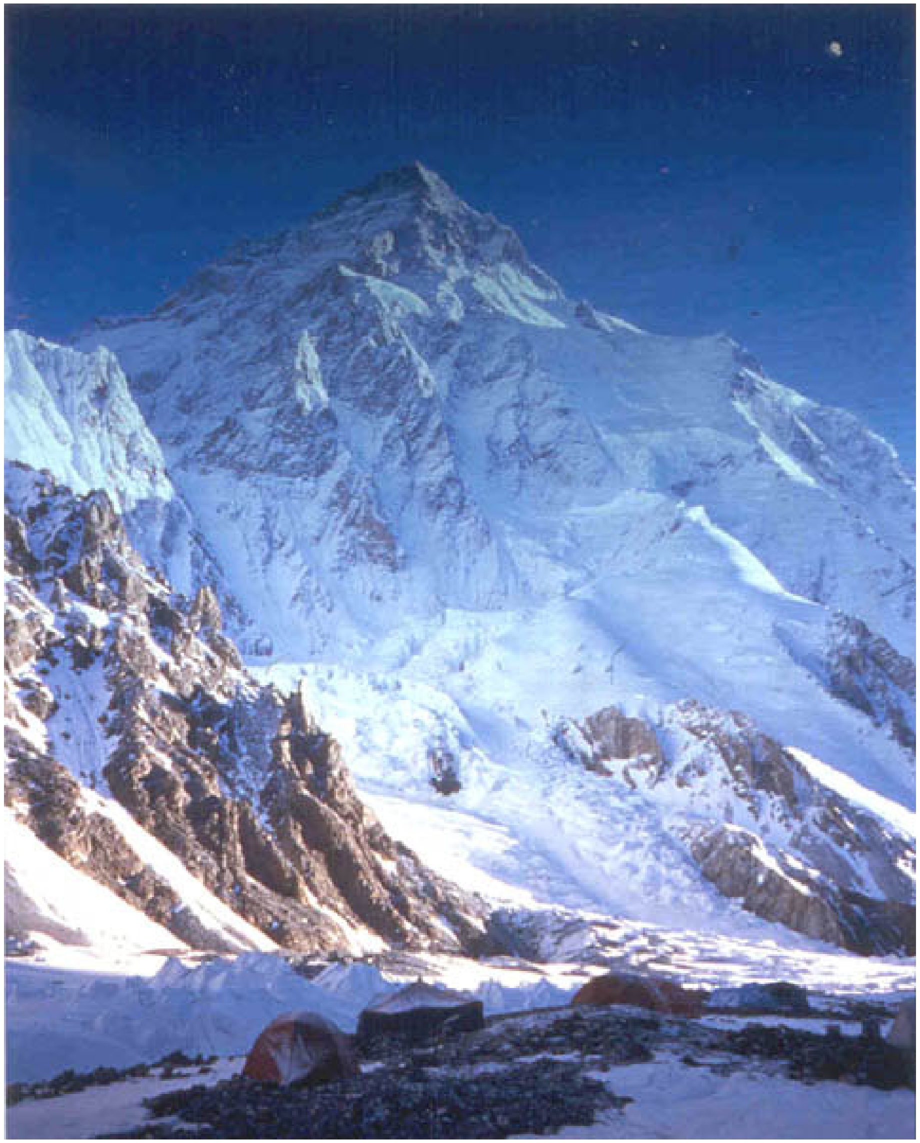
Problems with Pseudopure States

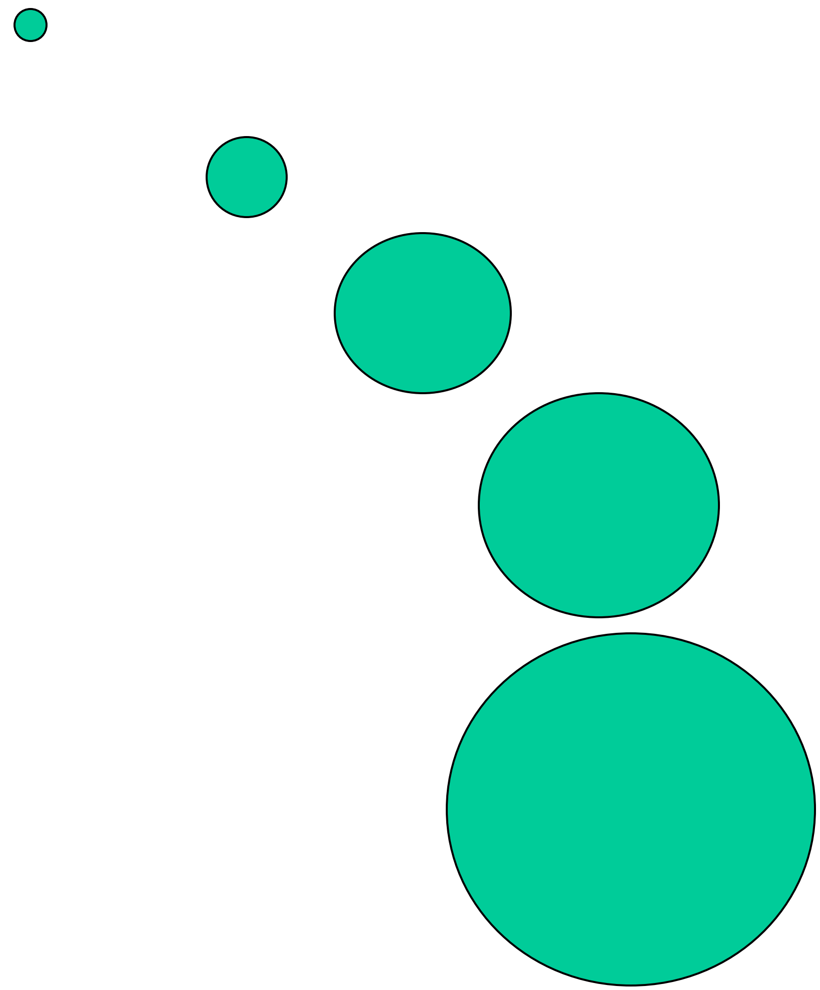
Scalability

Is NMR quantum mechanical at all?

S.L. Braunstein et al. Phys. Rev. Lett. **83**, (1999)
J.A. Jones, Fortsch. der Physik **48**, 909 (2002).

Climbing Mount Scalable



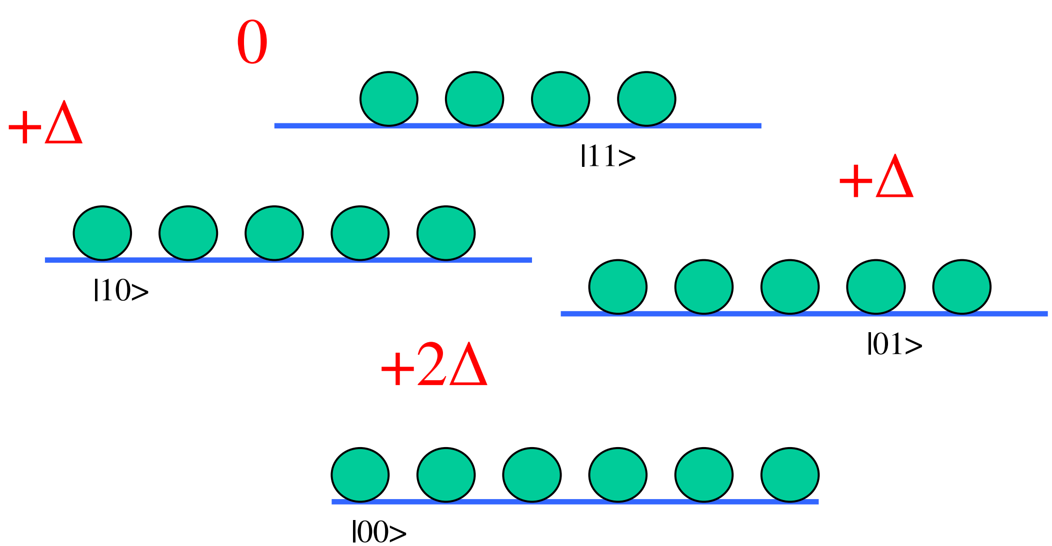


Scalability

Maximum pure state that can be extracted from thermal state

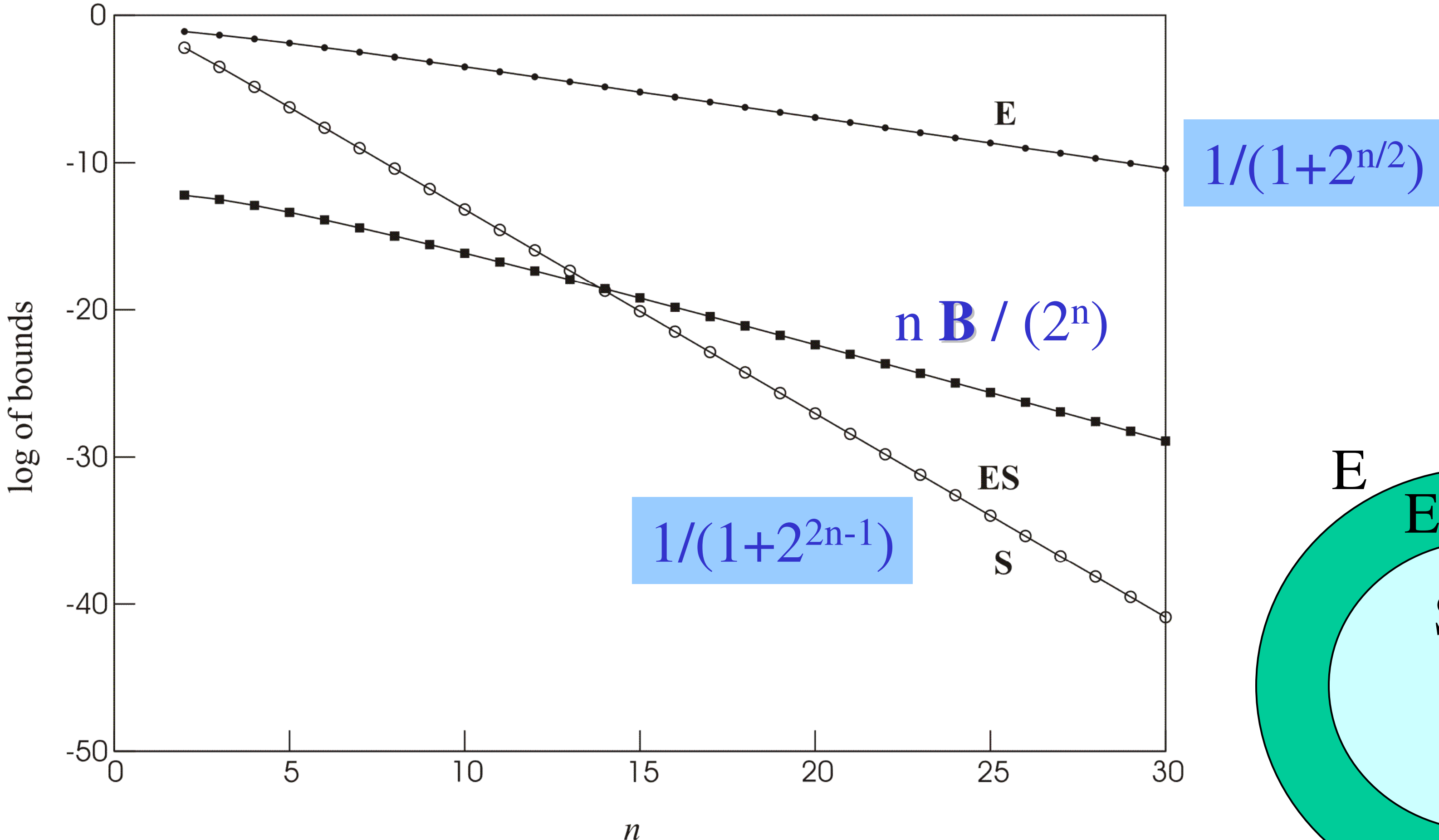
$$\rho_{ps}=(1-\varepsilon)\,\mathbf{1}\,/\,2^n + \varepsilon\,|\psi\rangle\langle\psi|$$

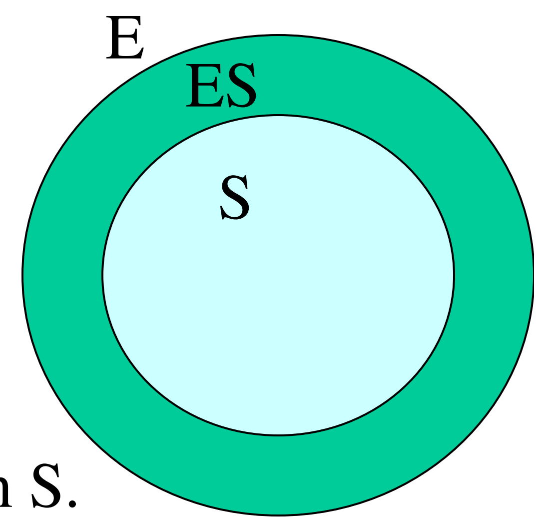
Warren proposed a theoretical maximum on ε:
$\varepsilon \sim n\mathbf{B} / (2^n)$ where n is the number of qubits.



W.S.Warren Science **277**, 1688 (1997).

Scalability and Separability





- Present day NMR implementations work in region S.
- We can enter ES if n > 11 (room temperature, 10T).
- We may never enter E with thermal states!

Methods for Increasing Polarization

High fields and low temperature $B = \hbar\omega / kT$

Algorithmic concentration of polarization

Polarization transfer from nuclear spins

Polarization transfer from electron spins

Chemically induced
dynamical nuclear polarization (CIDNP)

Is an NMR Device a Quantum Computer?

No entanglement

What makes a quantum computer quantum?

States or Dynamics?

Scaling of the Hilbert space dimensionality?

Superposition?

Other models of better than classical computing.

The para-hydrogen approach

Para-hydrogen Induced Polarization 1

Need for "non-thermal" distributions

Symmetrization postulate

$|\psi\rangle_t = |\psi\rangle_{tr} |\psi\rangle_{vib} |\psi\rangle_e |\psi\rangle_{ns} |\psi\rangle_r$

$|\psi\rangle_{ns}$ →

$|T_1\rangle = |00\rangle$

$|T_0\rangle = 1/2^{1/2}(|01\rangle + |10\rangle)$

$|S_0\rangle = 1/2^{1/2}(|01\rangle - |10\rangle)$

$|T_{-1}\rangle = |11\rangle$

$|\psi\rangle_r$ →

j=**0**,2,4,… even

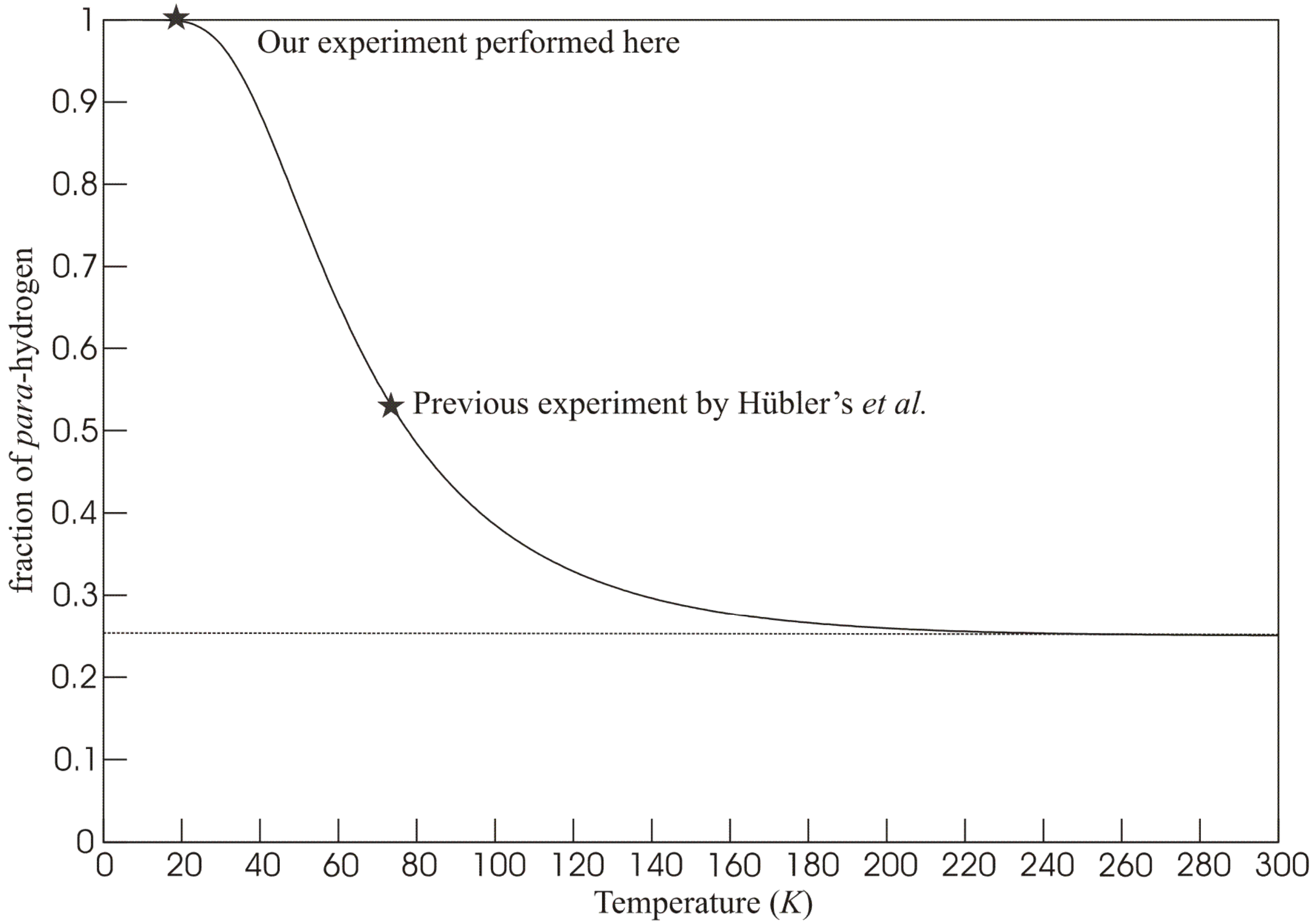
j=1,3,5,… odd

$(Y^j_m(\pi-\theta, \pi+\varphi) = (-1)^j Y^j_m(\theta, \varphi))$

Para-hydrogen Induced Polarization 2

j	$\|\psi_{rot}>$	$\|\psi_{ns}>$	o/p
0	s symmetrical	a asymmetrical	p
1	a	s	o
2	s	a	p
3	a	s	o

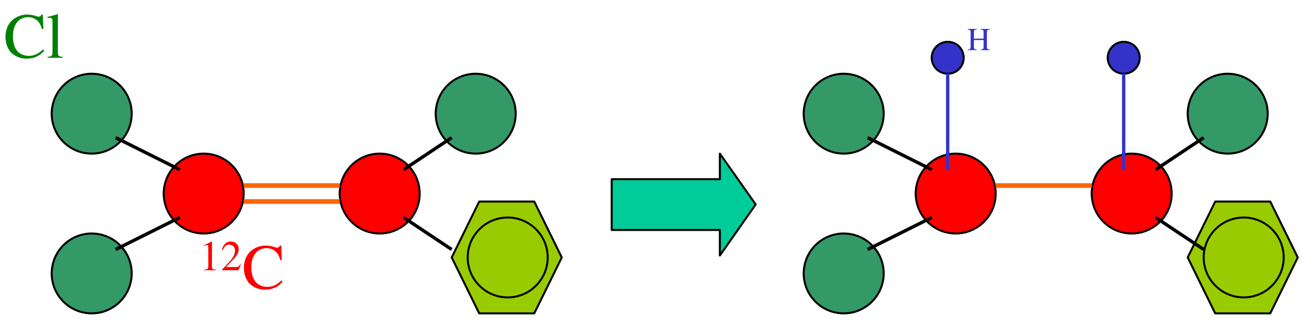
Making *Para*hydrogen



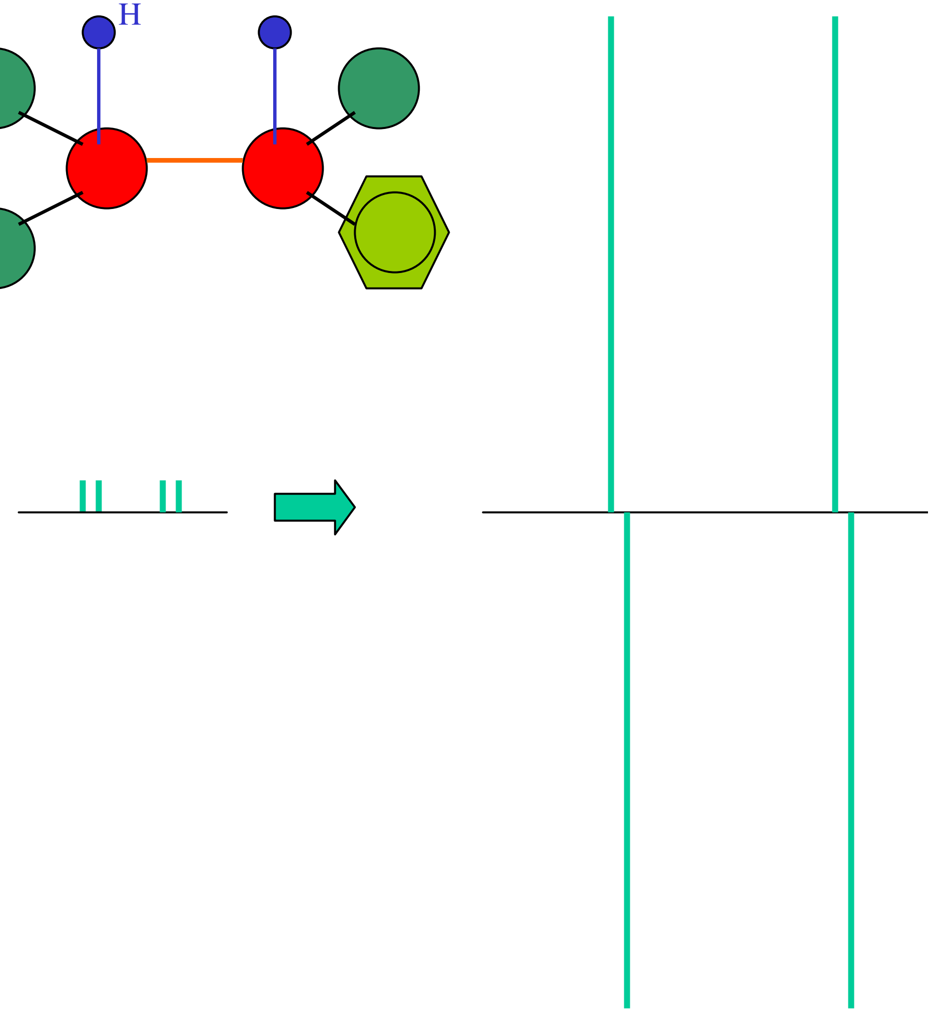
Para-hydrogen once is *para*-hydrogen forever!

Para-hydrogen Quantum Computer

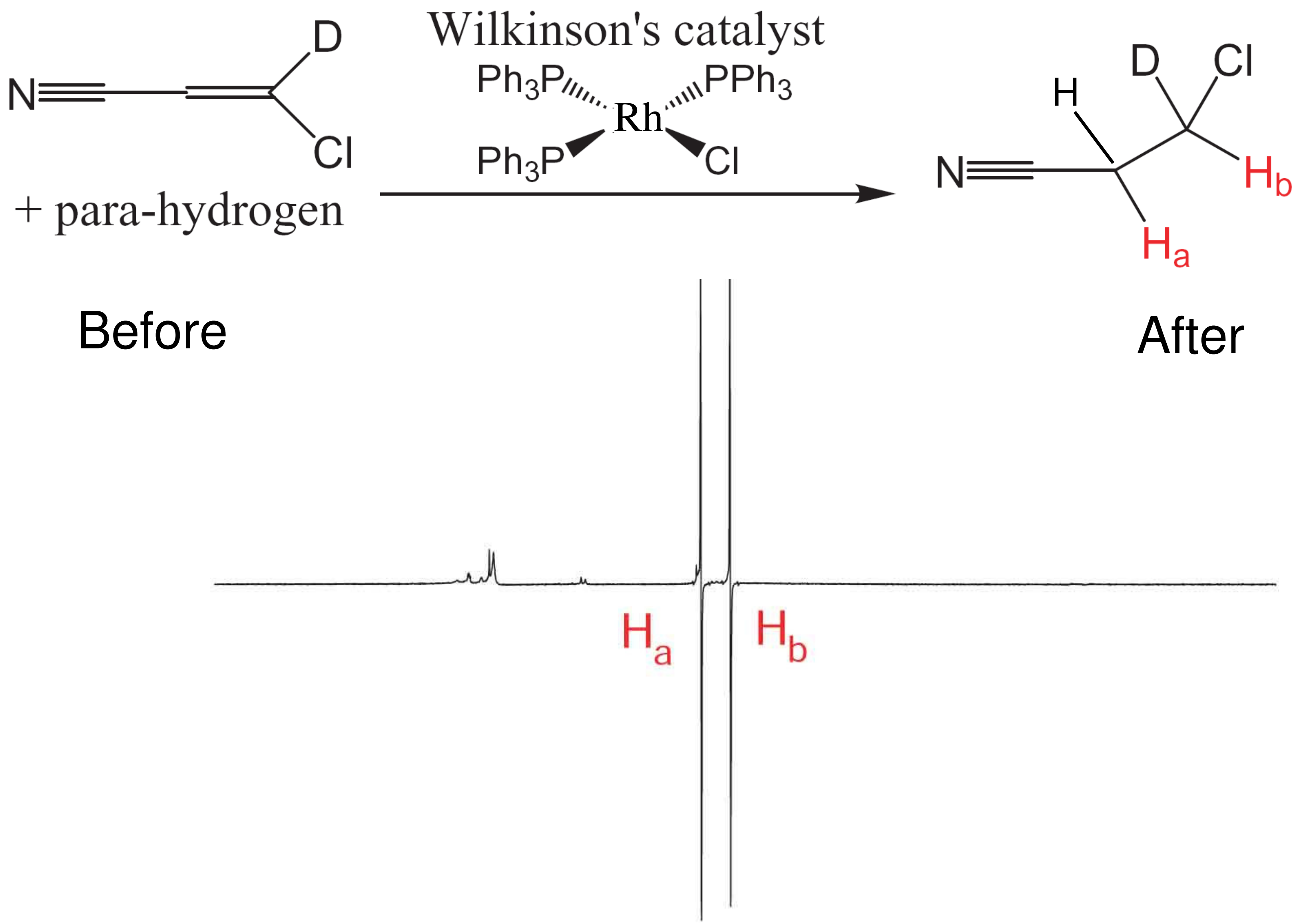
The PASADENA Experiment



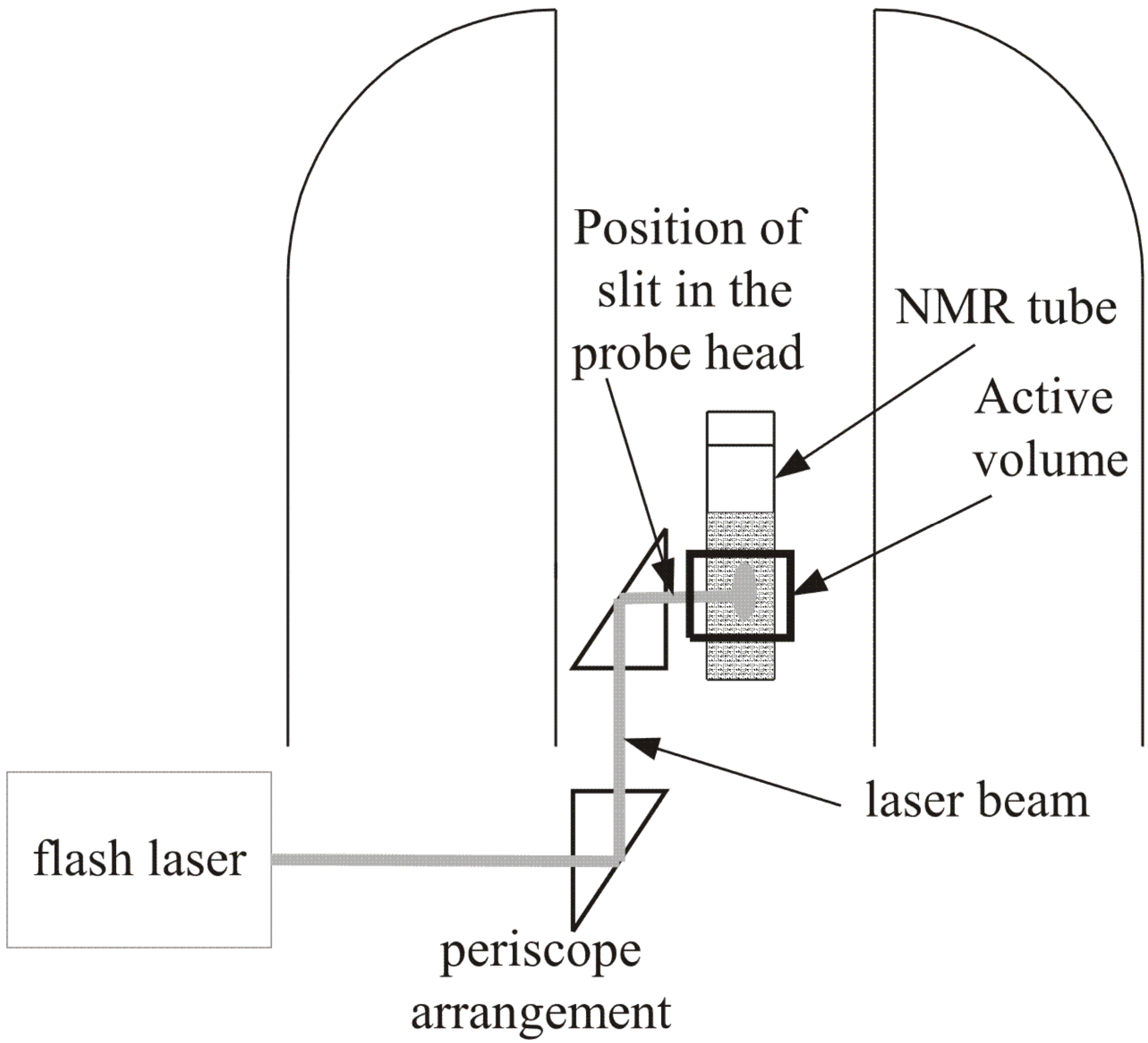
- pairwise addition
- assymetric environment
- enhanced polarizations



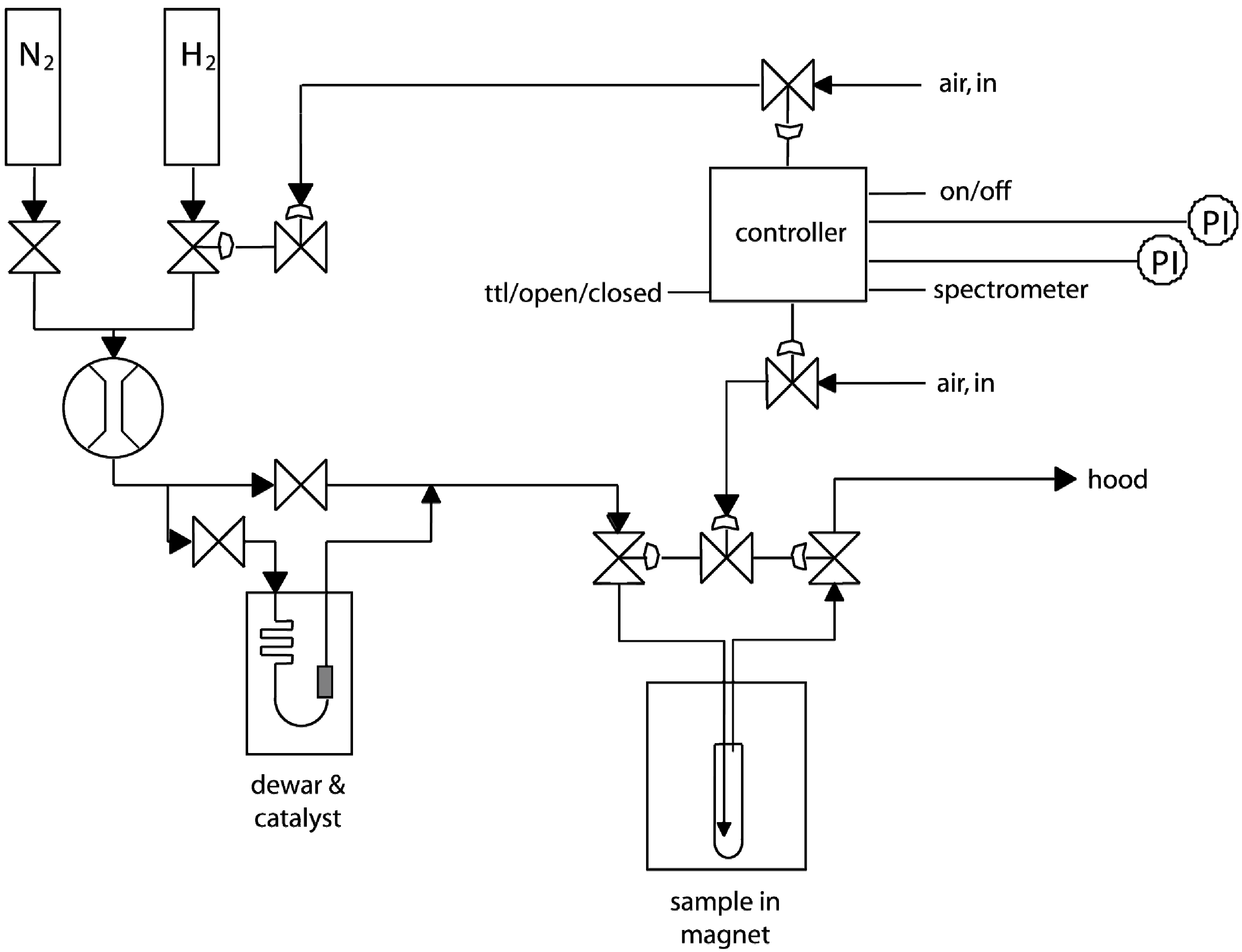
Example PASADENA spectrum



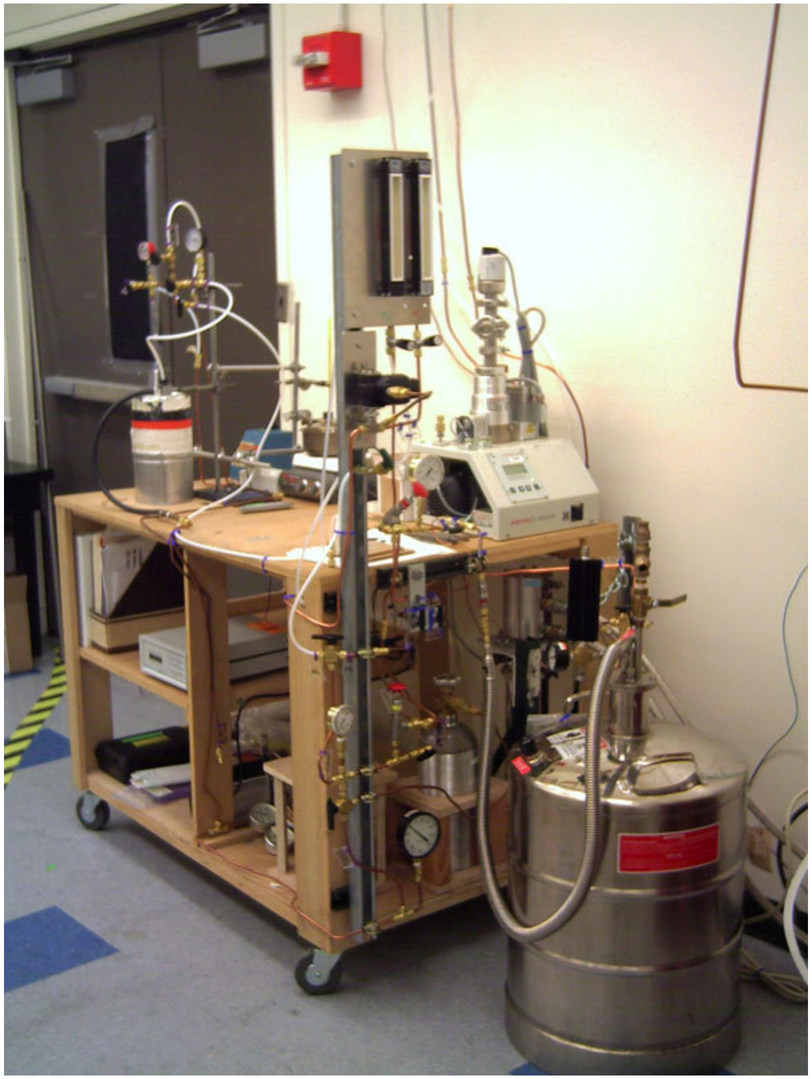
Experimental Setup

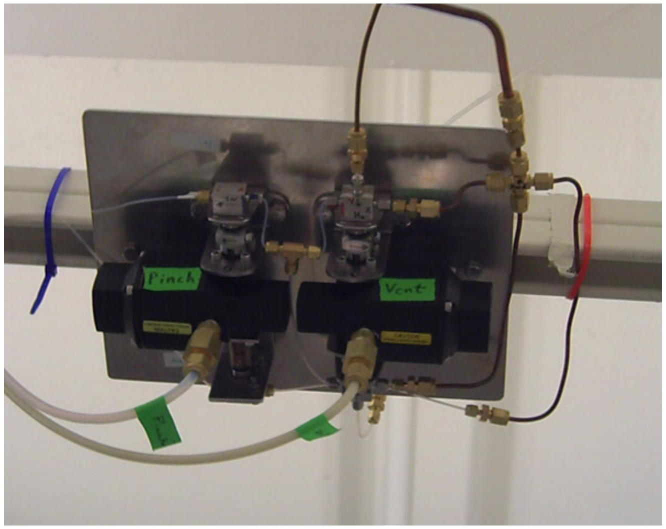


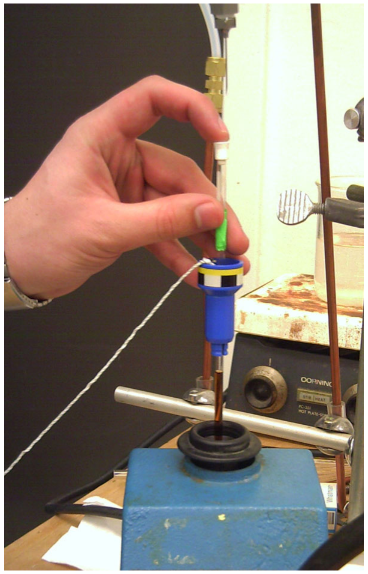
Schematic setup for the PASADENA Experiment



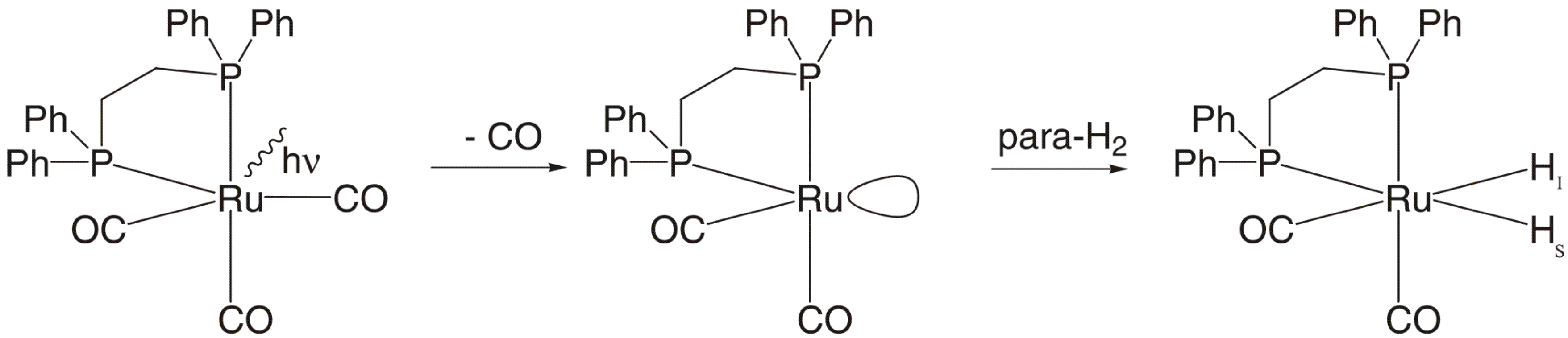
Some photographs depicting various units in the experiement







Flash Photolysis



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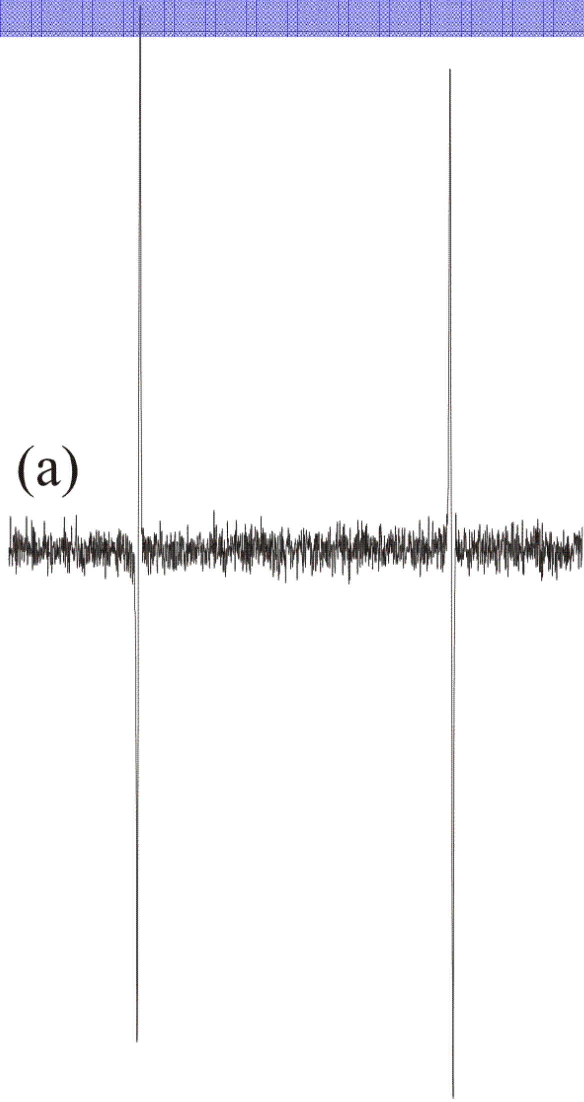
D. Blazina et al. Magn. Reson. Chem. **43**, 200 (2005)

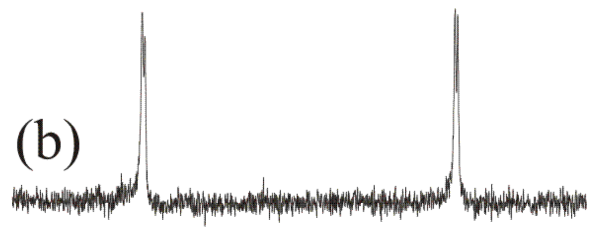
PHIP Spectra

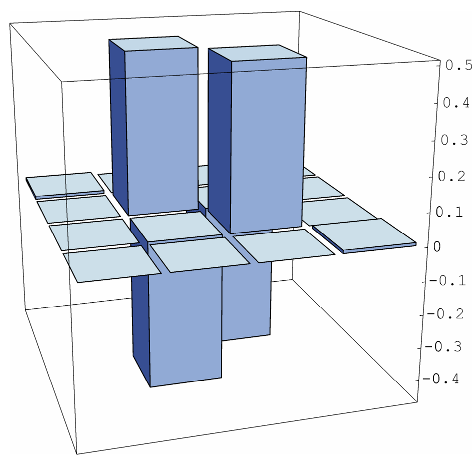
(a)



Spin Temperature = 6.4 mK
Effective Field = 0.45 MT
$\varepsilon = 0.916$

(b)



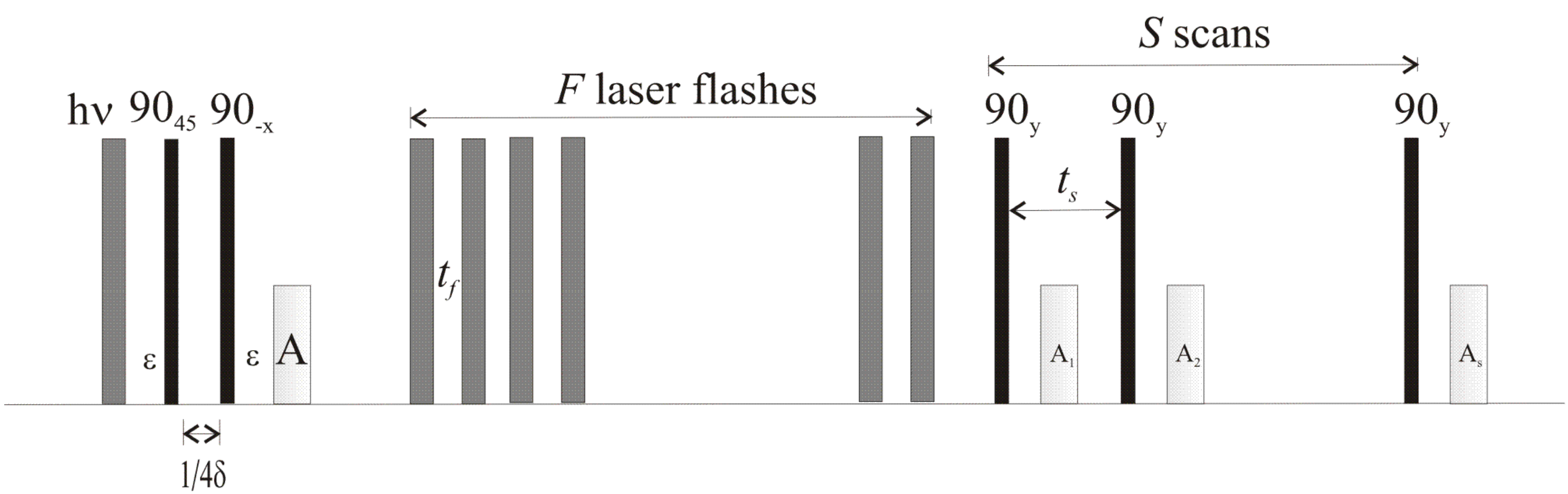


Tomography results

$$1/2\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Ideal singlet

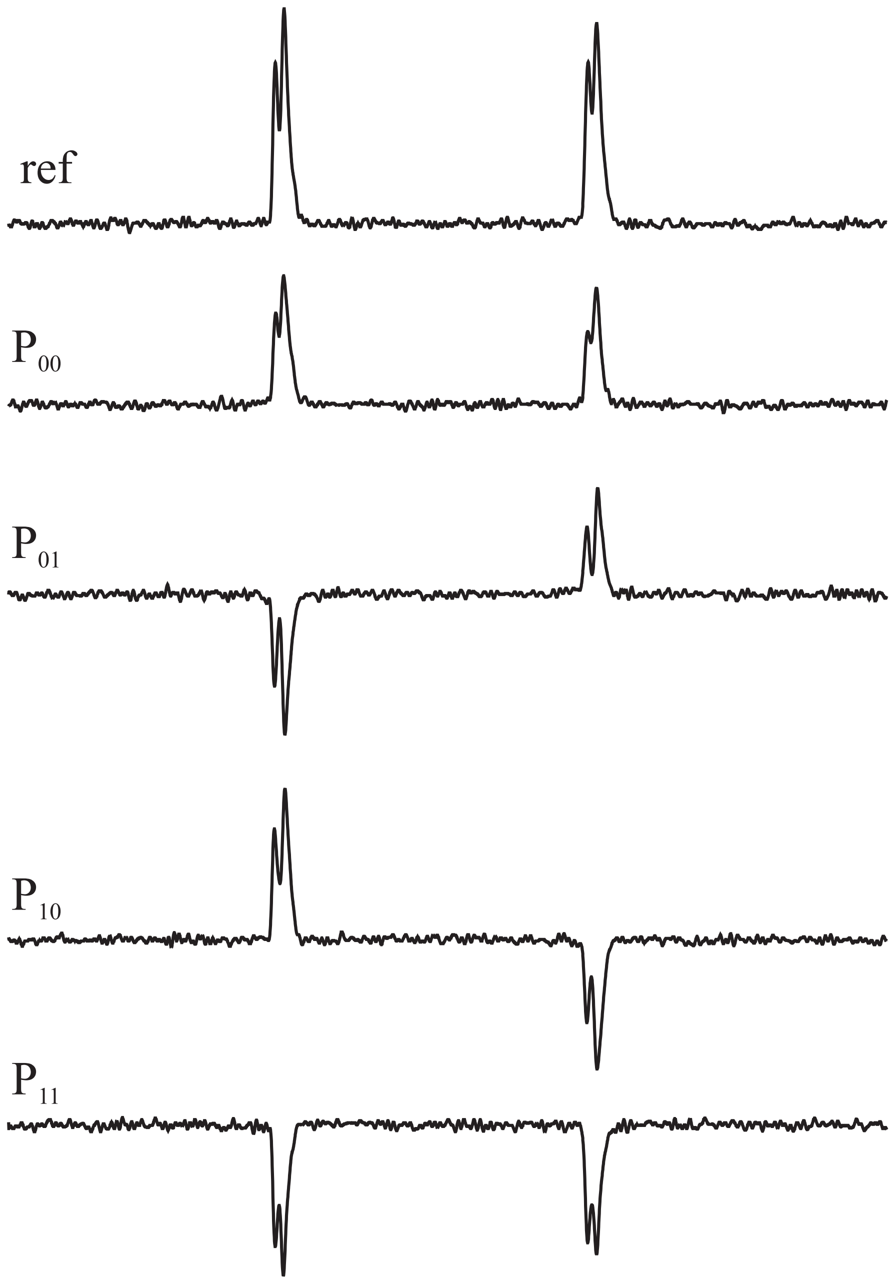
The NMR Experiment



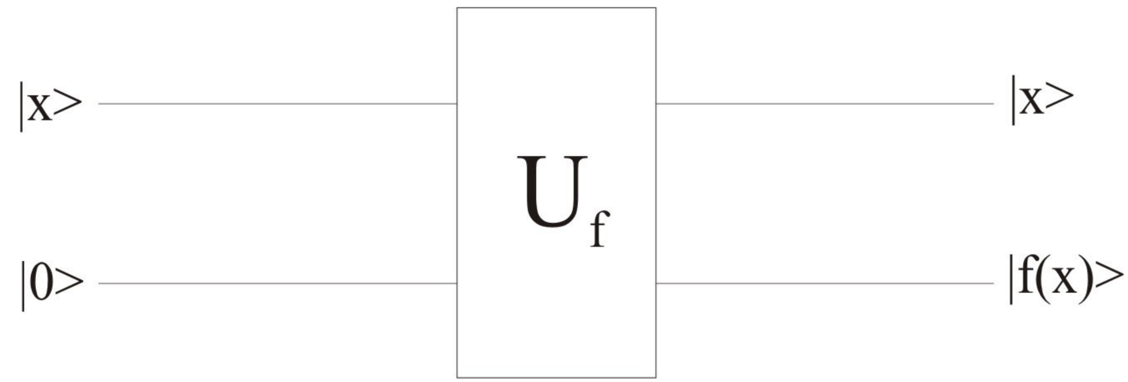
M.S. Anwar et al. Phys. Rev. Lett. **93**, 040501 (2004)

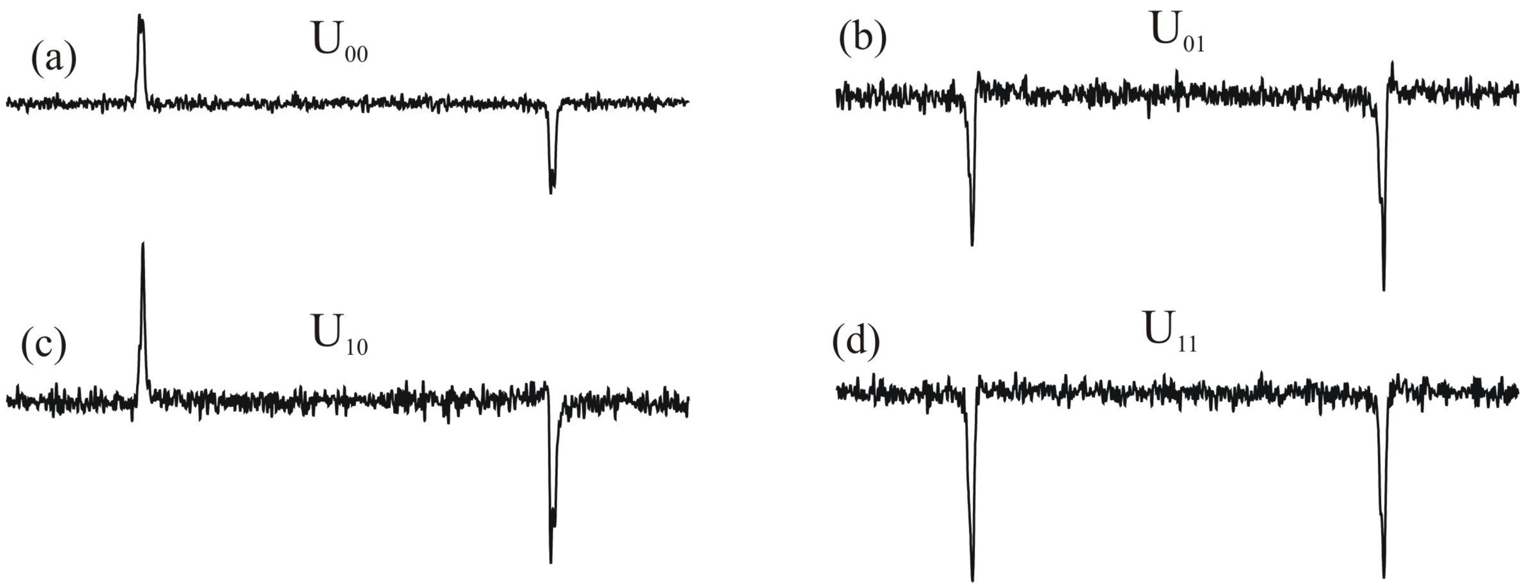
M.S. Anwar et al. Phys. Rev. A **71**, 032327 (2005)

Grover's algorithm

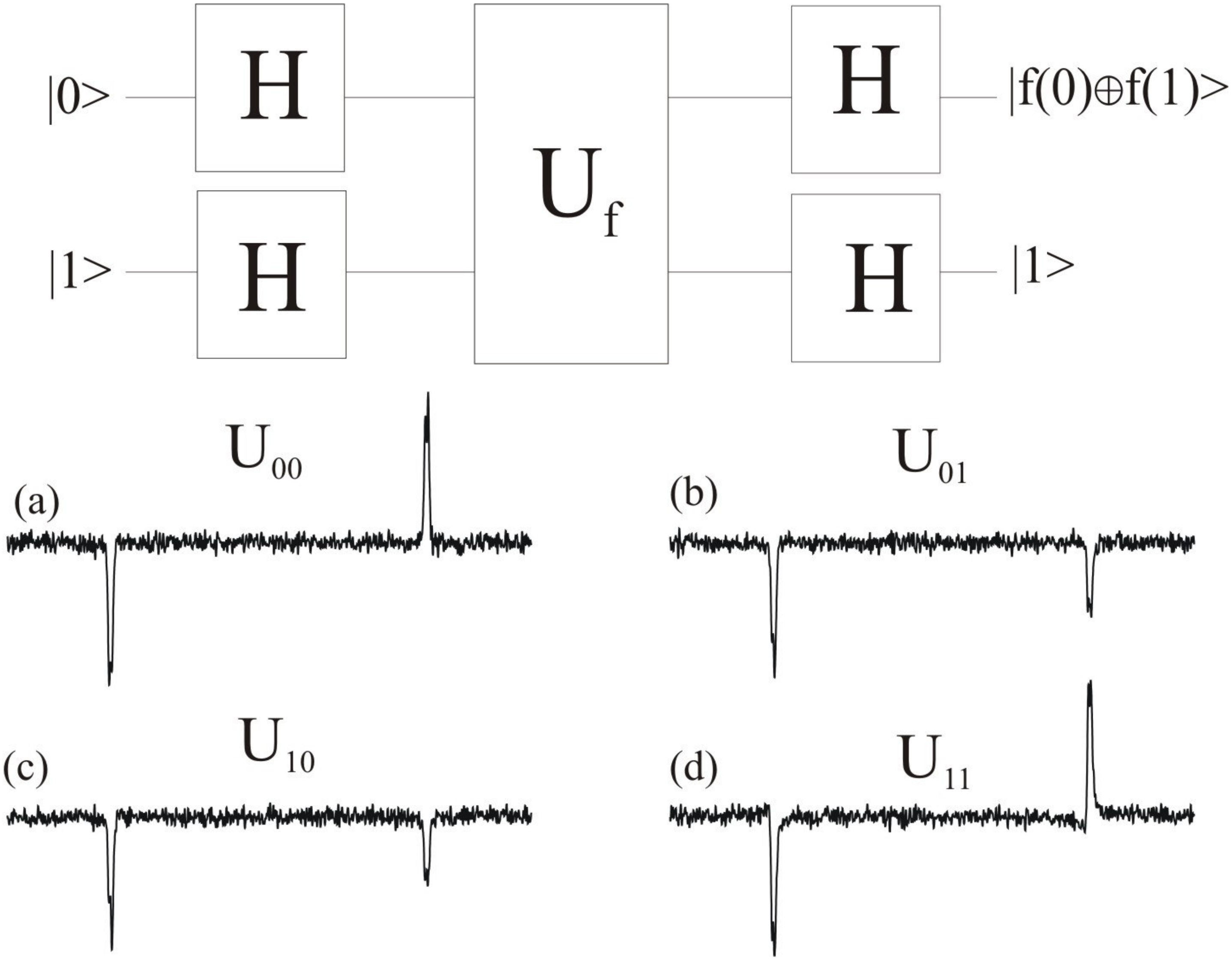


Classical Deutsch's Algorithm: *f(1)*



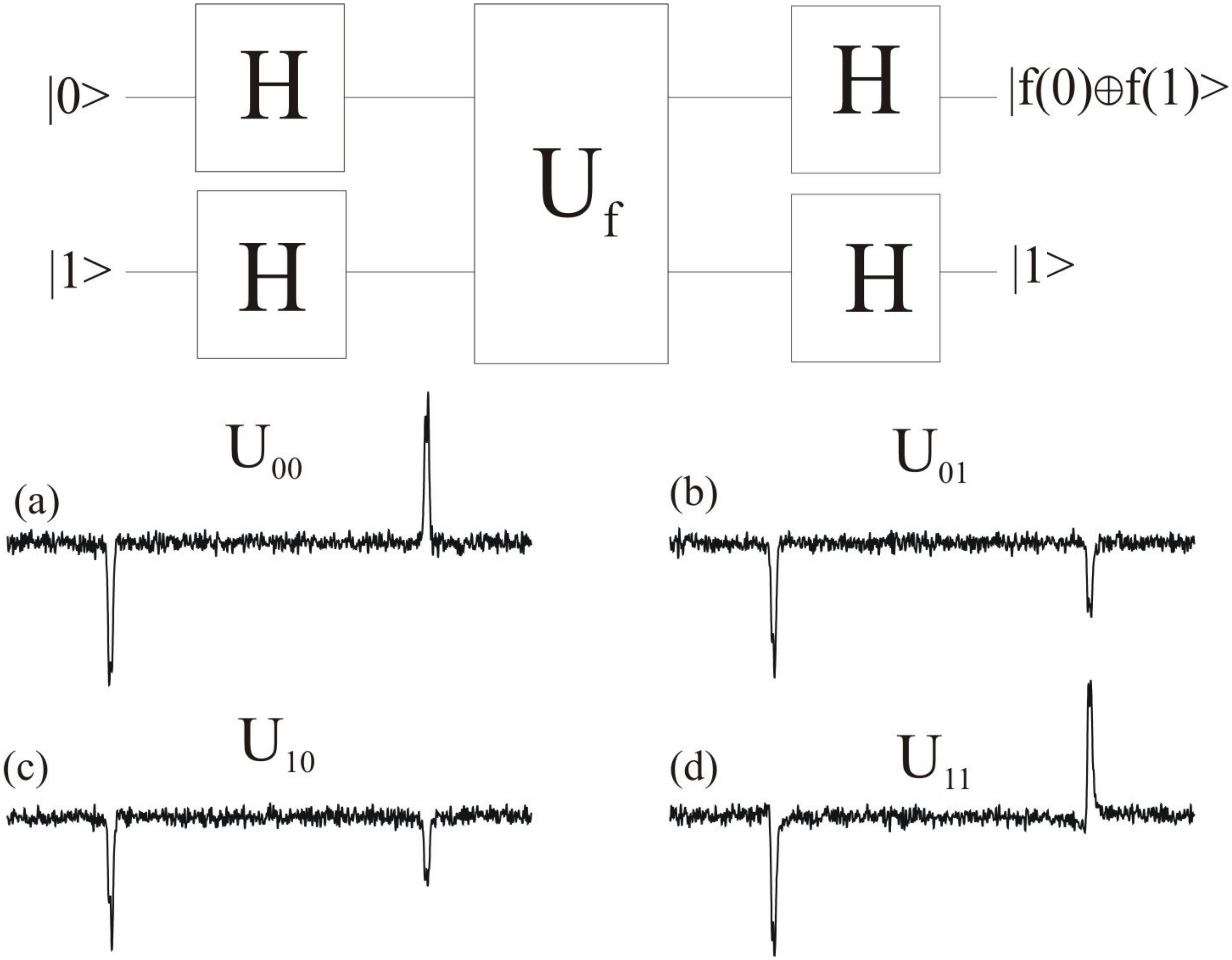


Quantum Deutsch's Algorithm



M.S. Anwar et al. Phys. Rev. A **70**, 032324 (2004)

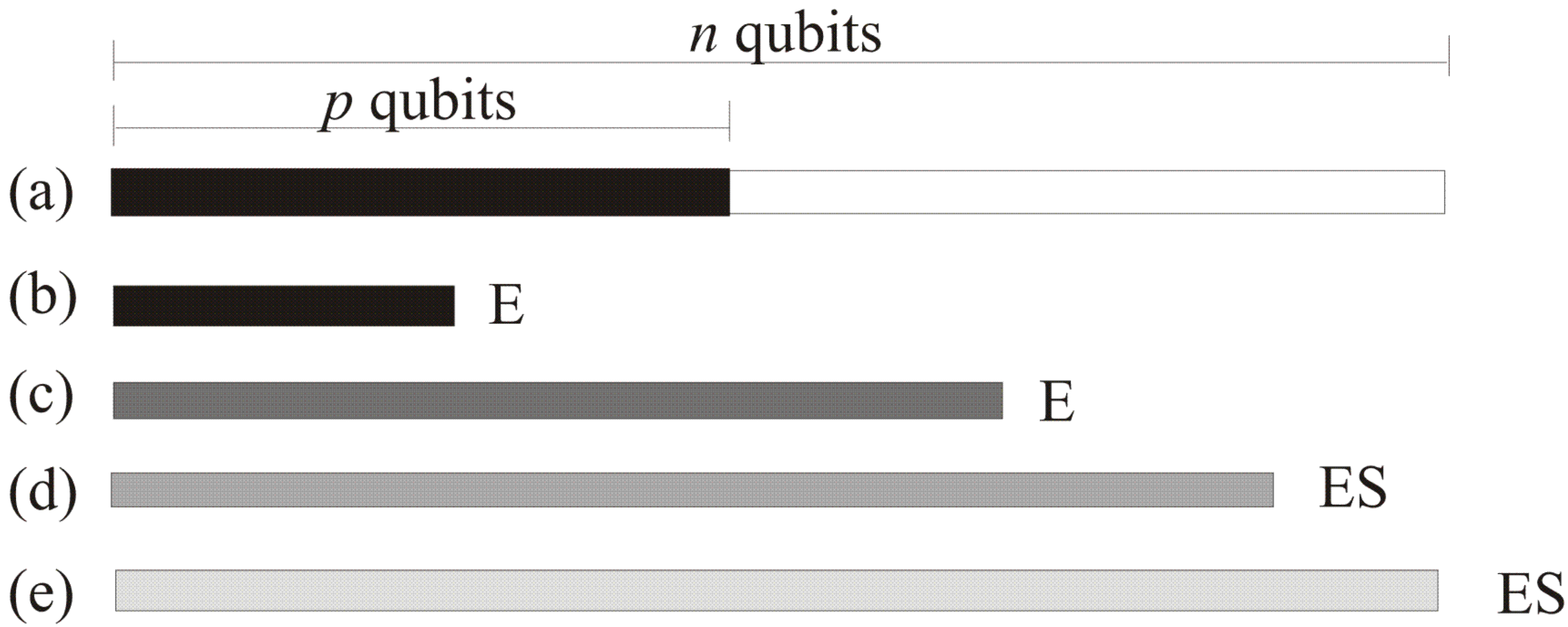
Quantum Deutsch's Algorithm



M.S. Anwar et al. Phys. Rev. A **70**, 032324 (2004)

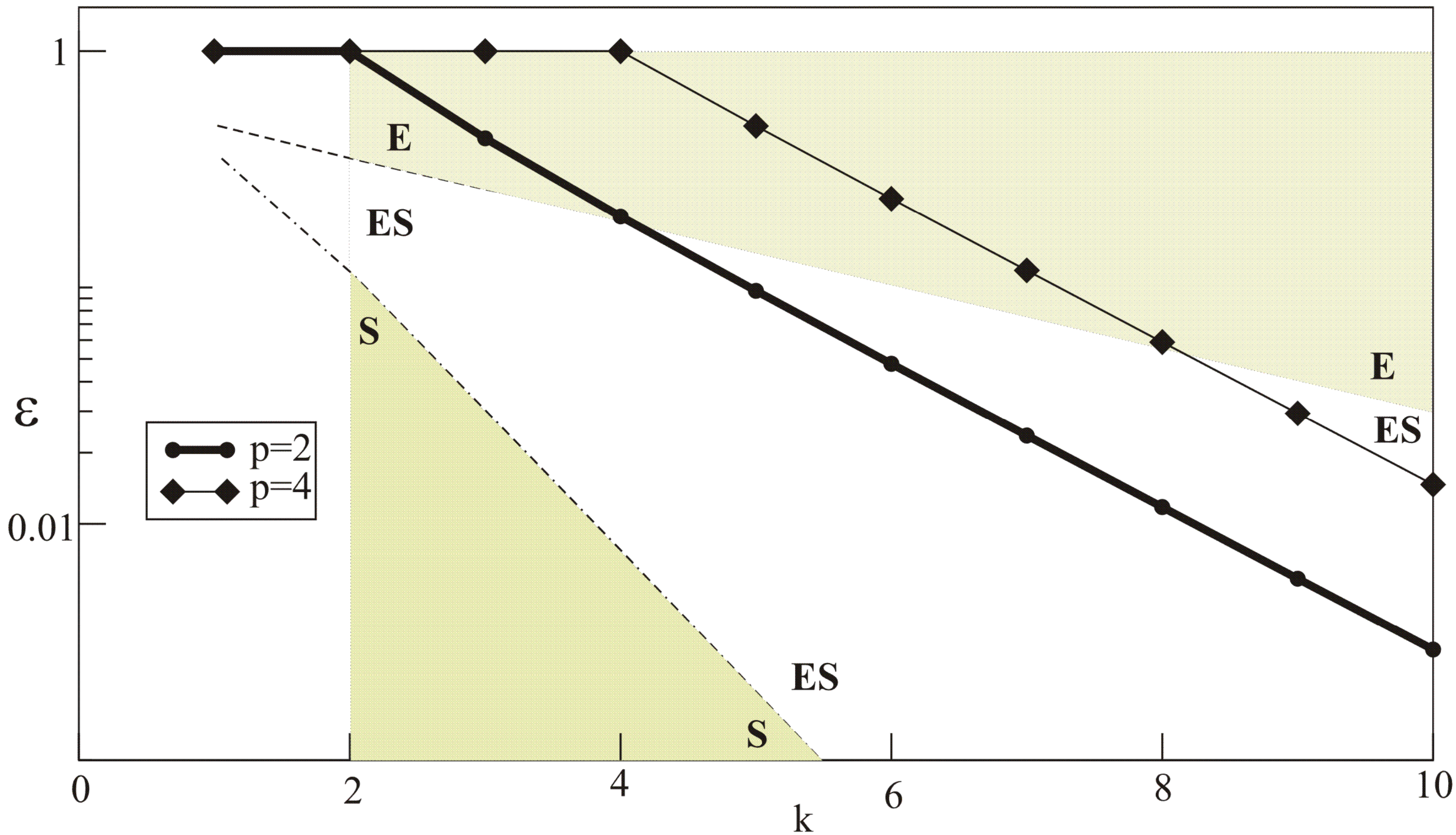
Purity dilution

Purity Sharing 1



M.S. Anwar et al. Phys. Rev. A **73**, 022322 (2006)

Purity Sharing 2



Purity Sharing 3