Optimal control of spin systems in NMR spectroscopy and quantum computing

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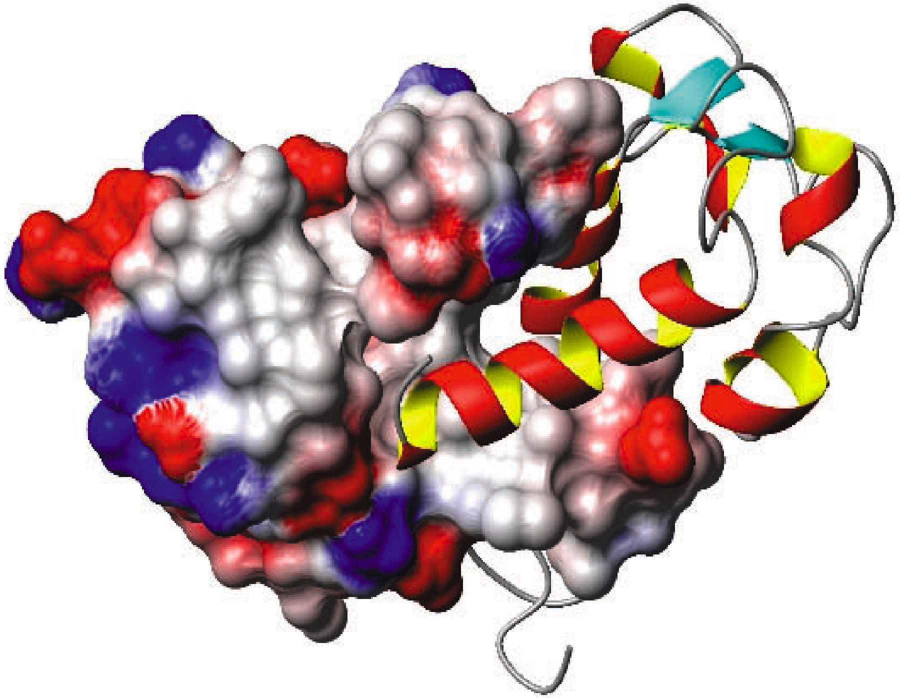
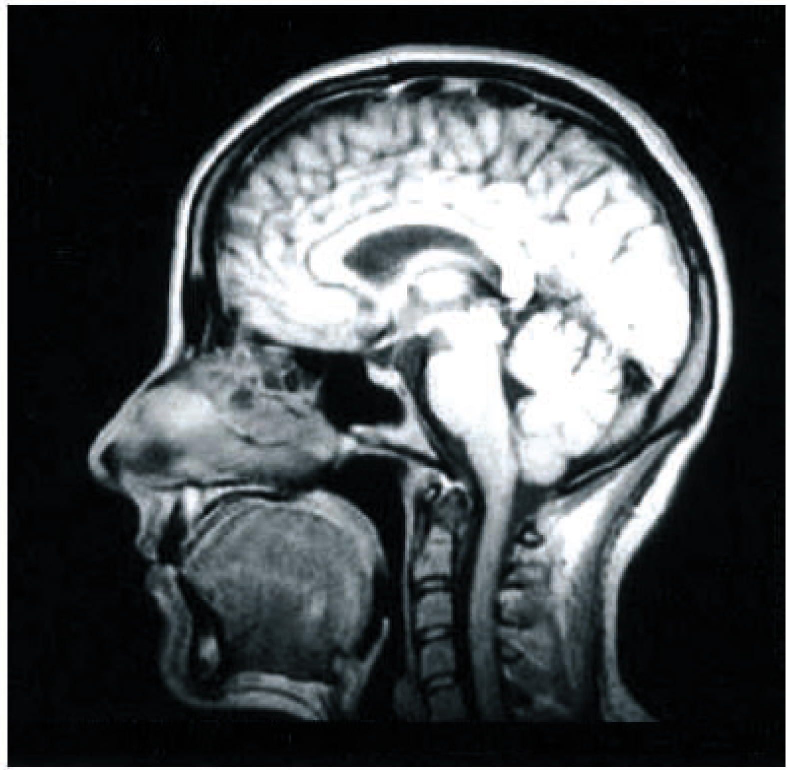
Technische Universität München

NMR spectroscopy and imaging

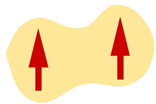




Nobel Prizes:

1952: Edward Purcell, Felix Bloch (Physics)
1991: Richard Ernst (Chemistry)
2002: Kurt Wüthrich (Chemistry)
2003: Paul Lauterbur, Peter Mansfield (Medicine)

Isolated quantum system



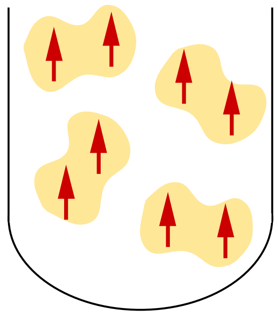
Pure state $|\Psi\rangle$

Measurement:

random *eigenvalue* of observable

(collapse of state function)

Ensemble of quantum systems



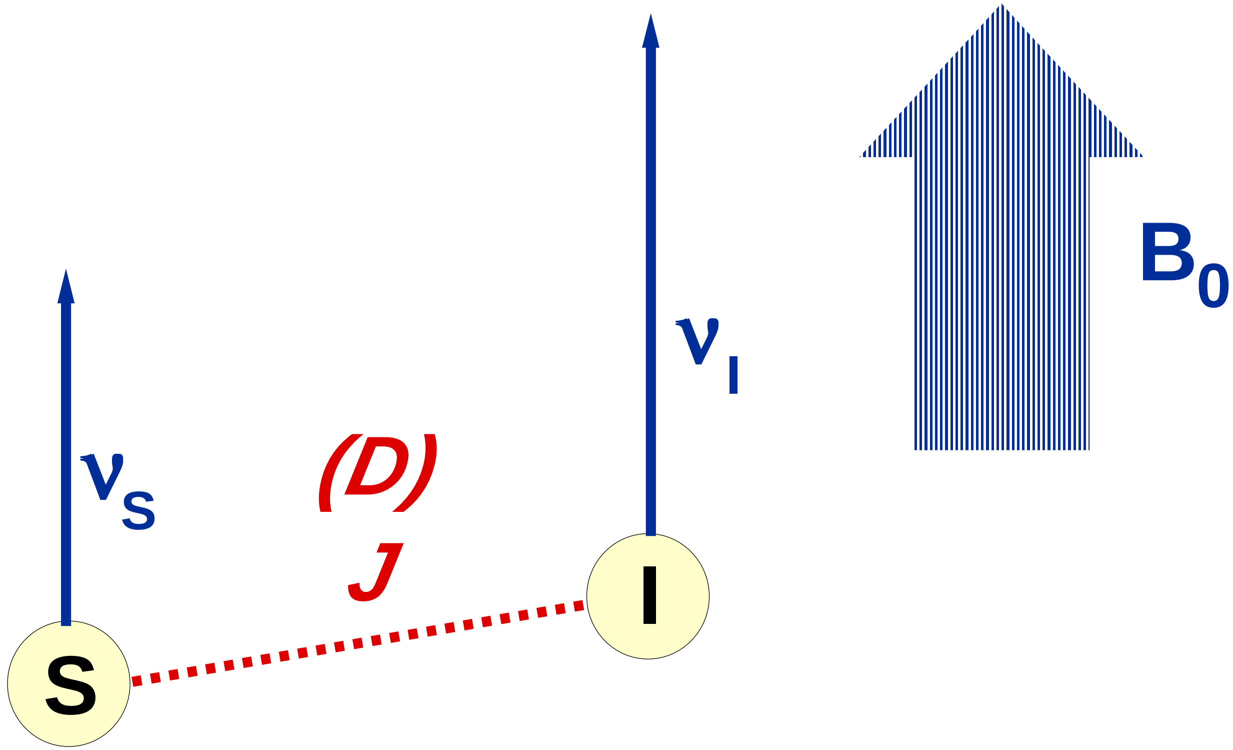
Density operator $\rho = \overline{|\Psi\rangle\langle\Psi|}$

Measurement:

expectation value of observable

(no collapse of state functions)

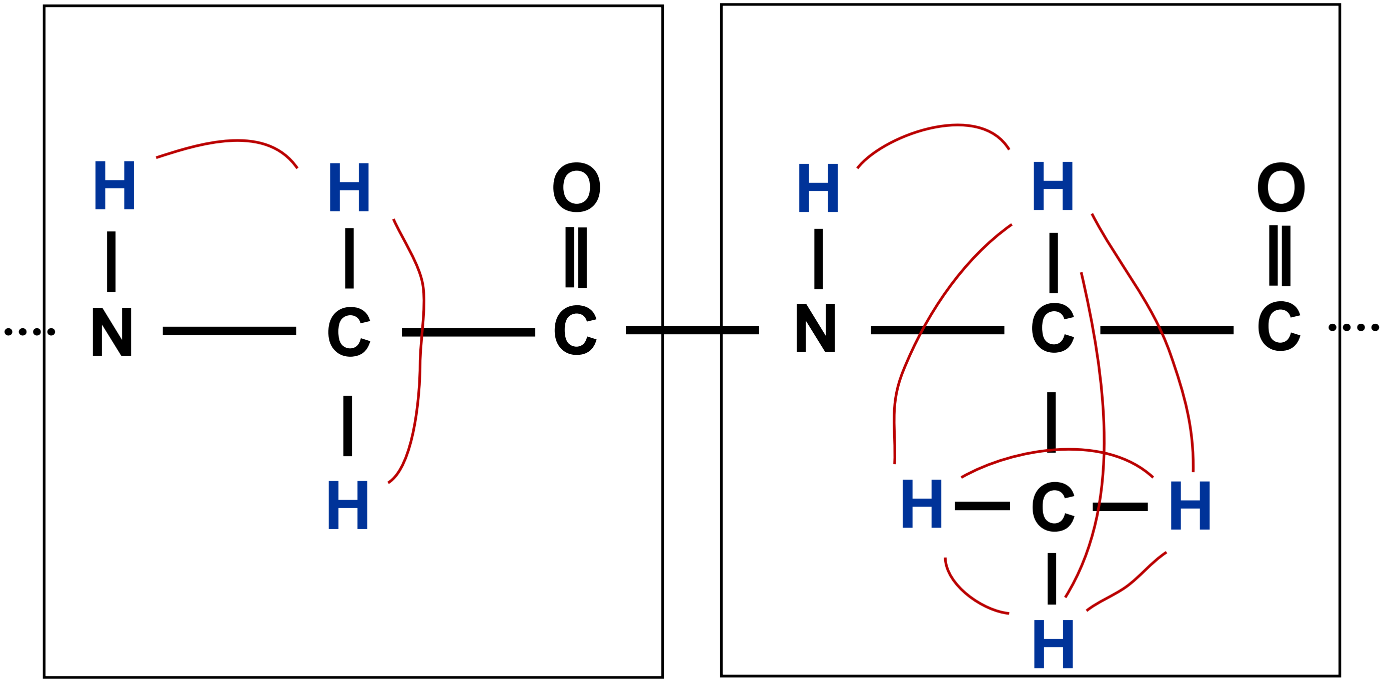
Interactions



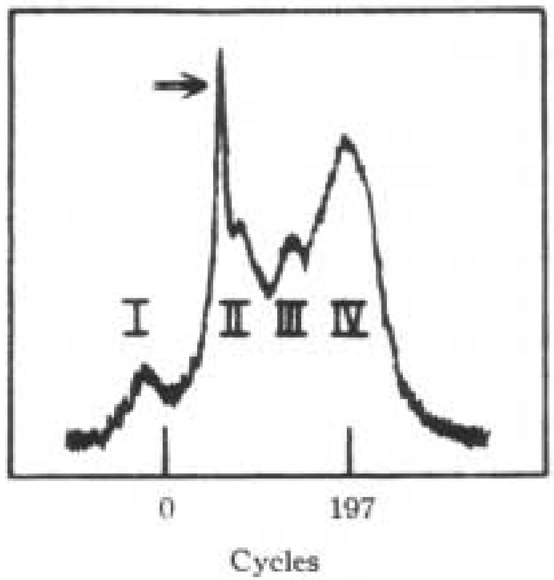
Spin Hamiltonian: $\mathbf{H_0}$

Resonance frequencies at 14 Tesla: ^{1}H 600 MHz

chemical shift range: ± 3 kHz



J couplings: 0-10 Hz

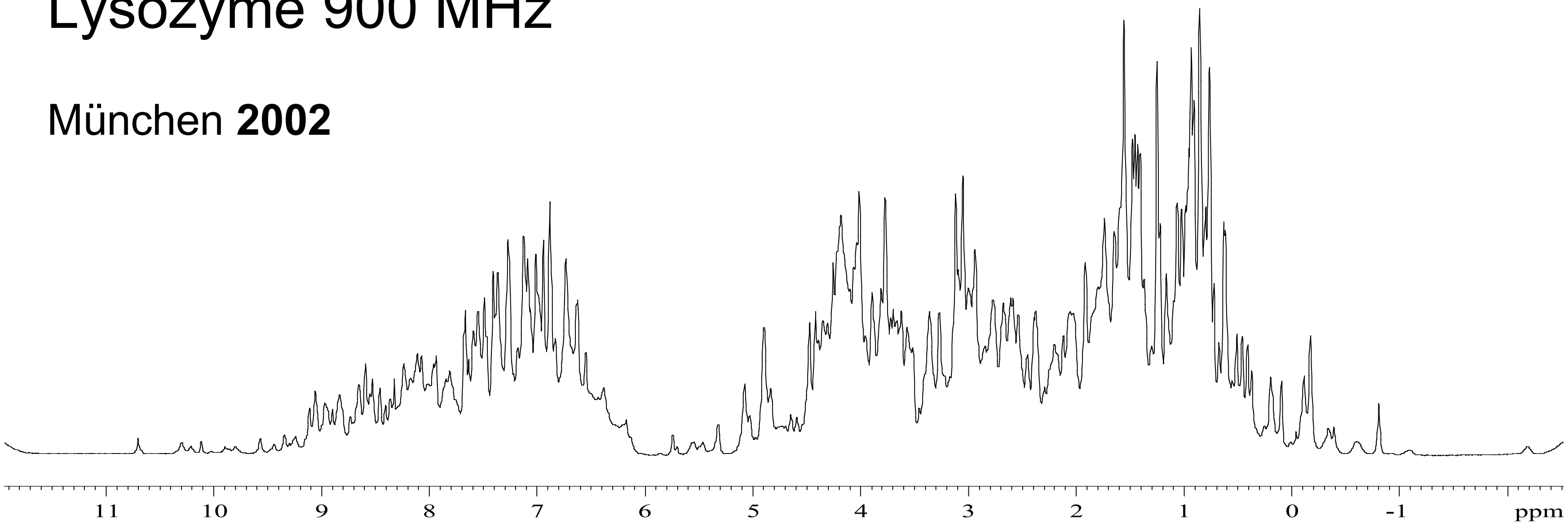


Ribonuclease 40 MHz

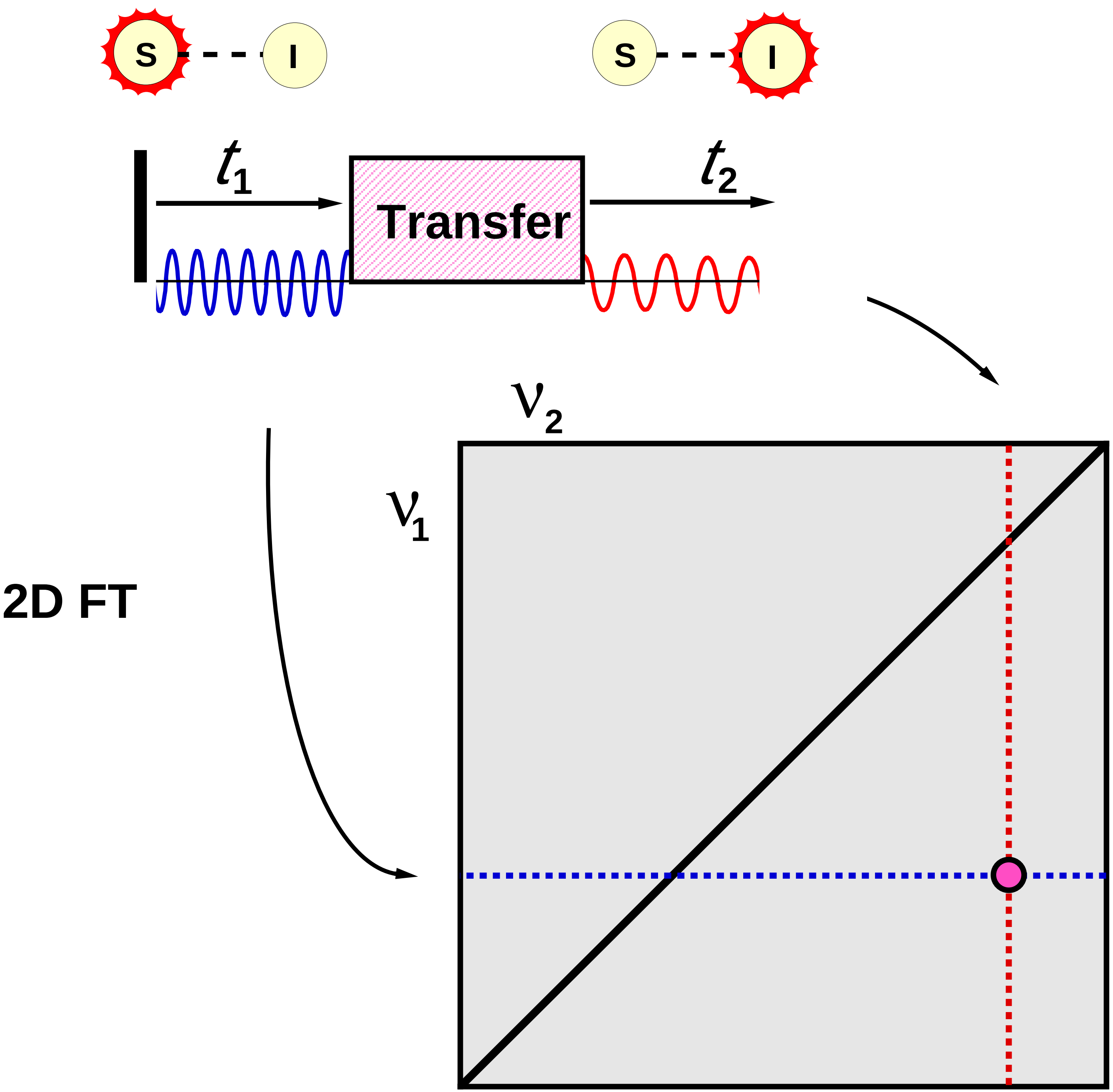
M. Saunders et al.
J.Amer.Chem.Soc. **1957**, *79*, 3289

Lysozyme 900 MHz

München **2002**

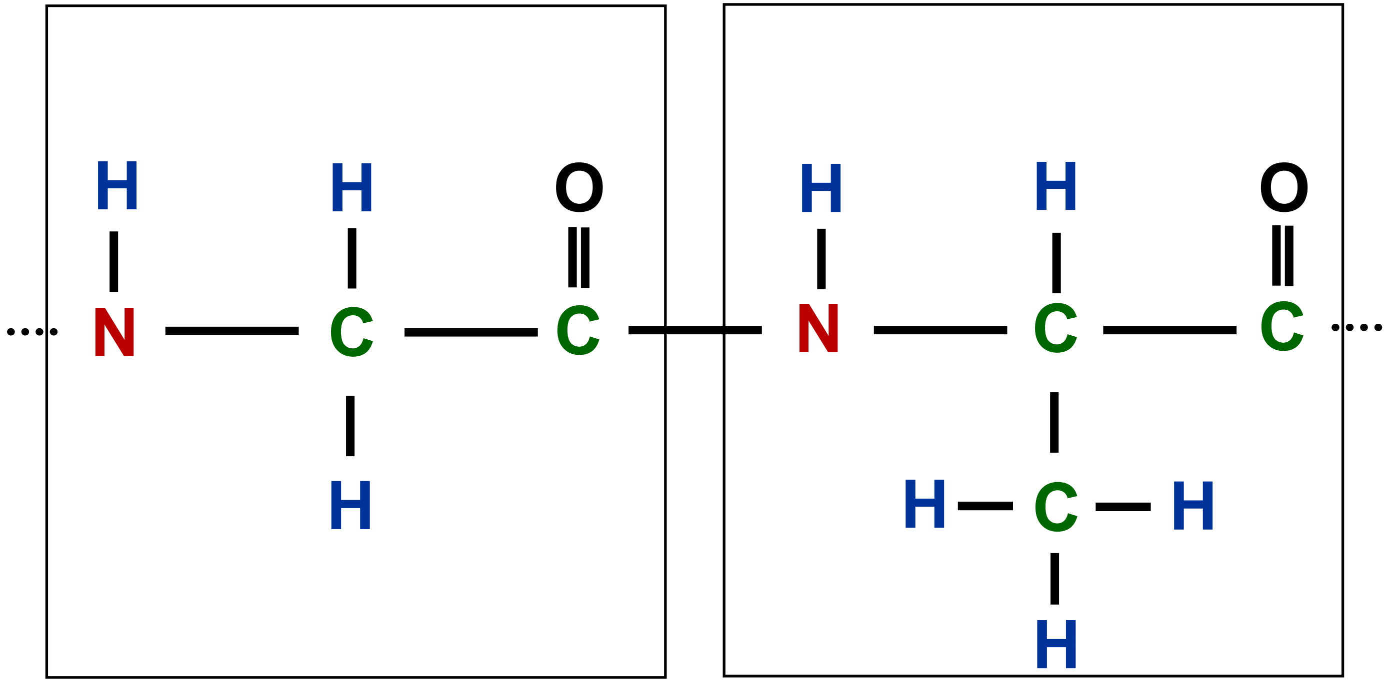


2D NMR

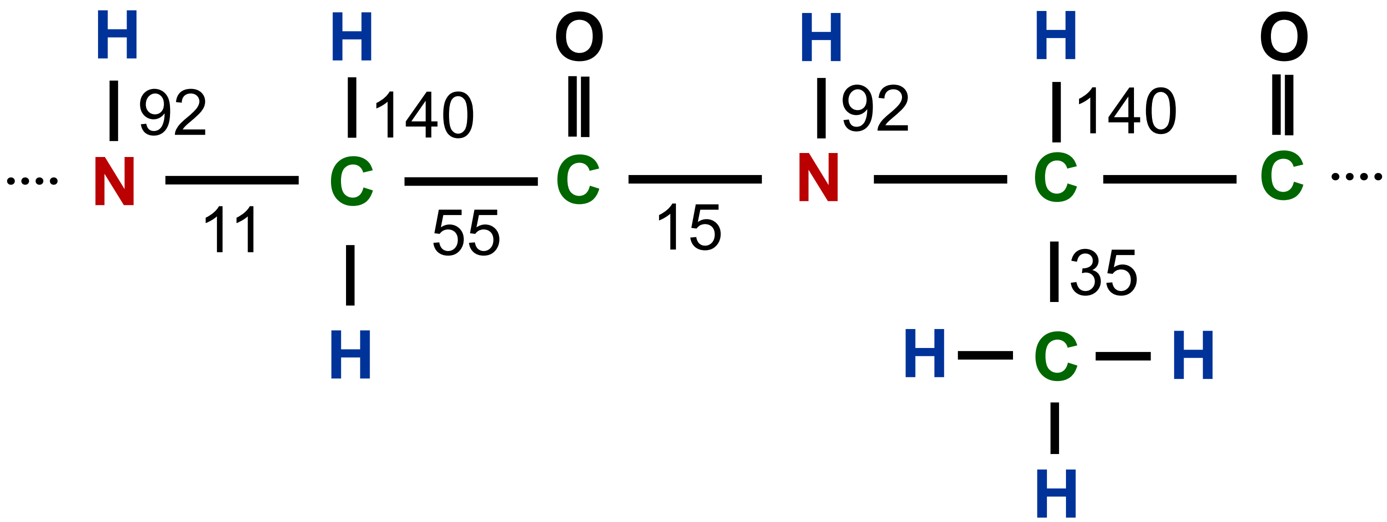


Resonance frequencies at 14 Tesla:

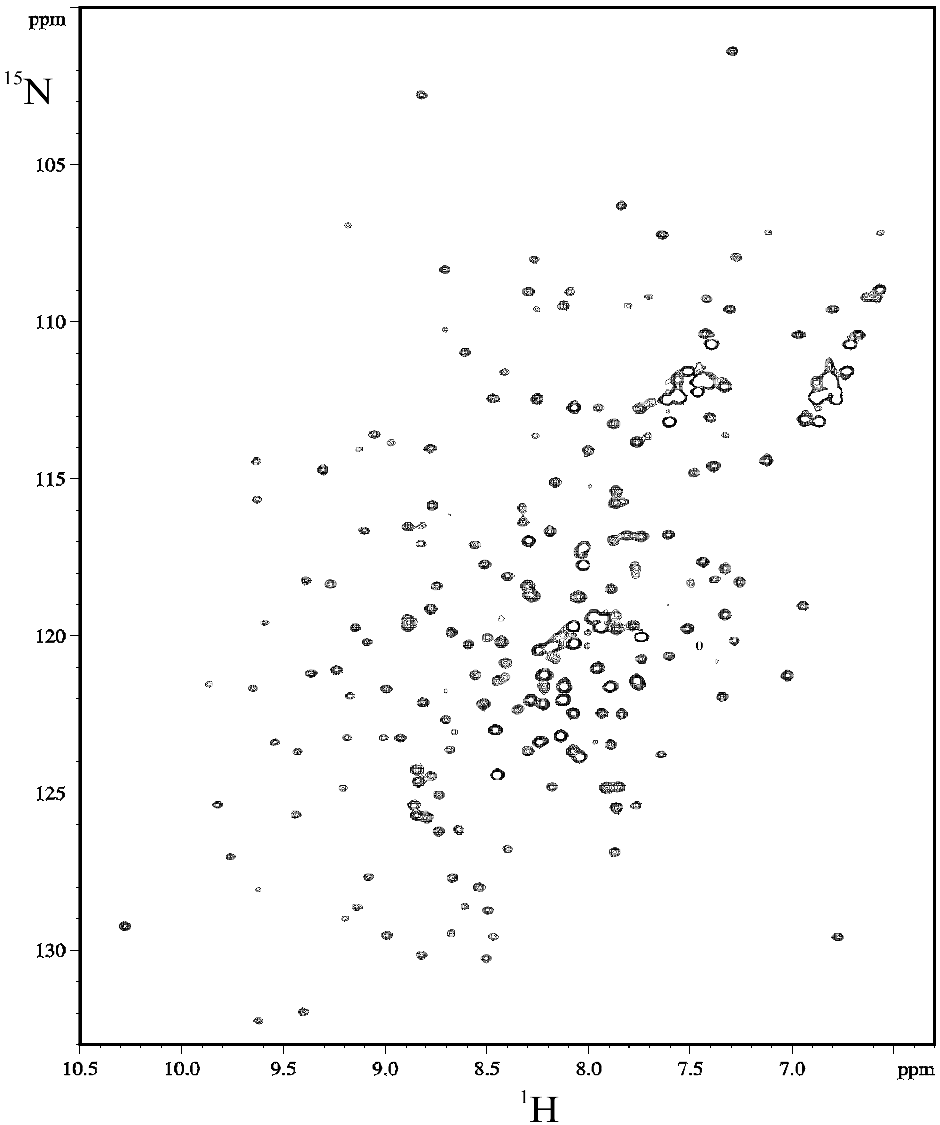
^{1}H	600 MHz
^{15}N	60 MHz
^{13}C	150 MHz



typical J couplings [Hz]



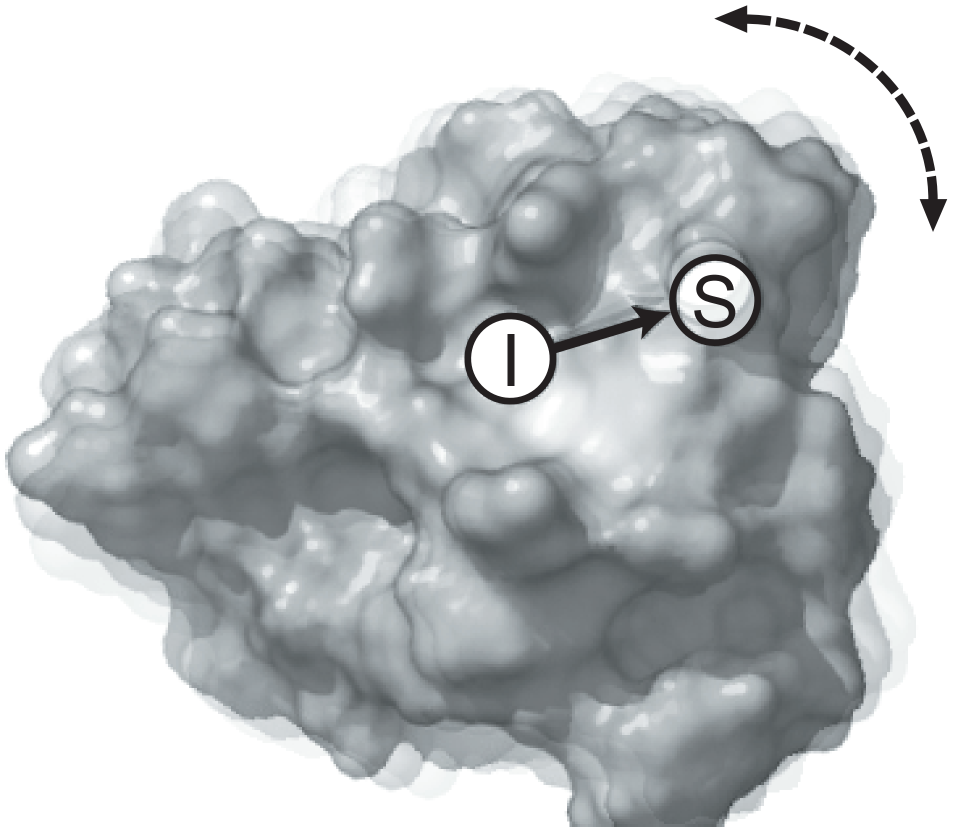
Example: ^{15}N-HSQC of p63



^{15}N labeling:

- all N atoms replaced by ^{15}N (ca. 95 % ^{15}N),
- characteristic fingerprint spectrum
- p63: 233 a.a. / 27 kDa
- measured at 750 MHz / 303 K

Relaxation rates k increase with molecular weight



NMR quantum computing

2 qubits (1996) *Cory et al., Gershenfeld et al.*

3 qubits (1998) *Linden et al.*

5 qubits (2000) *Marx et al.*

7 qubits (2001) *Vandersypen et al.*

... (**?**)

Scaling problem: Creation of pseudo-pure states based on thermal density operator: exponential signal loss

Solutions: Quantum algorithms based on thermal desity operator

Myers, Fahmy, Glaser, Marx, Phys. Rev. A 63, 032302 (2001)

Creation of pure states (e.g. using para hydrogen)

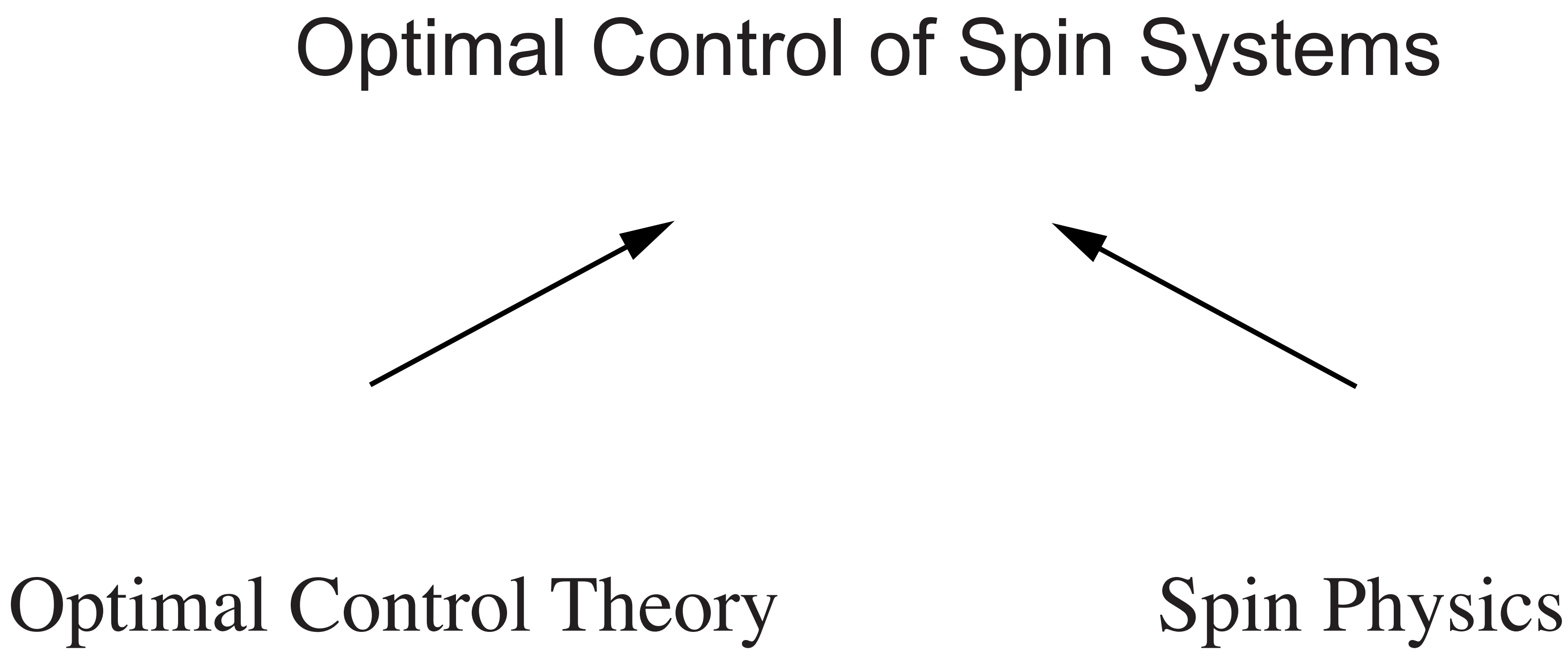
Hübler, Bargon, Glaser, J. Chem. Phys. 113, 2056 (2000)

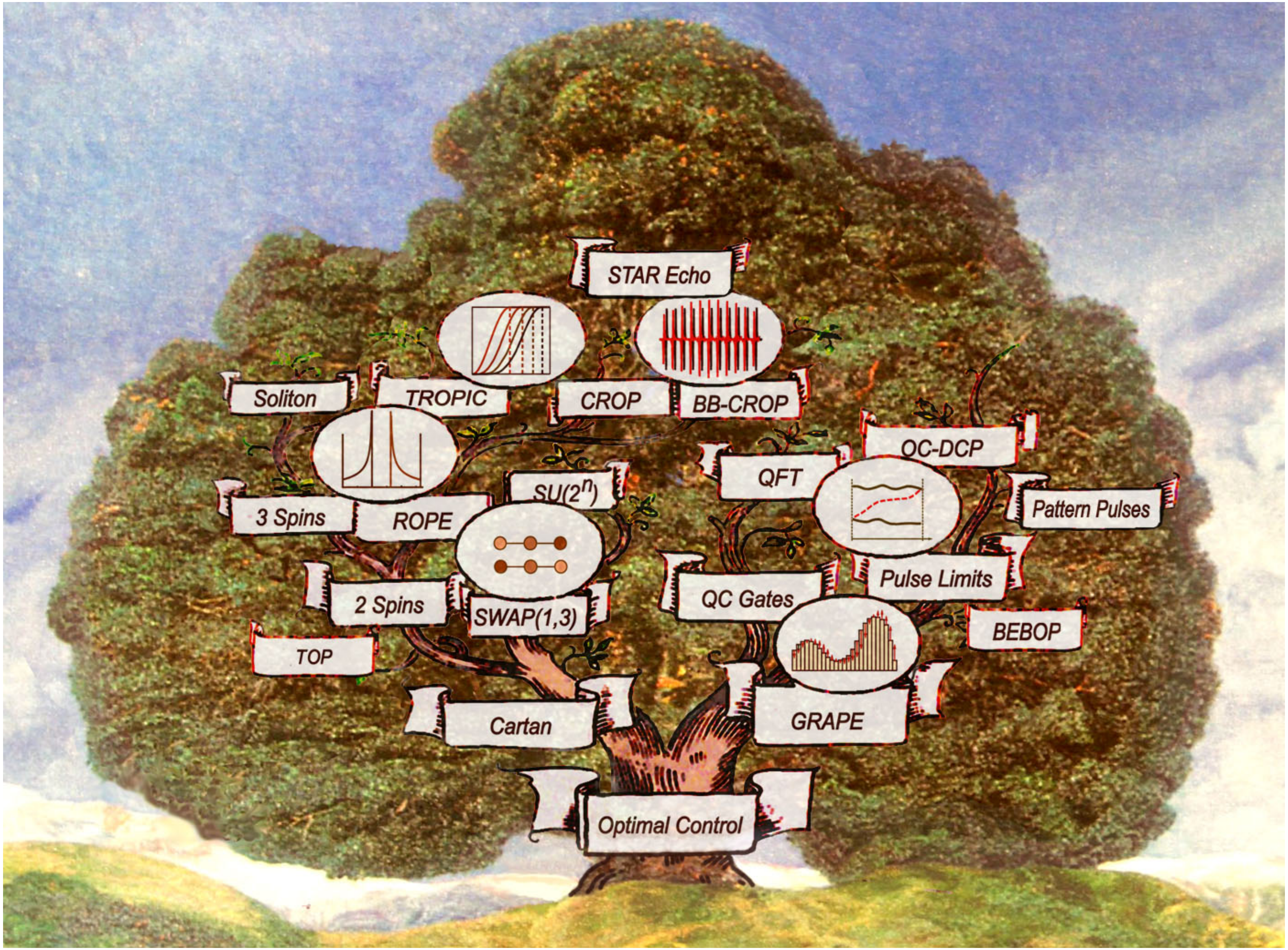
Practical problems: "hardware", molecules with suitable spin systems

"software", quantum algorithms

quantum "compilers"

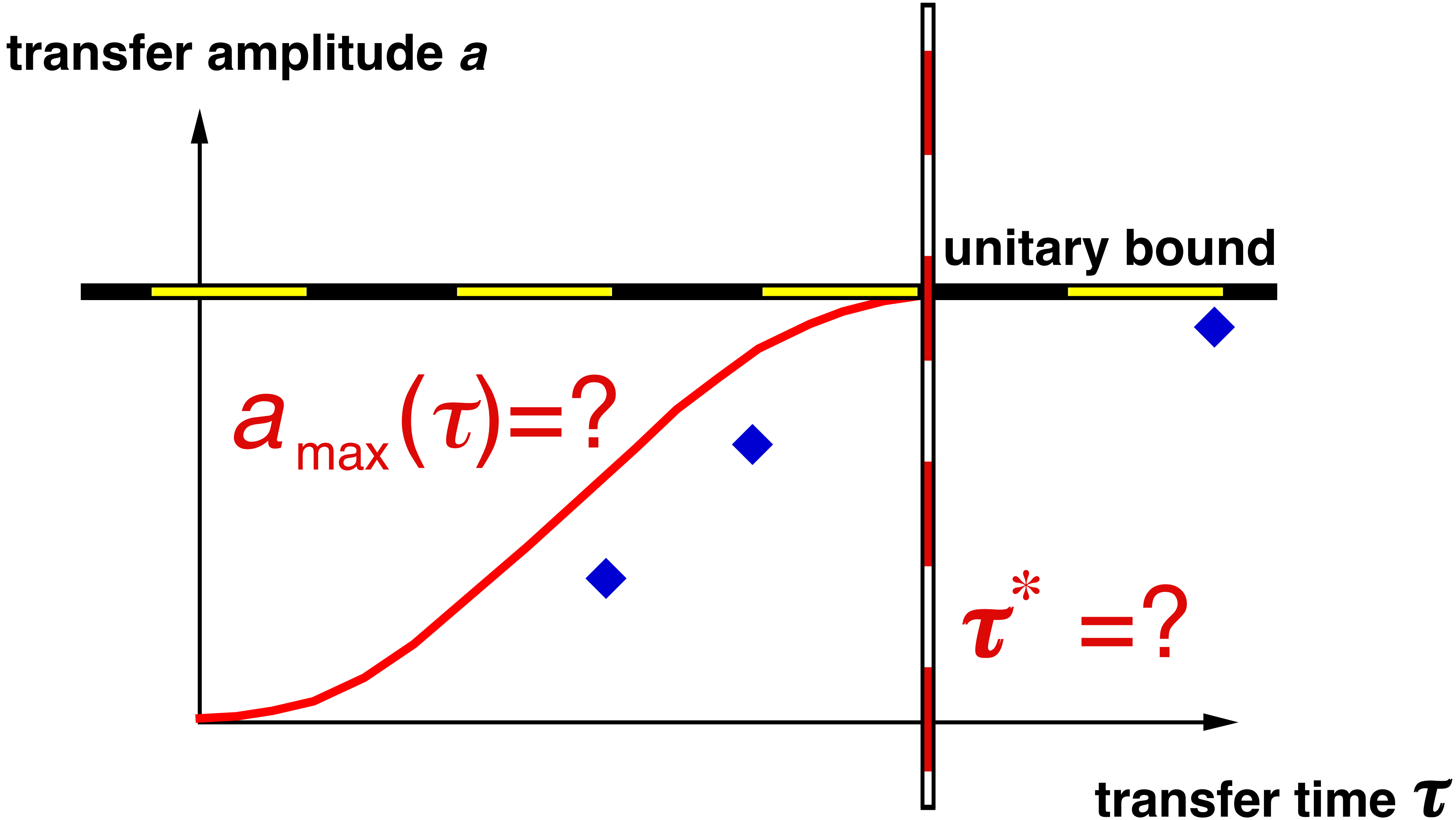
experimental imperfections, decoherence


Optimal Control of Spin Systems
Optimal Control Theory
Spin Physics

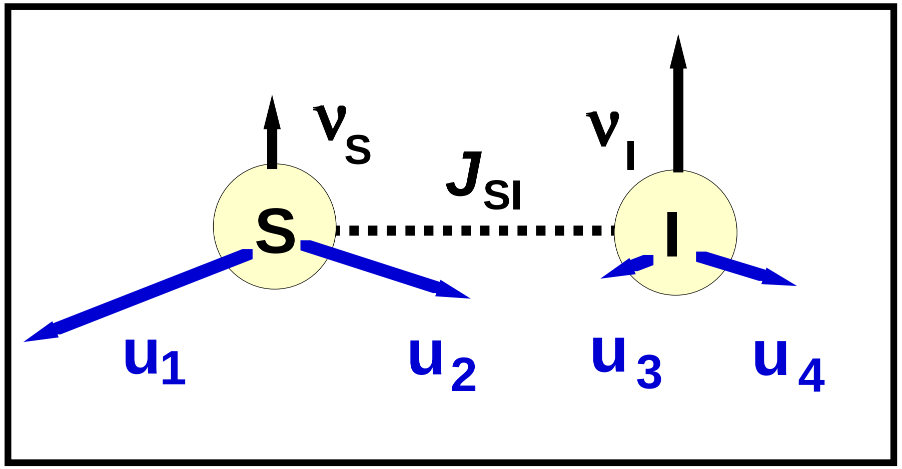

STAR Echo
Soliton
TROPIC
CROP
BB-CROP
OC-DCP
QFT
SU(2^n)
3 Spins
ROPE
Pattern Pulses
Pulse Limits
2 Spins
SWAP(1,3)
QC Gates
BEBOP
TOP
Cartan
GRAPE
Optimal Control

Time-optimal transfer

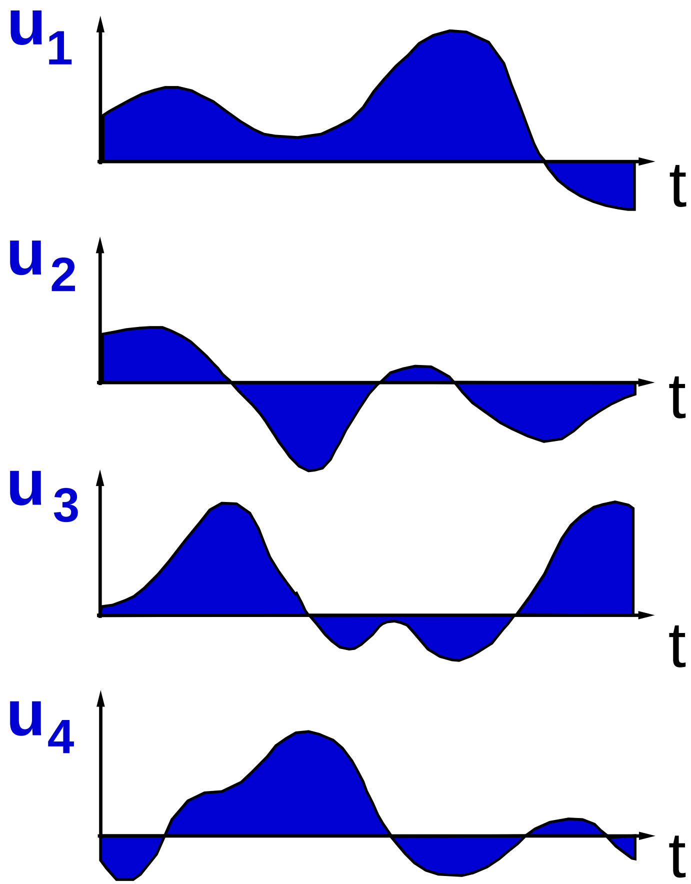
Unitary Quantum Evolution (no Relaxation)



Control Parameters $u_k(t)$



$$H_0 + \sum_k u_k(t)\, H_k$$



Time-Optimal Control of Two-Spin Systems

Strong-Pulse Limit: $H_{rf} >> H_C$ (2 time scales)

Cartan Decomposition

Characterization of ALL unitary operators
that can be created in time T

Derivation of - time-optimal transfer function (TOP curve)
- minimum time for maximum transfer
- pulse sequence

Khaneja, Brockett, Glaser (2001)

Khaneja, Kramer, Glaser (2005)

Propagators $U(t)$ that can be synthesized in time t

given: general coupling term

$$\mathcal{H}_c = 2\pi C(\mu_1 I_x S_x + \mu_2 I_y S_y + \mu_3 I_z S_z)$$

Theorem (Khaneja 2000): $U(t) = K_1 A(t) K_2$

K_1 and K_2 are local unitary transformations

$A(t) = \exp\{-\mathrm{i}2\pi Ct(\alpha I_x S_x + \beta I_y S_y + \gamma I_z S_z)\}$

(α, β, γ) in the convex cone generated by

(μ_1, μ_2, μ_3), $(\mu_1, -\mu_2, -\mu_3)$, $(-\mu_1, -\mu_2, \mu_3)$, $(-\mu_1, \mu_2, -\mu_3)$, ...

Maximum transfer efficiency $\eta^*(t)$ and minimum time $t_{\min}$ for complete transfer

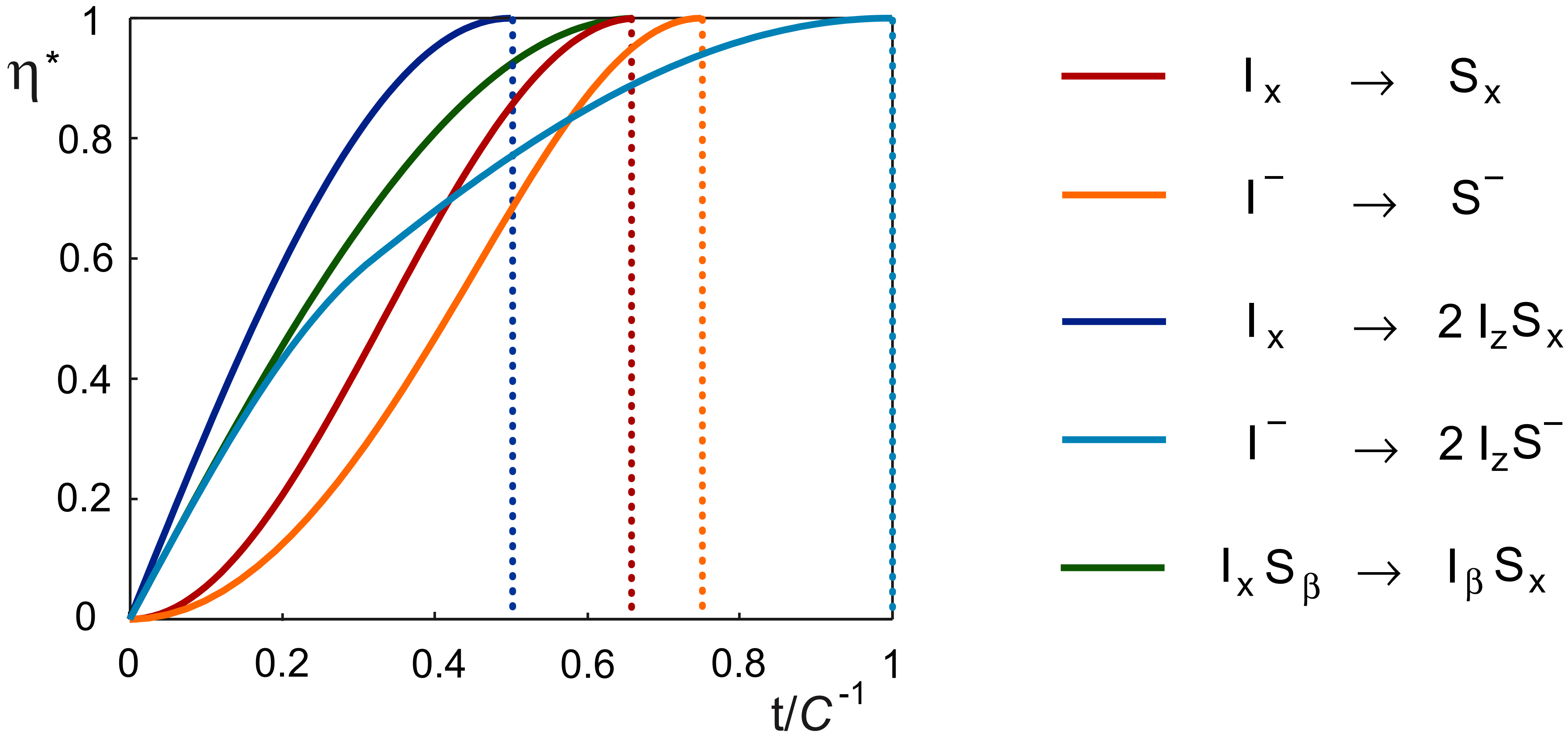
Transfer	$\eta^*(t)$	$t_{\min}^{-1}$
$I_x \rightarrow S_x$	$\sin^2(\frac{\pi}{2}C(\lvert\mu_3\rvert + \lvert\mu_2\rvert)t)$	$C(\lvert\mu_3\rvert + \lvert\mu_2\rvert)$
$I^- \rightarrow S^-$	$\sin(\pi C a)\sin(\pi C b)$	$\frac{2}{3}C(\lvert\mu_3\rvert + \lvert\mu_2\rvert + \lvert\mu_1\rvert)$
$I_x \rightarrow 2I_zS_x$	$\sin(\pi C\lvert\mu_3\rvert t)$	$2C\lvert\mu_3\rvert$
$I^- \rightarrow 2I_zS^-$	$\max_x \sin(\frac{\pi}{2}C\{\lvert\mu_3\rvert + \lvert\mu_2\rvert - \lvert\mu_1\rvert + x\}t)\cos(\pi C t x)$	$C(\lvert\mu_3\rvert + \lvert\mu_2\rvert - \lvert\mu_1\rvert)$
$I_xS_\beta \rightarrow I_\beta S_x$	$\sin(\frac{\pi}{2}C(\lvert\mu_3\rvert + \lvert\mu_2\rvert)t)$	$C(\lvert\mu_3\rvert + \lvert\mu_2\rvert)$
$I^-S_\beta \rightarrow I_\beta S^-$	$\sin(\frac{\pi}{2}C(\lvert\mu_3\rvert + \lvert\mu_2\rvert)t)$	$C(\lvert\mu_3\rvert + \lvert\mu_2\rvert)$

Note: $I^- = I_x - \mathrm{i}I_y$ and $I_\beta = \frac{\mathbf{1}}{2} - I_z$. For the transfer $I^- \rightarrow S^-$, the optimal values of a and b are completely characterized by the two conditions $a + 2b = (\lvert\mu_3\rvert + \lvert\mu_2\rvert + \lvert\mu_1\rvert)\,t$ and $\tan(\pi C a) = 2\tan(\pi C b)$.

Khaneja, Kramer, Glaser (2005)

TOP (time-optimal pulse) curves for dipolar coupling

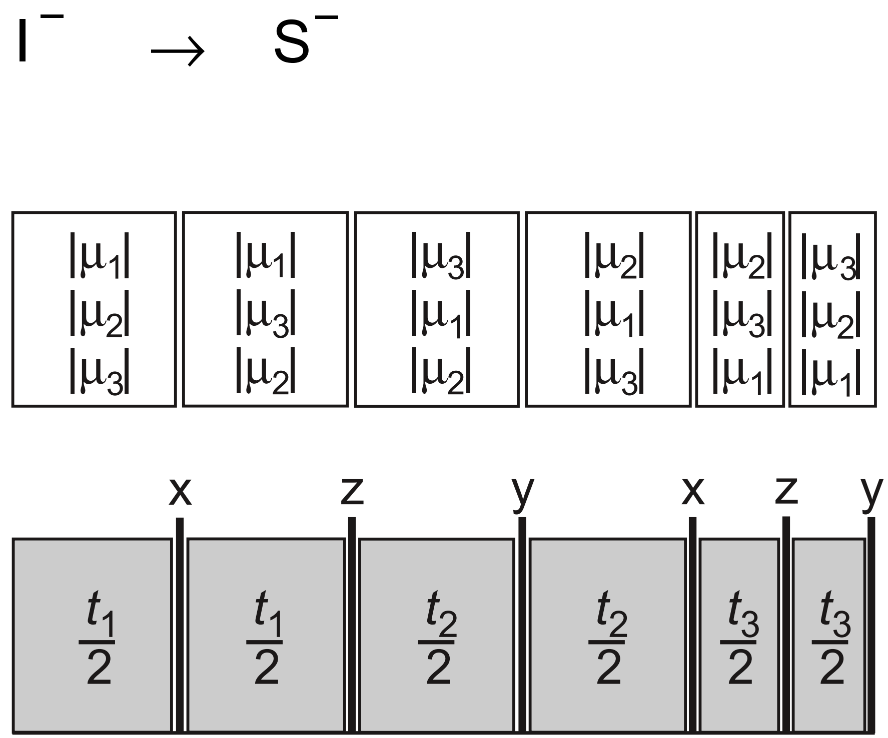
$$(\mu_1, \mu_2, \mu_3) = (-1/2,\ -1/2,\ 1)$$



Khaneja, Kramer, Glaser (2005)

Optimal sequence of effective Hamiltonians

Pulse sequences



Optimal durations t_1, t_2, t_3 for a given

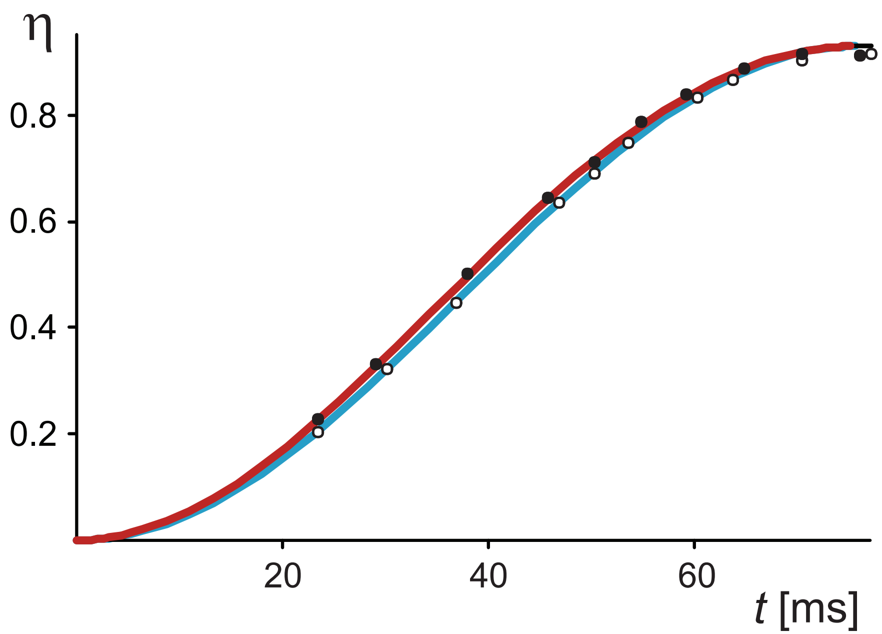
transfer time $t = t_1 + t_2 + t_3$

$$t_1 = t_2 \quad \text{and} \quad \tan(\pi C a) = 2\,\tan(\pi C b)$$

$$\text{with } a = (|\mu_2| + \mu_3|)t_2 + |\mu_1| t_3$$

$$b = (|\mu_2| + \mu_3|)(t_2 + t_3)/2 + |\mu_1| t_2$$

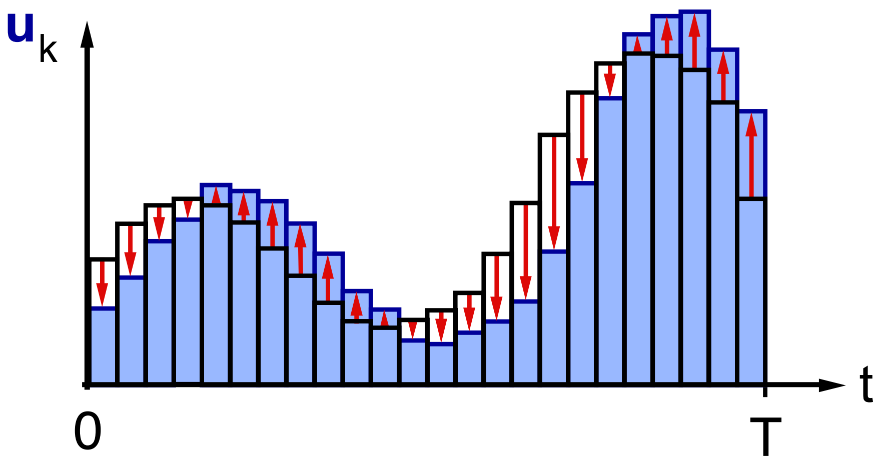
TOP (time optimal pulse) curve



Model system:
Cytosine in liquid crystal
C=10.8 Hz
μ_1=0.03, μ_2=0.88, μ_3=0.88

Khaneja, Kramer, Glaser (2004)

GRAPE (Gradient Ascent Pulse Engineering)



desired transfer: $A \longrightarrow C$

performance: $\langle C \mid \rho(T) \rangle$

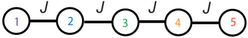
$\rho(0) = A$

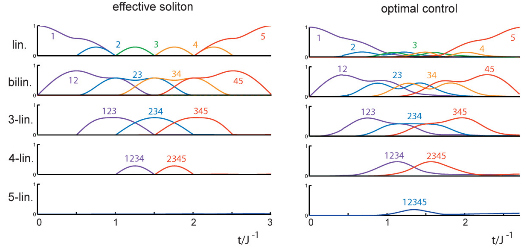
$\lambda(T) = C$

$$\mathbf{u}_k(t) \longrightarrow \mathbf{u}_k(t) + \varepsilon \left\langle \lambda(t) \middle| [-i\, H_k, \rho(t)] \right\rangle$$

Khaneja, Reiss, Kehlet, Schulte-Herbrüggen, Glaser, J. Magn. Reson. 172, 296-305 (2005)

Time-optimal $I_1^- \rightarrow I_n^-$ transfer along Ising spin chains

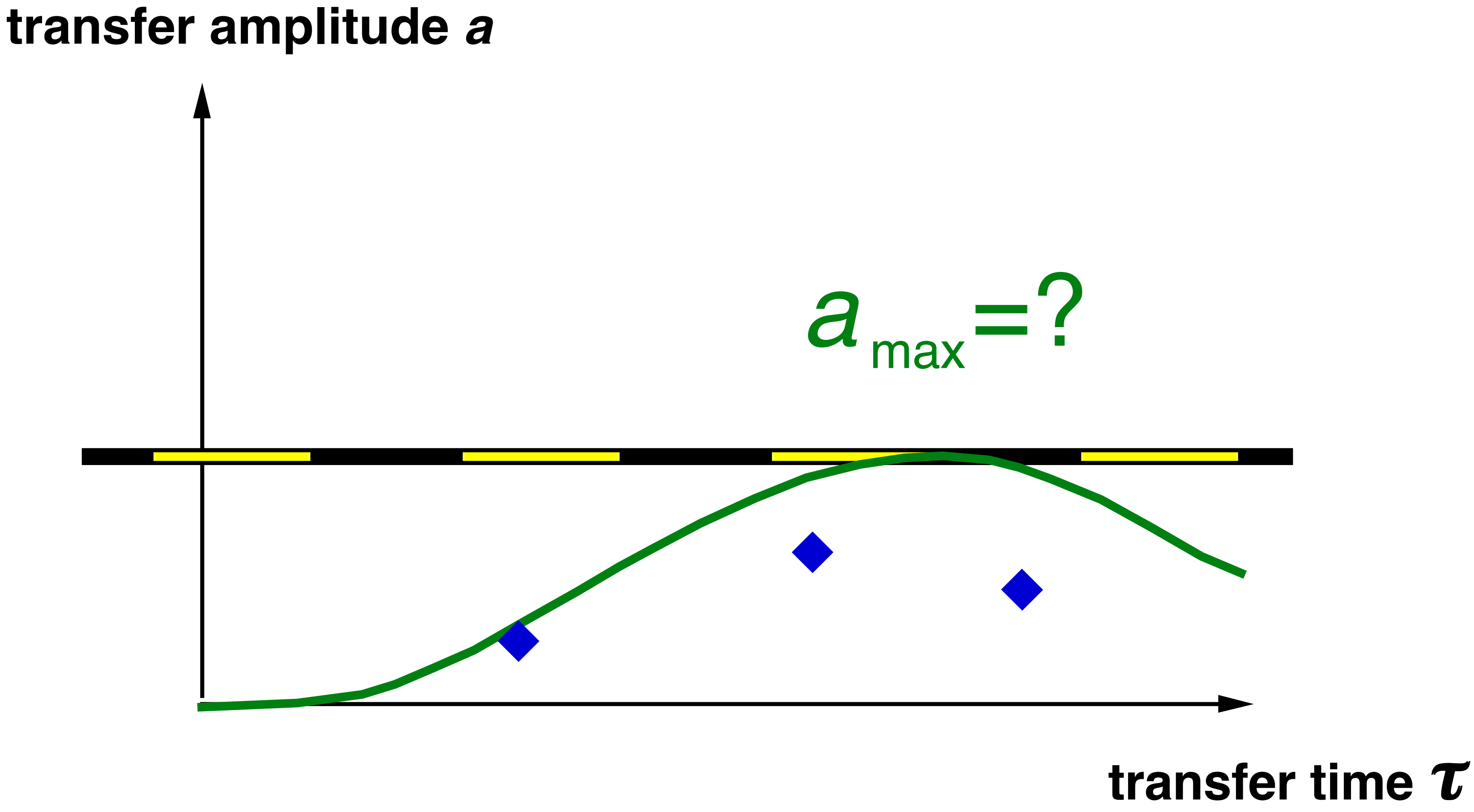


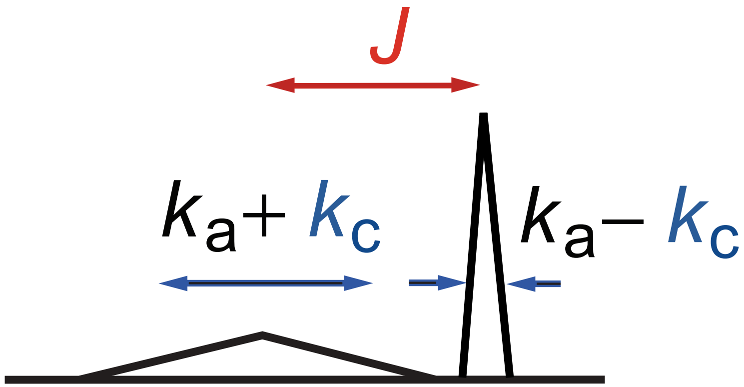


Khaneja, Glaser (2002)

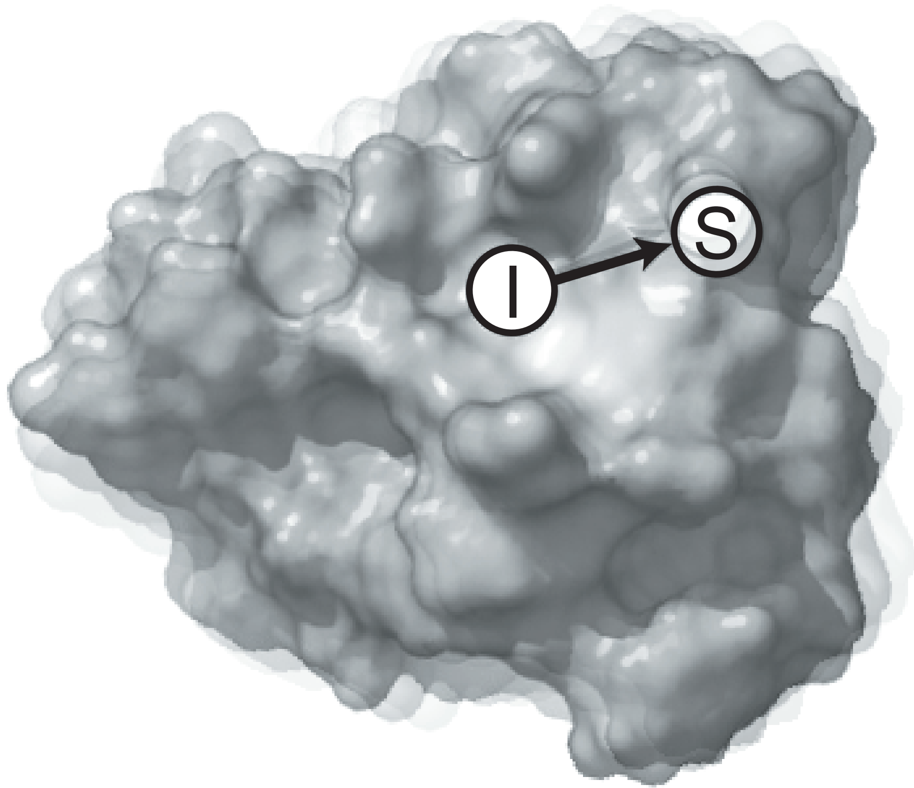
Relaxation-optimized transfer

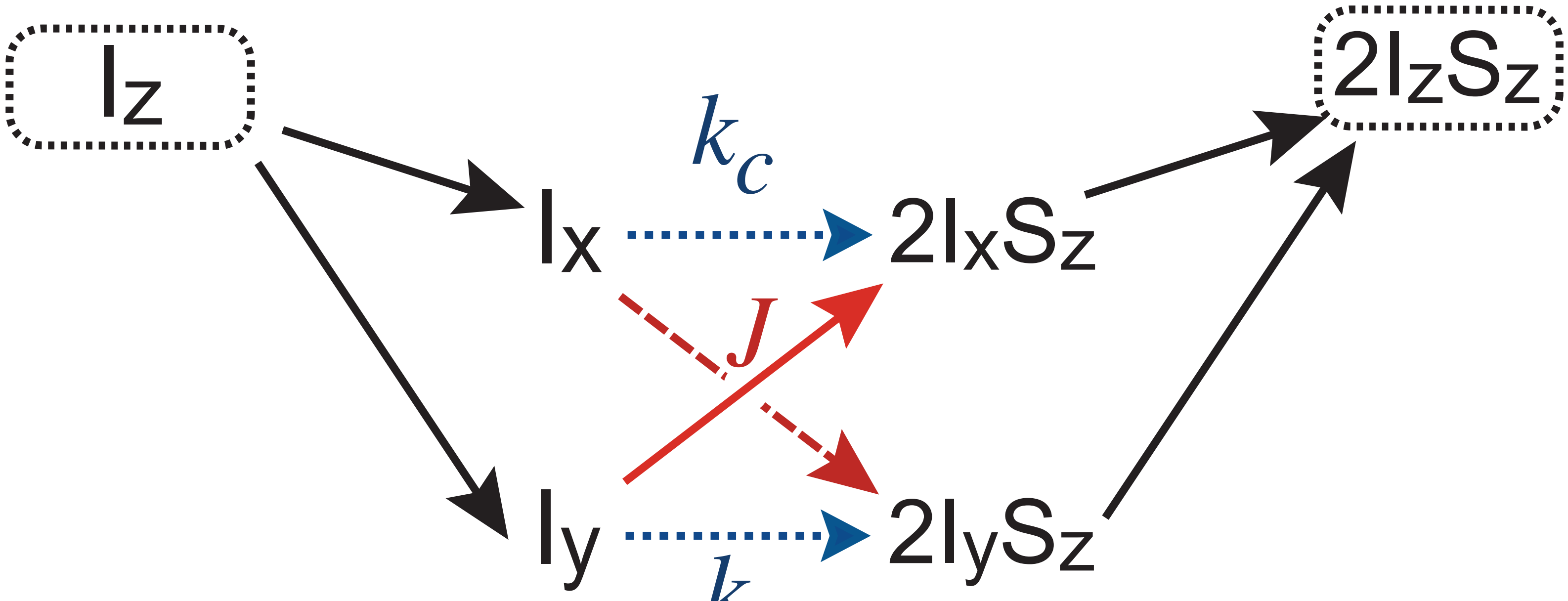
Quantum Evolution in Presence of Relaxation





Multiplet of Spin I




Iz
Ix
Iy
kc
kc
J
2IxSz
2IySz
2IzSz

Optimal transfer efficiency η from I_z to $2 I_z S_z$:

$$\eta = \sqrt{1 + \xi^2} - \xi$$

with $\xi^2 = \frac{k_a^2 - k_c^2}{J^2 + k_c^2}$

Khaneja, Luy, Glaser, *Proc. Natl. Acad. Sci.* (2003)

maximum transfer efficiency:

$$\eta = \sqrt{1 + \xi^2} - \xi$$

formal proof (based on principles of optimum control theory):

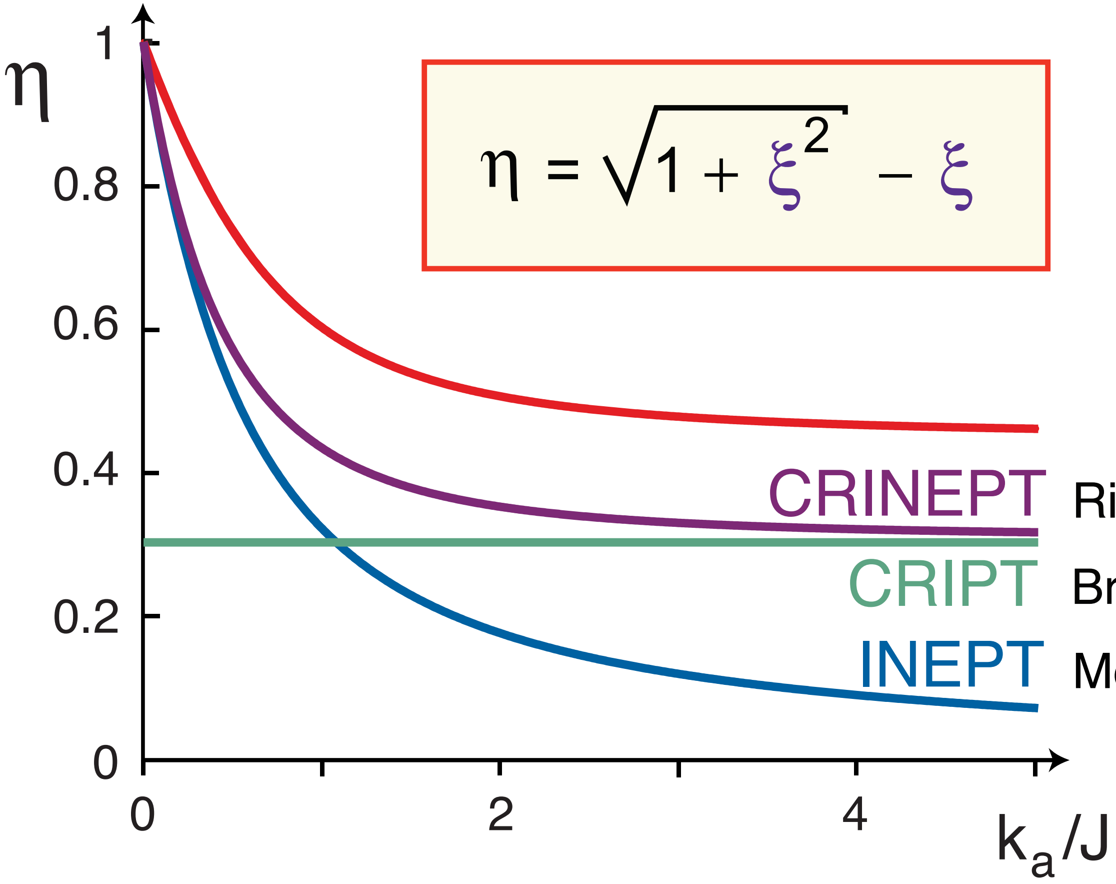
optimal return function $V(r_1, r_2)$

Hamilton-Jacobi-Bellman equation

$$\max_{u_1, u_2} \left[\frac{\partial V}{\partial r_1} \delta r_1 + \frac{\partial V}{\partial r_2} \delta r_2 \right] = 0$$

Transfer Efficiency η for $k_c / k_a = 0.75$

$$\eta = \sqrt{1 + \xi^2} - \xi$$

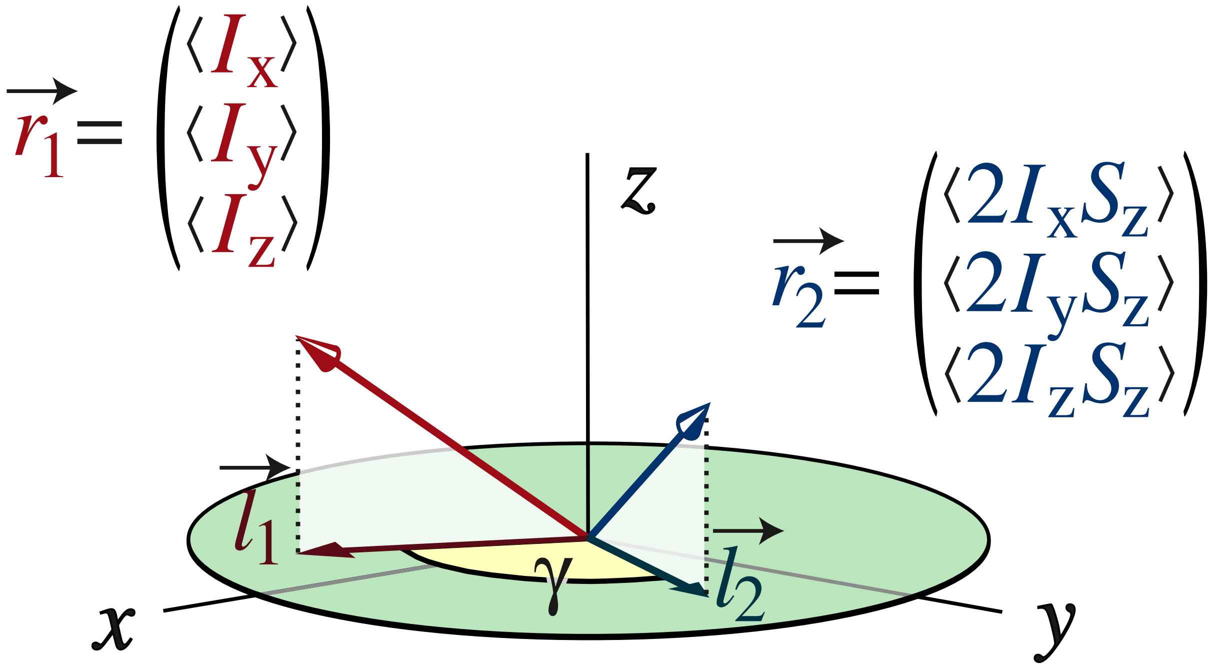


CRINEPT Riek, Wider, Pervushin, Wüthrich (1999)

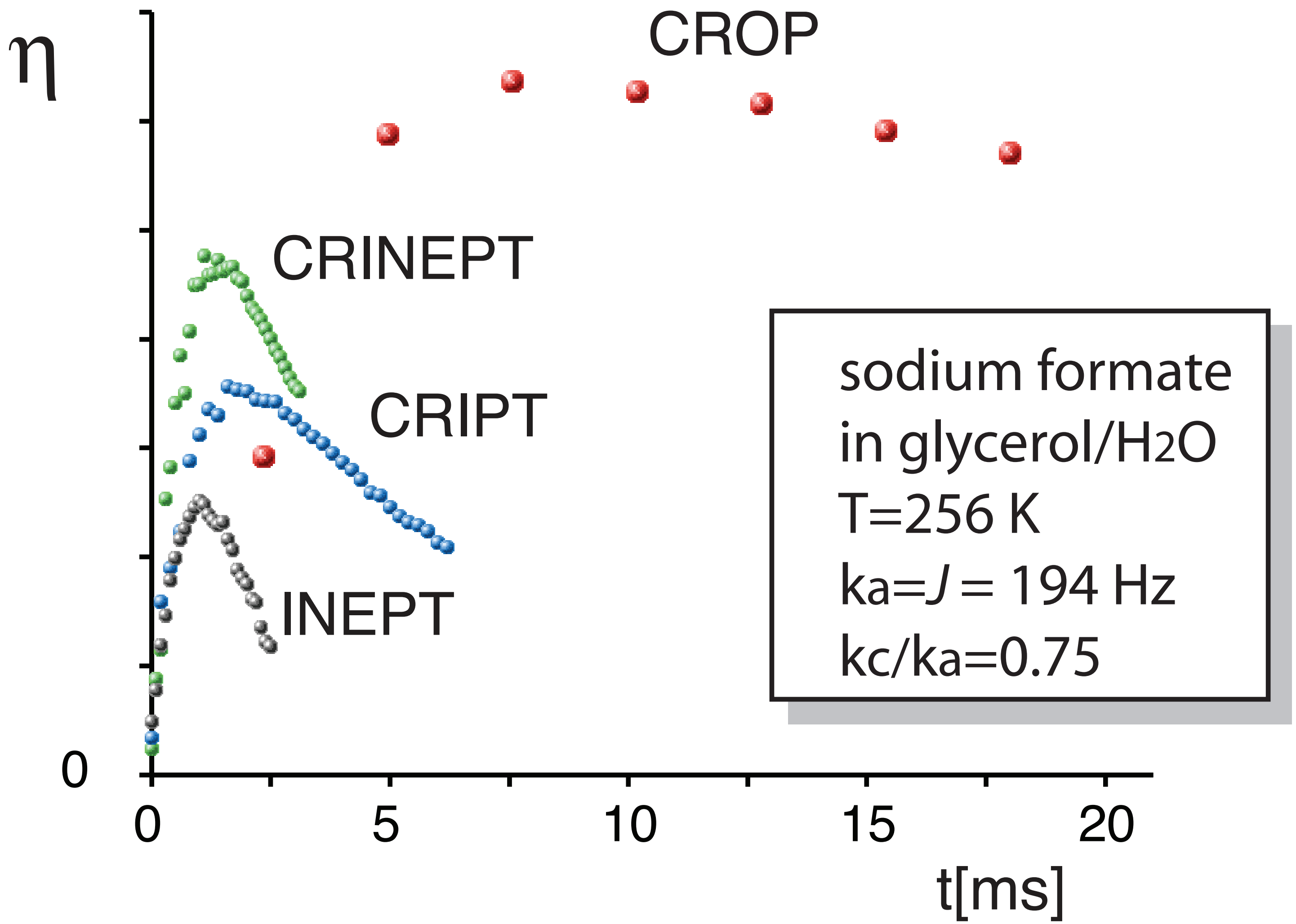
CRIPT Brüschweiler, Ernst (1992)

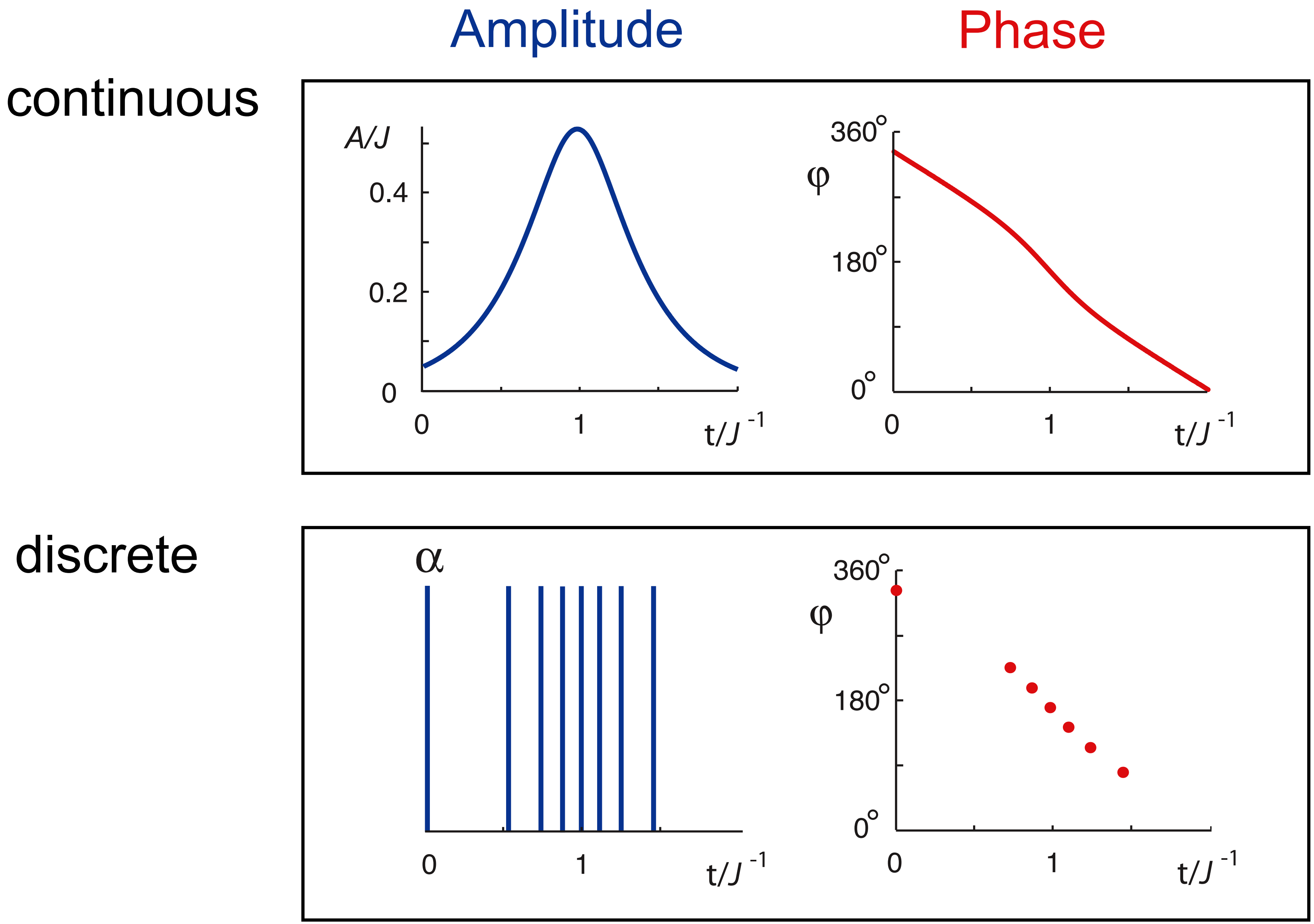
INEPT Morris, Freeman (1979)

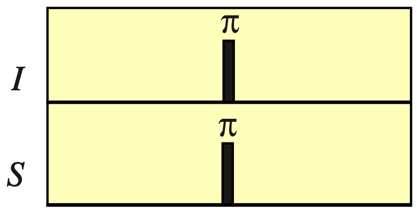
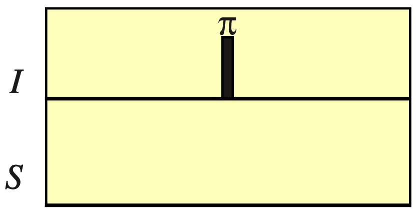
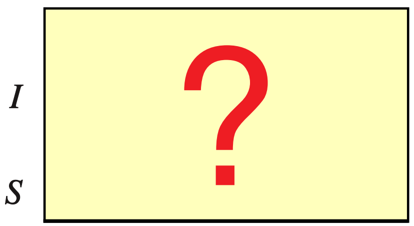
Optimal trajectory preserves ratio $\frac{l_2}{l_1} = \eta$ and angle γ



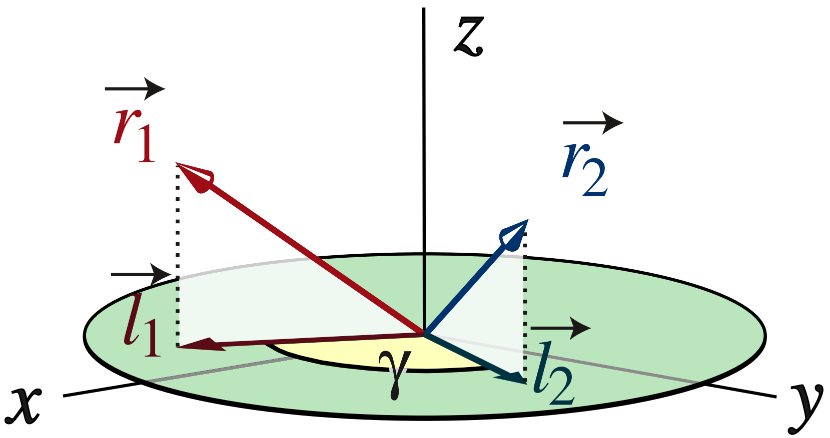
Experimental Transfer Functions

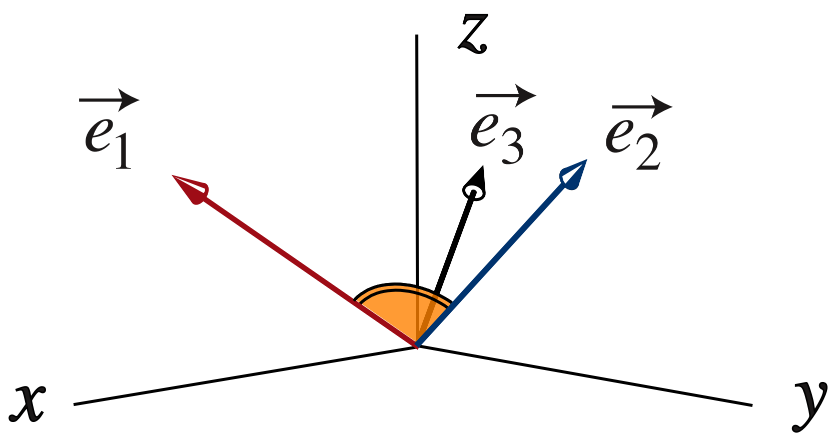



Amplitude
Phase
continuous
discrete
A/J
0.4
0.2
0
0
1
t/J -1
360°
180°
0°
φ
0
1
t/J -1
α
0
1
t/J -1
360°
180°
0°
φ
0
1
t/J -1

	chemical shift	J coupling	cross-correlated relaxation
	$H_{cs} \sim I_z$	$H_J \sim I_z S_z$	$k_c \sim [I_z,[I_z S_z, \rho]]$
	$\overline{H}_{cs} = 0$ ✓	$\overline{H}_J = H_J$ ✓	$\overline{k}_c = 0$ ↯
	$\overline{H}_{cs} = 0$ ✓	$\overline{H}_J = 0$ ↯	$\overline{k}_c = k_c$ ✓
	$\overline{H}_{cs} = 0$ ✓	✓	✓

Optimal trajectory preserves ratio $\frac{l_2}{l_1} = \eta$ and angle γ





time-dependent,

specific trajectory adapted

frame of reference

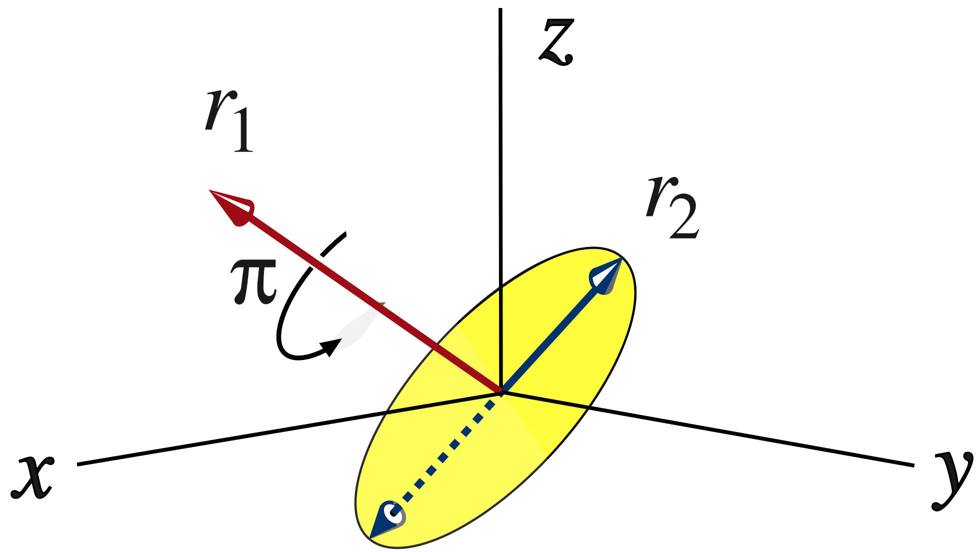
Trajectory adapted 180° rotations preserve

the ratio $\frac{l_1}{l_2}$ and the angle γ

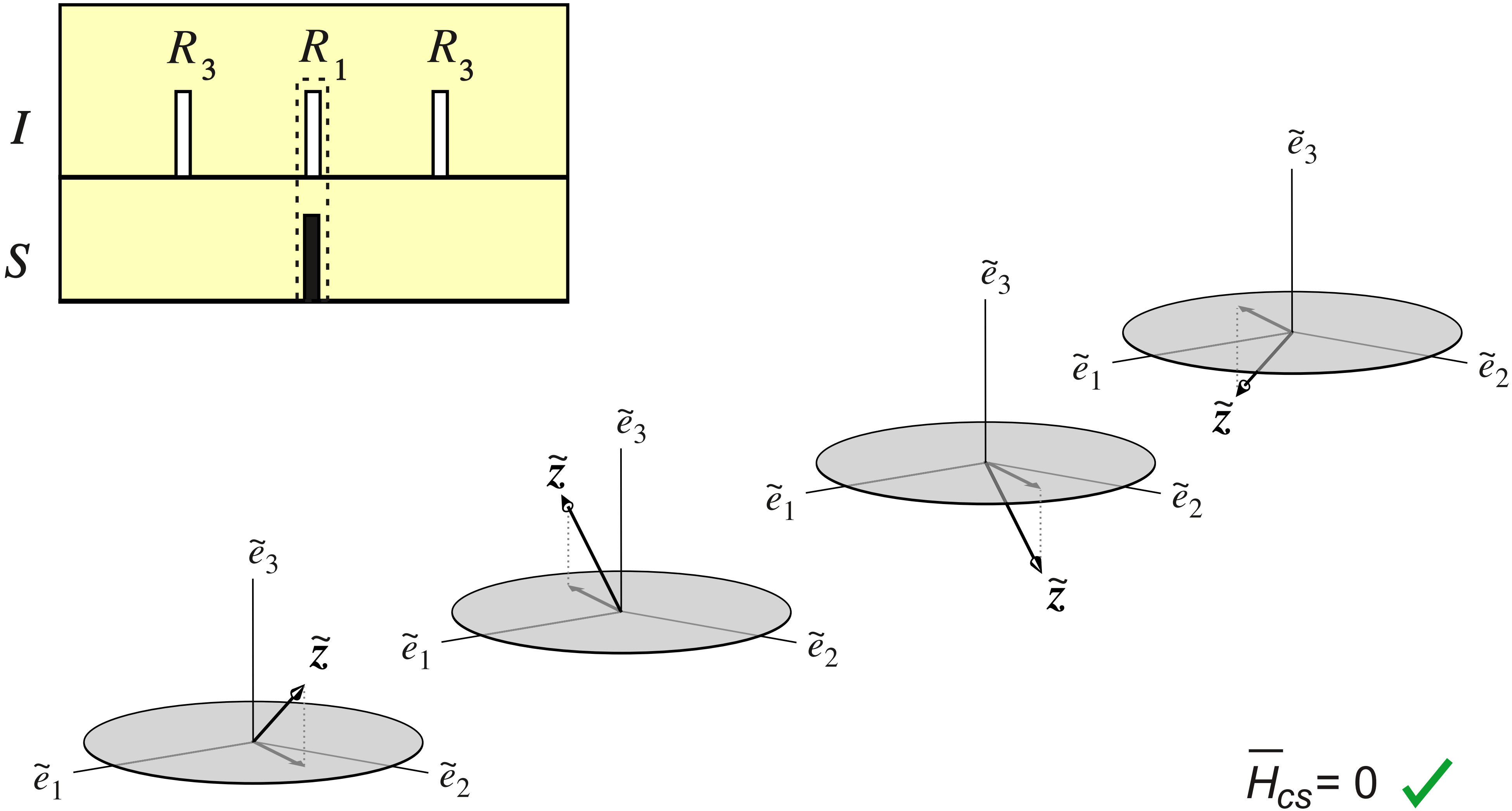
$$R_1 = \pi(\overrightarrow{e_1})\,\pi(S)$$

$$R_2 = \pi(\overrightarrow{e_2})\,\pi(S)$$

$$R_3 = \pi(\overrightarrow{e_3})$$



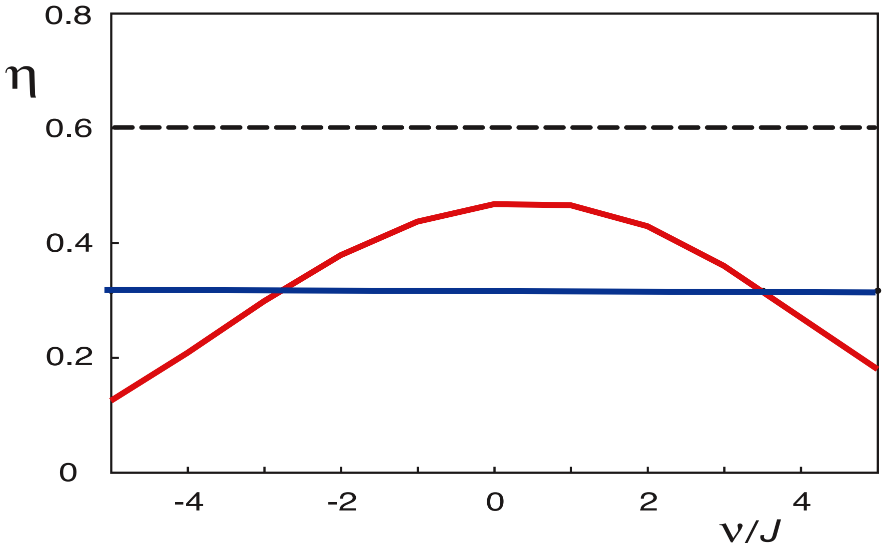
STAR Echo



$\overline{H}_{cs} = 0$ ✓

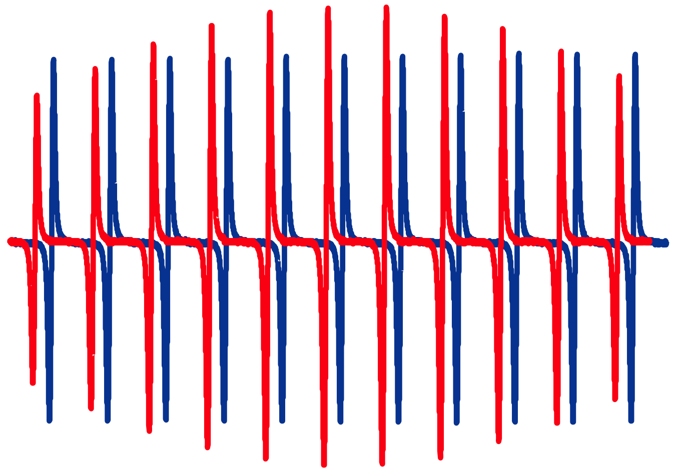
Model system: sodium formate in glycerol

Simulation



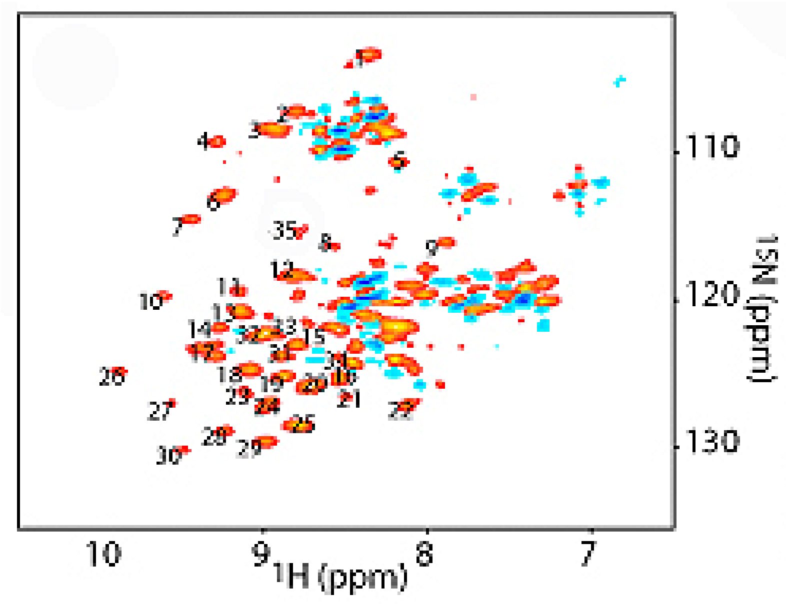
BB-CROP vs. INEPT

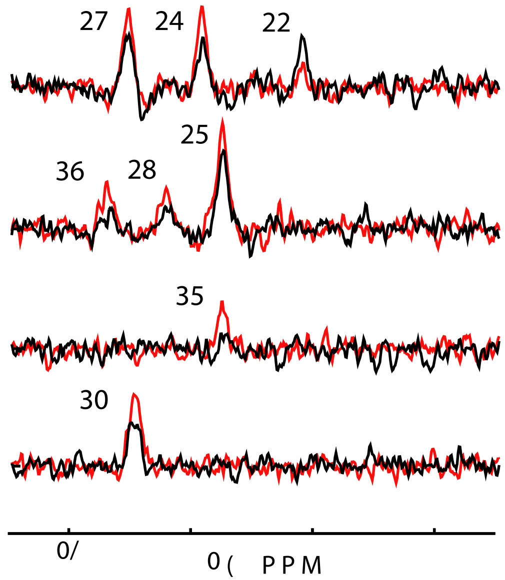
Experiment



(offset range: 1 kHz)

[^{15}N, ^{1}H]-TROPIC-TROSY of GroEL (800 kDa)

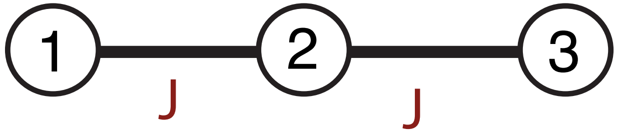




Früh, Ito, Li, Wagner, Glaser, Khaneja, J. Biomol. NMR (2005)

Time-optimal unitary transformations

Time-Optimal Simulation of Trilinear Coupling Terms



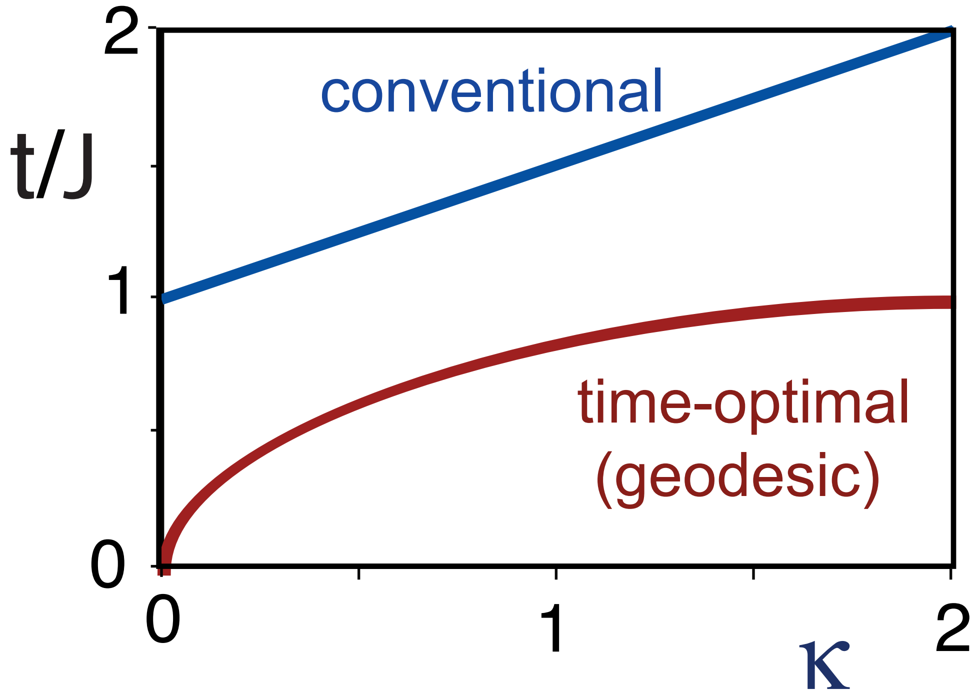
given:

$$H = 2\pi J\,(I_{1z} I_{2z} + I_{2z} I_{3z})$$

desired:

$$H_{eff} = 2\pi J_{eff}\,(I_{1z} I_{2z} I_{3z})$$

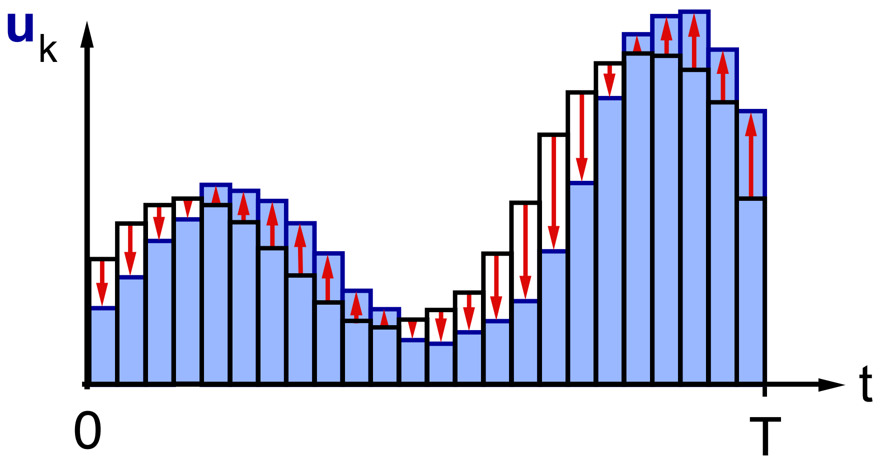
$$U = \exp\{-i\,\kappa\, 2\pi\, I_{1z} I_{2z} I_{3z}\}$$



Tseng, Somaroo, Sharf, Knill, Laflamme, Havel, Cory, Phys. Rev. A 61, 012302 (2000)

Khaneja, Glaser, Brockett, Phys. Rev. A 65, 032301 (2002)

GRAPE (Gradient Ascent Pulse Engineering)



desired propagator: U_F

performance: $\left| \langle U_F \,|\, U(T) \rangle \right|^2$

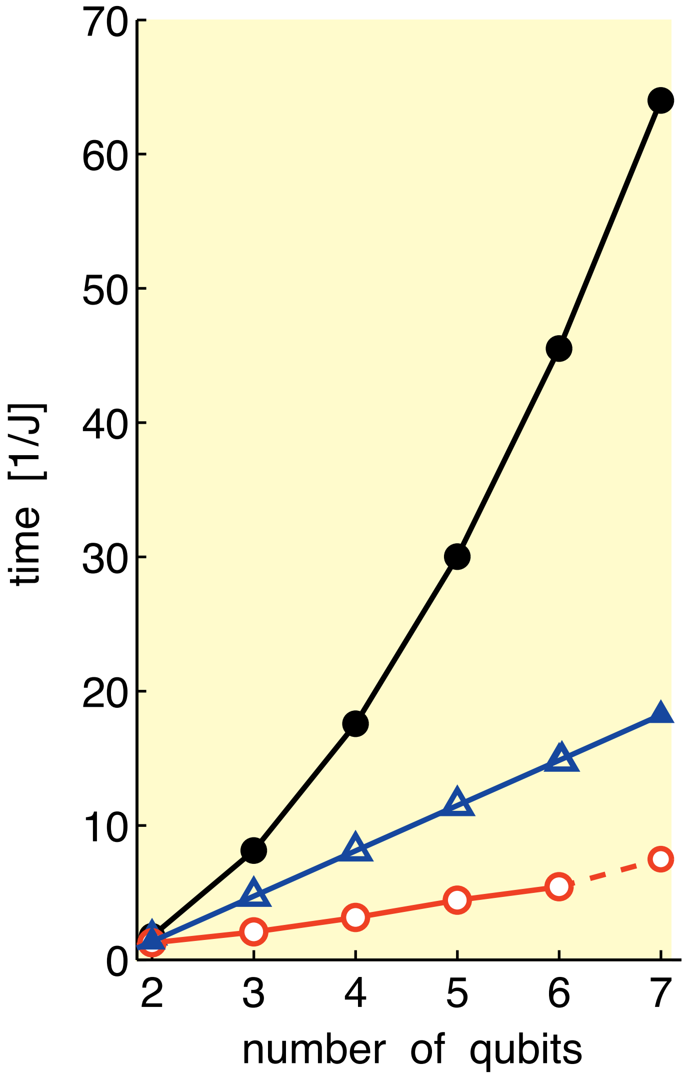
$U(0) = \mathbf{1}$

$P(T) = U_F$

$$u_k(t) \longrightarrow u_k(t) + \varepsilon \, Re \left\{ \langle P(t) \,|\, -i\, H_k U(t)] \rangle \langle U(t) \,|\, P(t)] \rangle \right\}$$

Khaneja, Reiss, Kehlet, Schulte-Herbrüggen, Glaser, J. Magn. Reson. 172, 296-305 (2005)

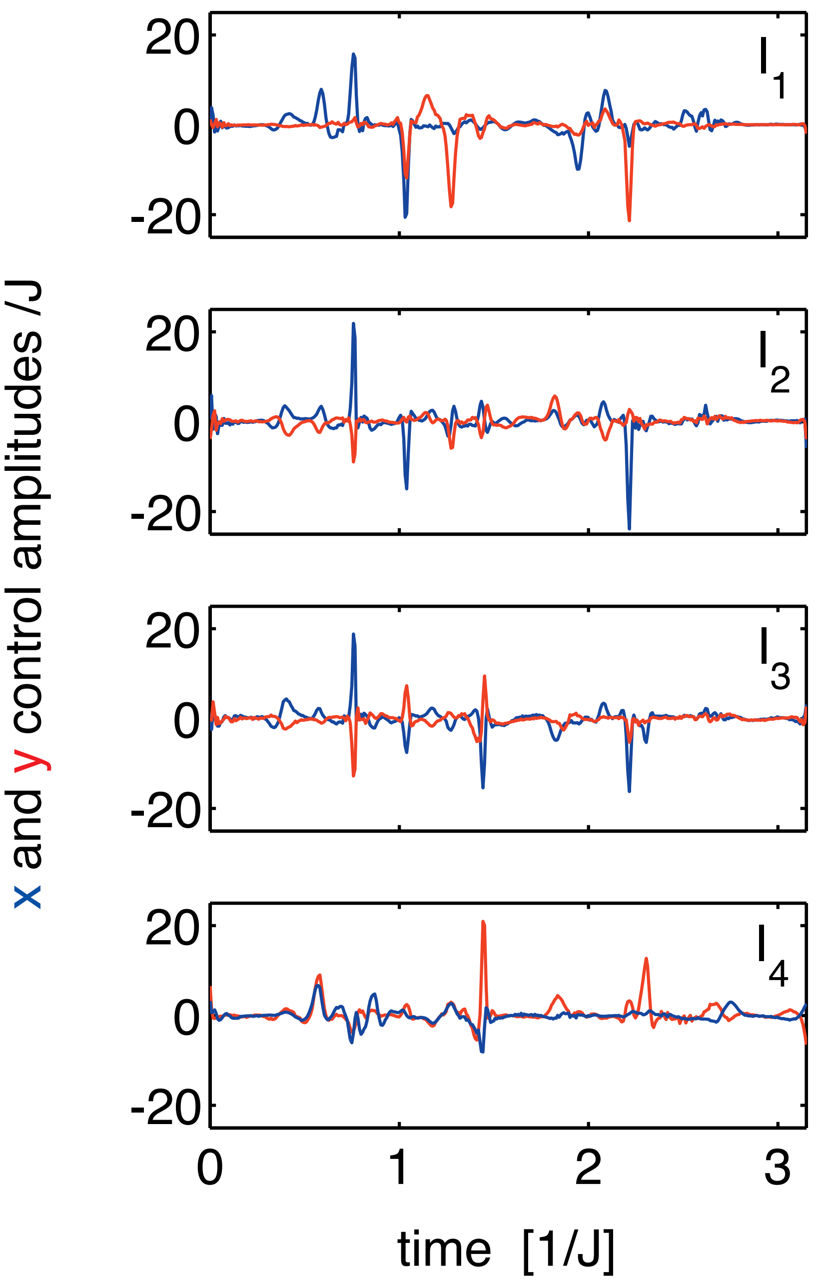
Time-optimal implementation of the quantum Fourier transform



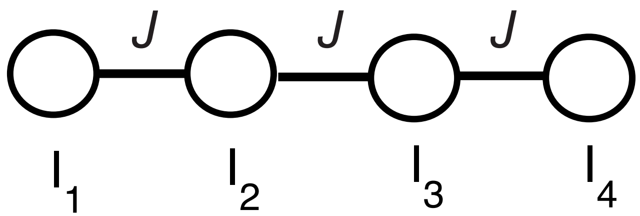
Saito et al. (2000)
quant-ph/0001113

Blais (2001)
PRA 64, 022312

Schulte-Herbrüggen et al. (2005)
quant-ph/0502104

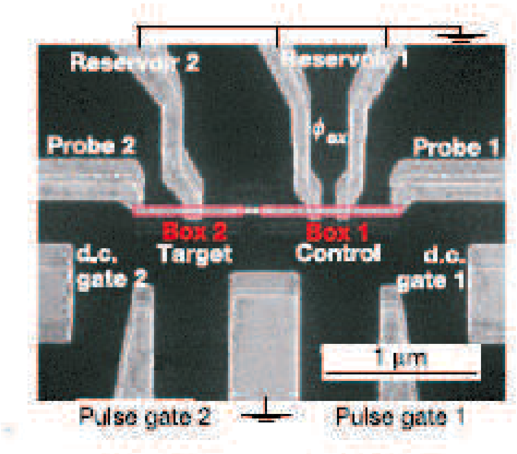


Pulse sequence for
time-optimal implementation
of the
quantum Fourier transform
for n=4 qubits



Schulte-Herbrüggen et al.
quant-ph/0502104

Quantum Gates for Coupled Josephson Charge Qubits



Pioneering "CNOT" by Yamamoto, Pashkin, Astaviev, Nakamura, Tsai

250 ps pulse duration for "CNOT":

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

Yamamoto et al., Nature 425, 2003

Makhlin et al., Rev. Mod. Phys. 73, 2001

Pseudo-Spin Hamiltonian for Coupled Josephson Qubits

$$H_{\text{drift}} = \boldsymbol{a}_1 I_{1z} + \boldsymbol{a}_2 I_{2z} + b_1 I_{1x} + b_2 I_{2x} + c\, I_{1z} I_{2z}$$

$$H_{\text{control}} = u_1 (\boldsymbol{d}_1 I_{1z} + c\, I_{2z}) + u_2 (\boldsymbol{d}_2 I_{2z} + c\, I_{1z})$$

gate charges u_k controlled via external voltages

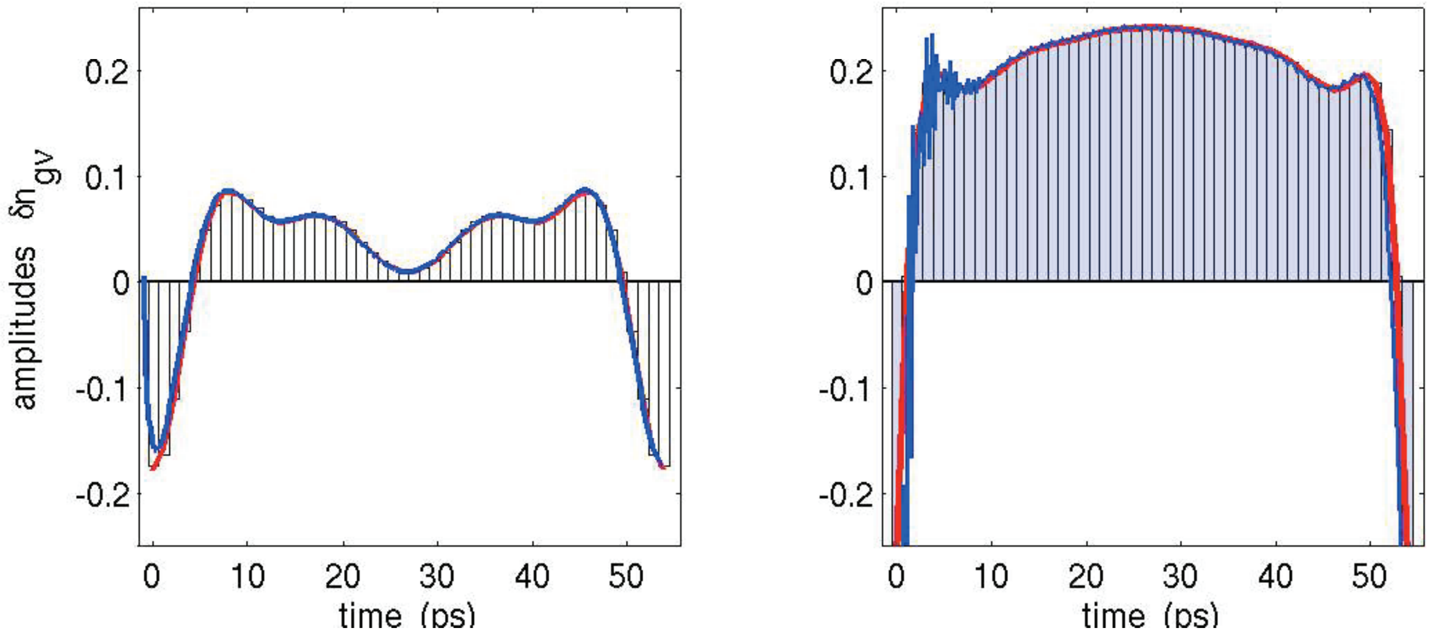
$$\boldsymbol{a}_k = -\boldsymbol{E}_k^{\text{qubit}} - E^{\text{coup}}/2 \qquad b_k = -E_k^{\text{tunnel}}$$

$$\boldsymbol{d}_k = 2\,\boldsymbol{E}_k^{\text{qubit}} \qquad c = E^{\text{coup}}$$

Makhlin, Schön, Shnirman, Rev. Mod. Phys. 73 (2001)

Spörl, Schulte-Herbrüggen, Glaser, Bergholm, Storcz, Ferber, Wilhelm, quant-ph/0504202

Time-Optimal cNOT for Coupled Charge Qubits



five times faster: duration T=55 ps (correct relative phases)

cNOT with trace fidelity > $1\text{-}10^{-9}$

pulse realisable with standard network theory (8 LCR and 2 low-pass filters)

Spörl, Schulte-Herbrüggen, Glaser, Bergholm, Storcz, Ferber, Wilhelm, quant-ph/0504202

Extension to Three Coupled Charge Qubits:

Toffoli Gate on Linear 3-Spin Chain

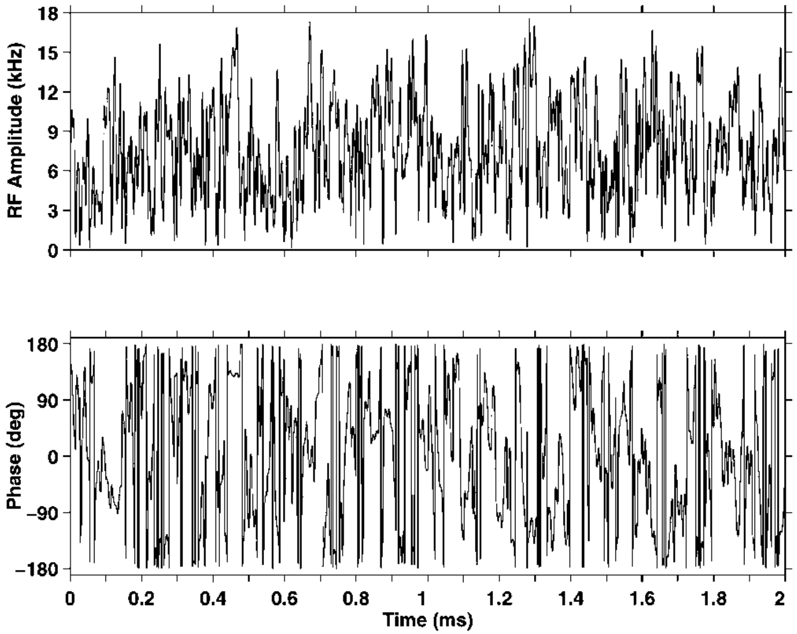
- very fast ($T = 180$ ps)
  - 13 times faster than 9 of Nakamura's cNOTs (2250 ps)
  - 2.7 times faster than 9 of timeoptimised cNOTs (495 ps)
- Toffoli with trace fidelity $> 1 - 10^{-5}$

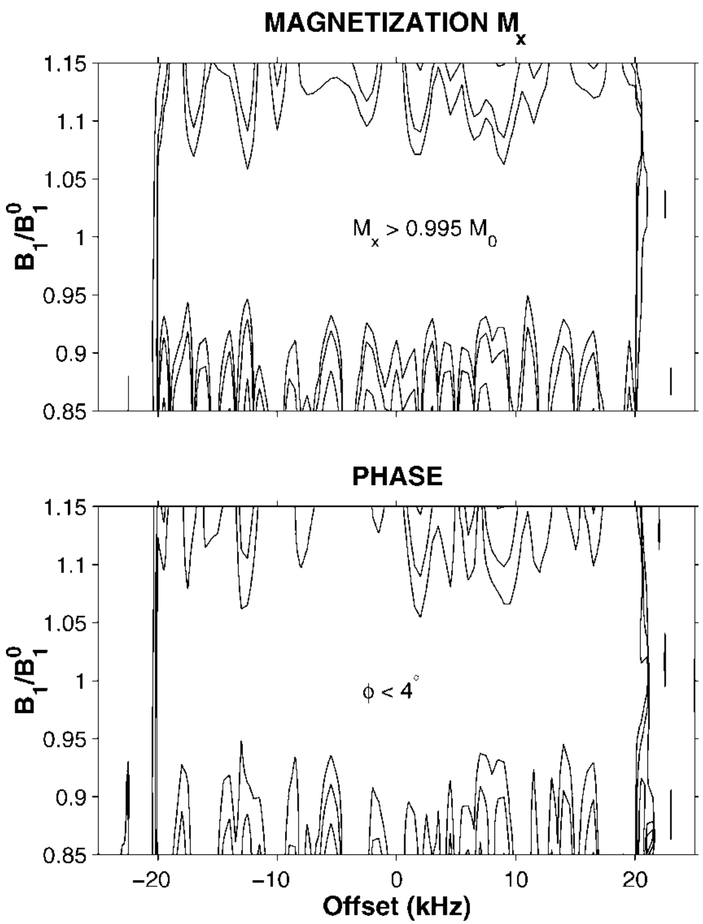
quant-ph/0504202

Robust control

Robust control of a single spin

Control fields

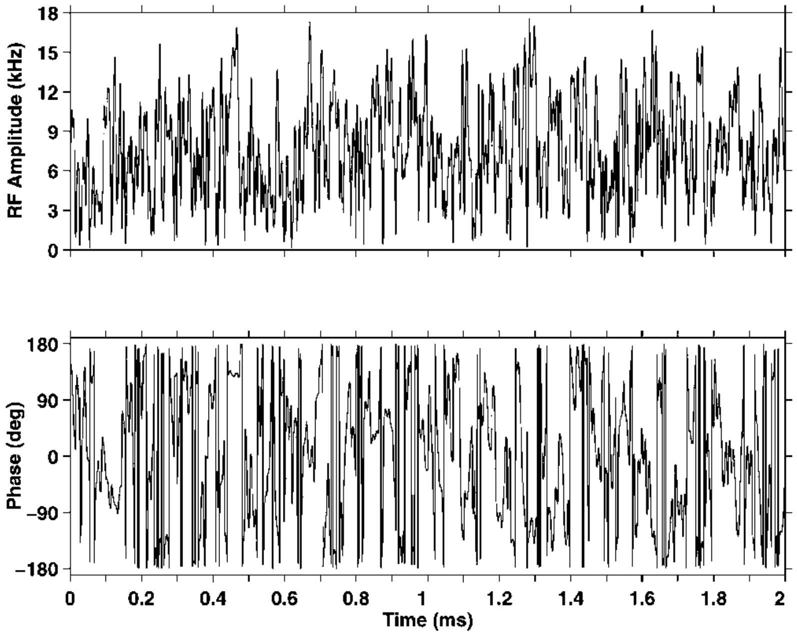


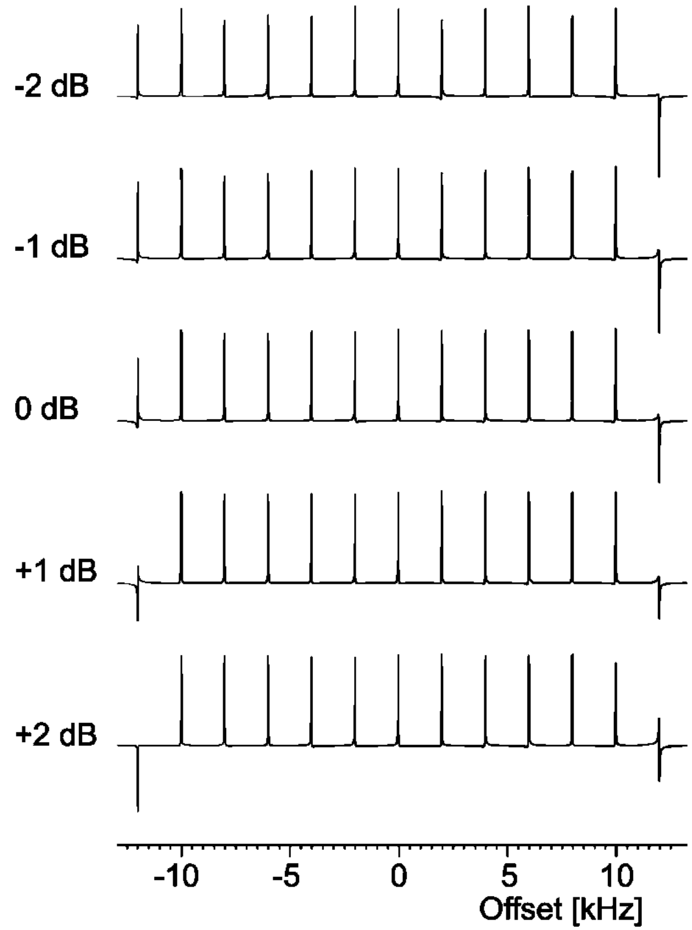


Skinner, Reiss, Khaneja, Luy, Glaser (2003)

Robust control of a single qubit

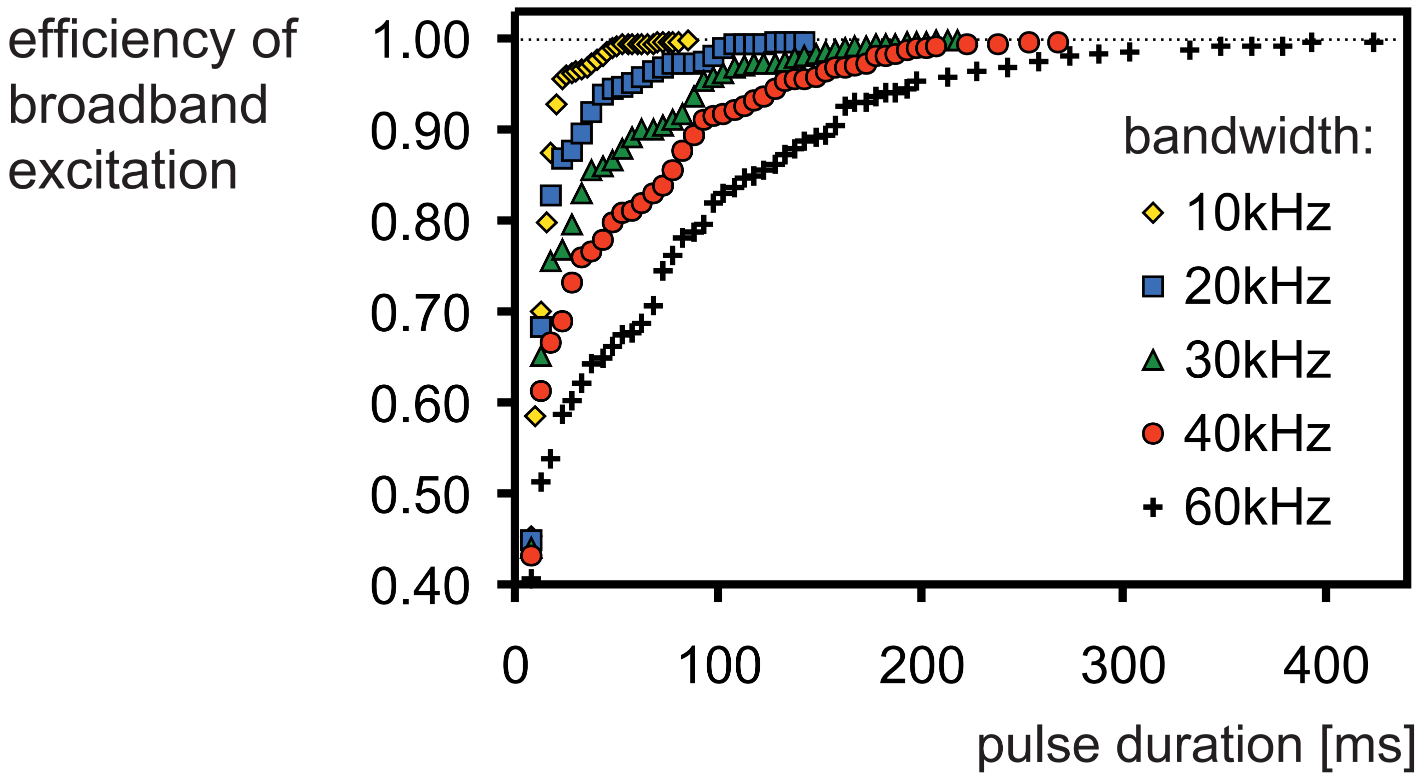
Control fields





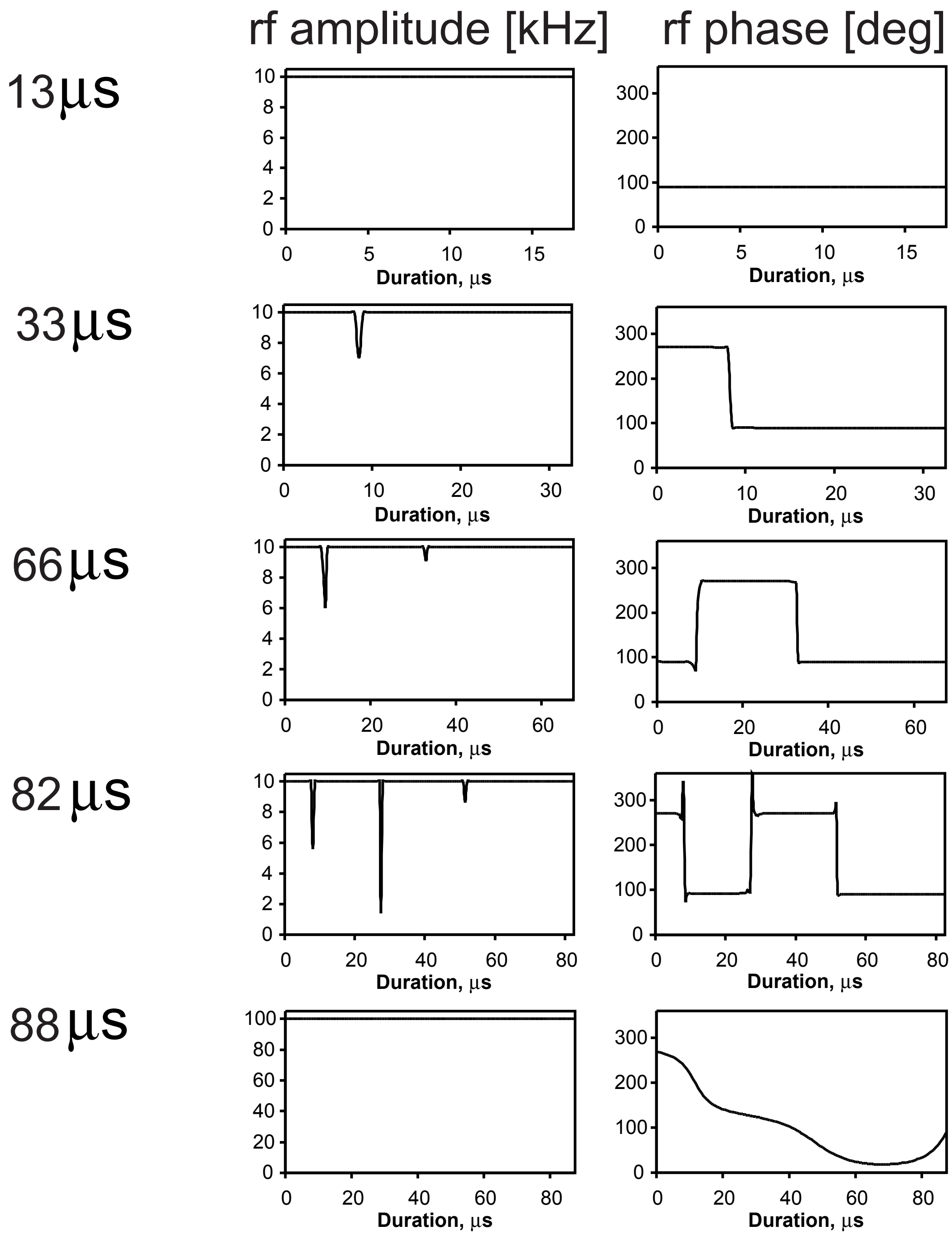
Skinner, Reiss, Khaneja, Luy, Glaser (2003)

Larger excitation bandwidths require longer pulses for same performance



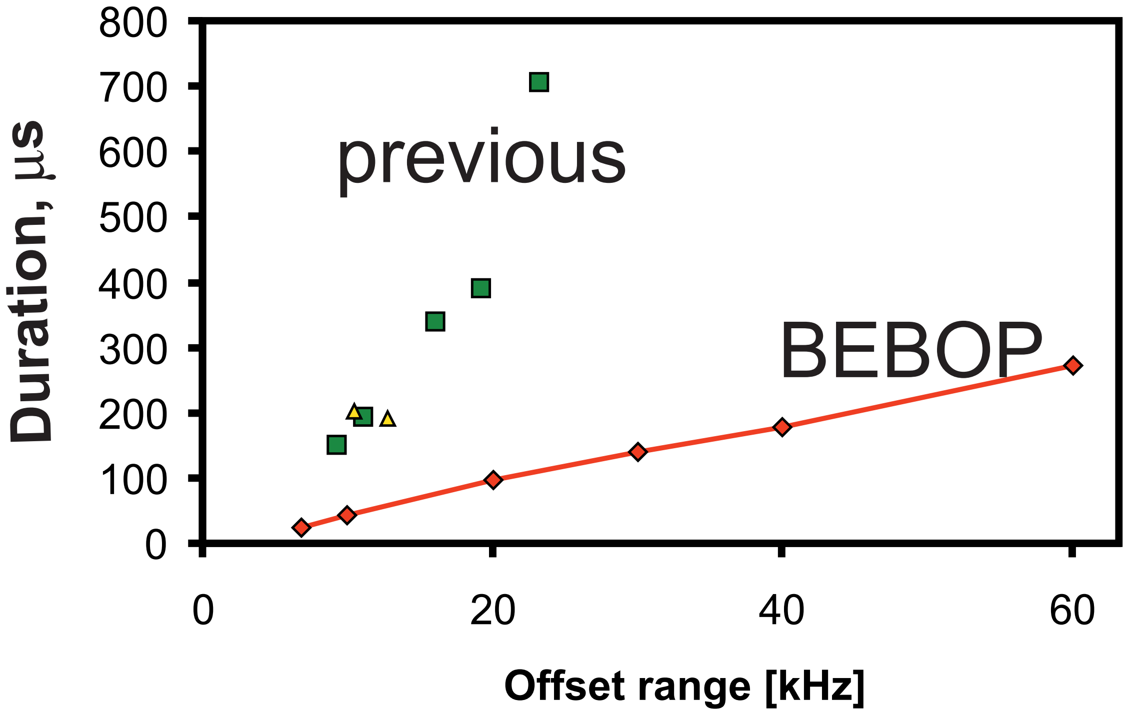
(max. rf amplitude: 10 kHz, no rf inhomogeneity)

Longer pulse durations allow for more complex phase variations



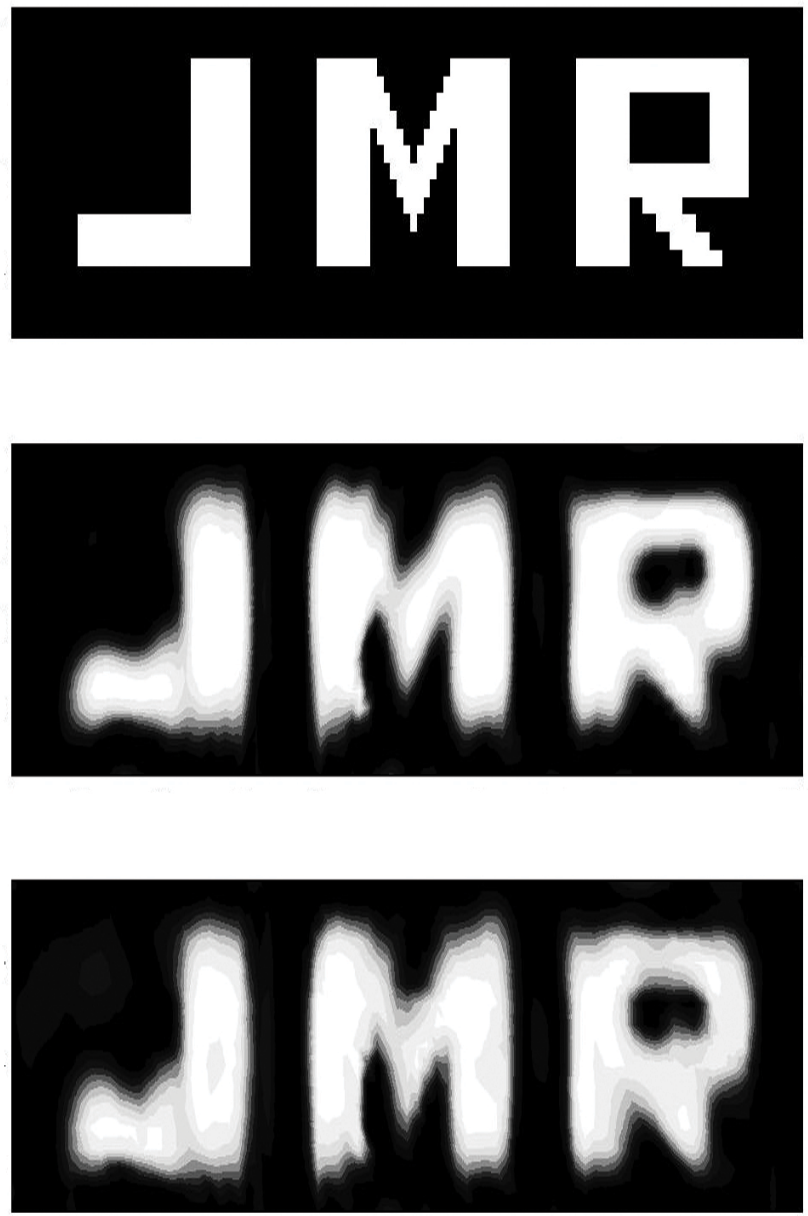
excitation bandwidth: 20 kHz
no rf inhomogeneity

Time-optimal excitation pulses are significantly shorter compared to previously known composite pulses

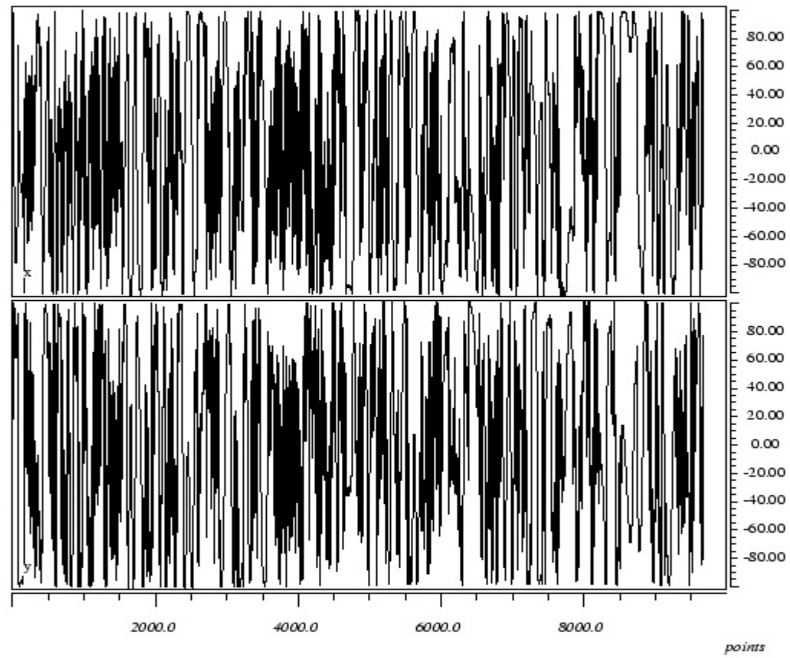


(excitation efficiency: 98%, max. rf amplitude: 10 kHz, no rf inhomogeneity)

Pattern Pulses



rf amplitude (x)

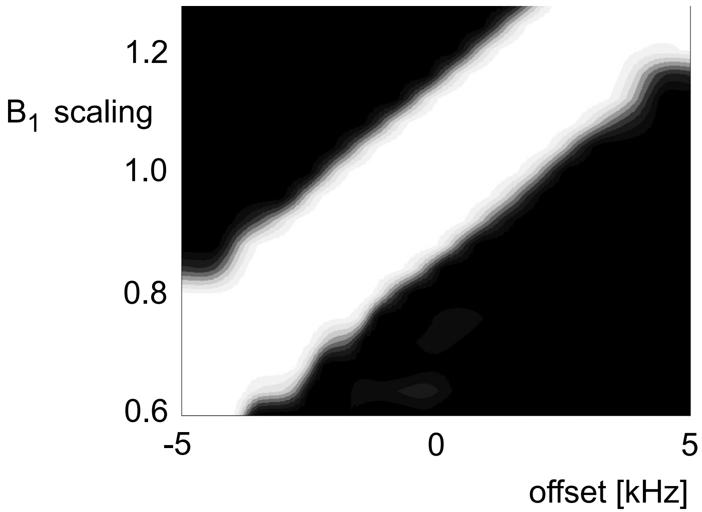


rf amplitude (y)

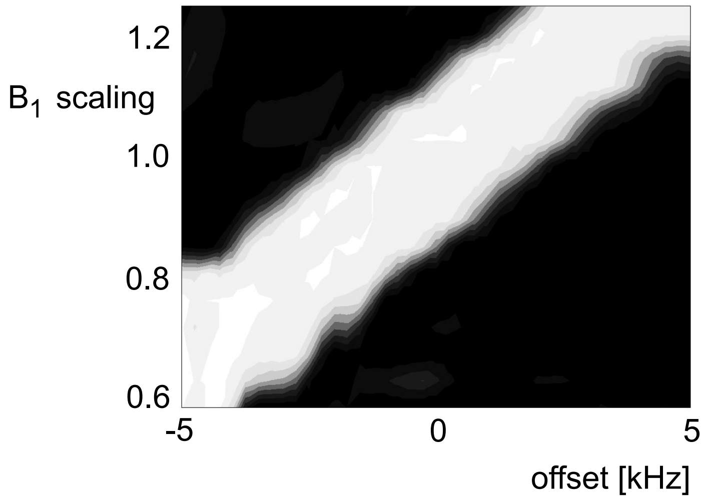
Kobzar et al., J. Magn. Reson. (2005)

NMR Test Patterns (Excitation)

Simulation



Experiment



Harvard

N. Khaneja, D. Stefanatos, Jr-S. Li, H. Yuan, A. Johnson

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H. Kessler, A. Frank

Ludwig-Maximilians-Universität München (LMU)

F. Wilhelm, M. Storcz, J. Ferber

Funding: DFG, FCI, DAAD

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For a complete list of references including papers on composite pulses, decoupling, polarization and coherence transfer, see http://www.org.chemie.tu-muenchen.de/glaser/Publ.html

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