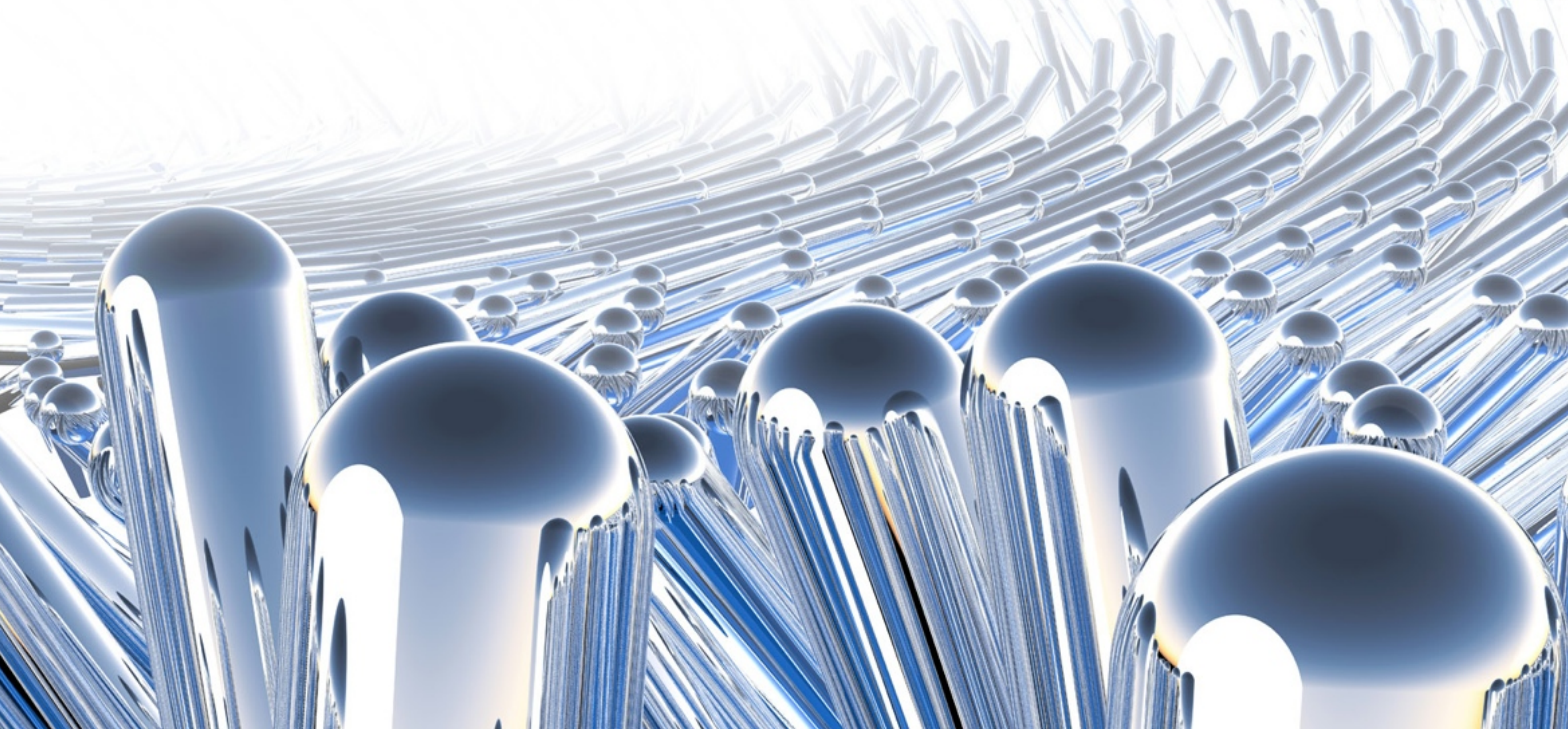
# Optimal Control of Spin and Pseudo-Spin Systems

*Steffen Glaser, TU München*



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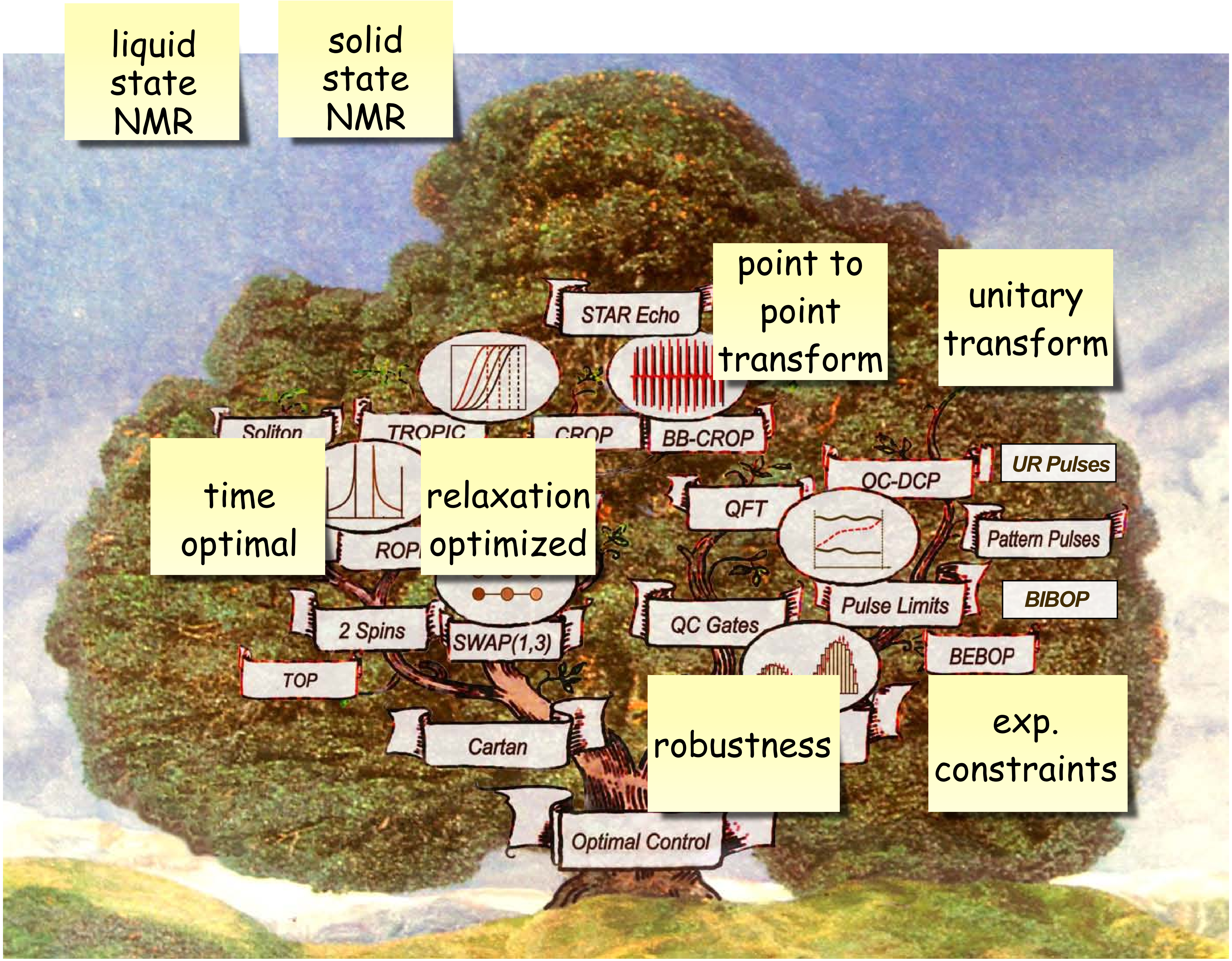
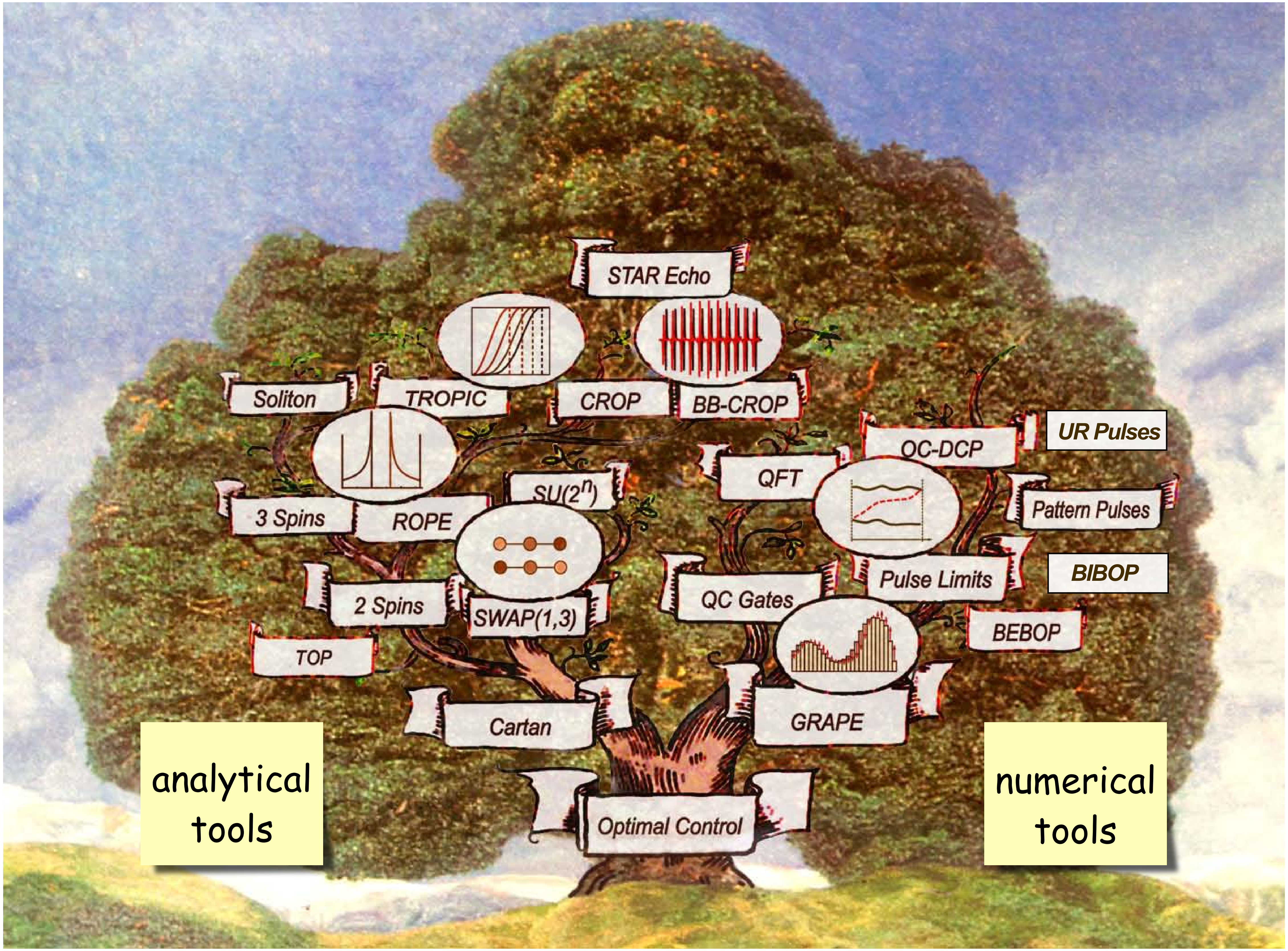


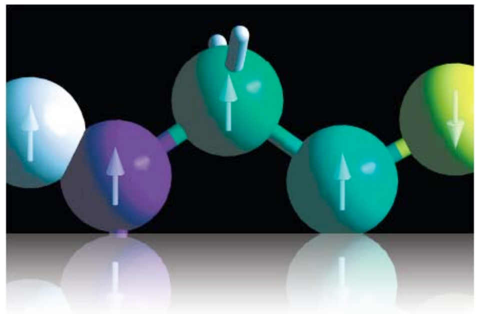
liquid state NMR
solid state NMR
STAR Echo
point to point transform
unitary transform
Soliton
TROPIC
CROP
BB-CROP
UR Pulses
QC-DCP
QFT
time optimal
relaxation optimized
Pattern Pulses
Pulse Limits
BIBOP
2 Spins
SWAP(1,3)
QC Gates
BEBOP
TOP
Cartan
robustness
exp. constraints
Optimal Control



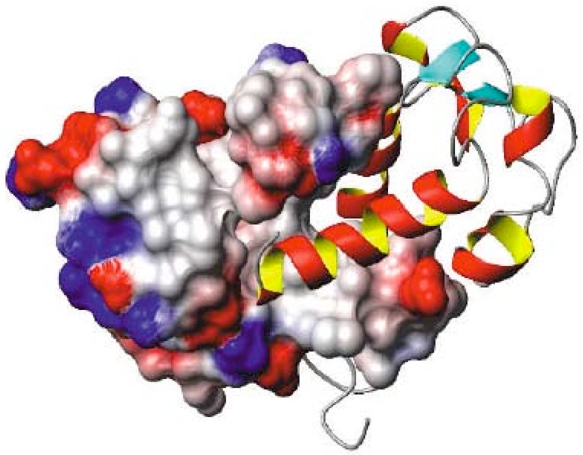
STAR Echo
Soliton
TROPIC
CROP
BB-CROP
UR Pulses
QC-DCP
QFT
SU(2^n)
3 Spins
ROPE
Pattern Pulses
Pulse Limits
BIBOP
QC Gates
2 Spins
SWAP(1,3)
BEBOP
TOP
Cartan
GRAPE
analytical tools
numerical tools
Optimal Control

# Optimal Control of Spin Systems

physical limits of spin dynamics



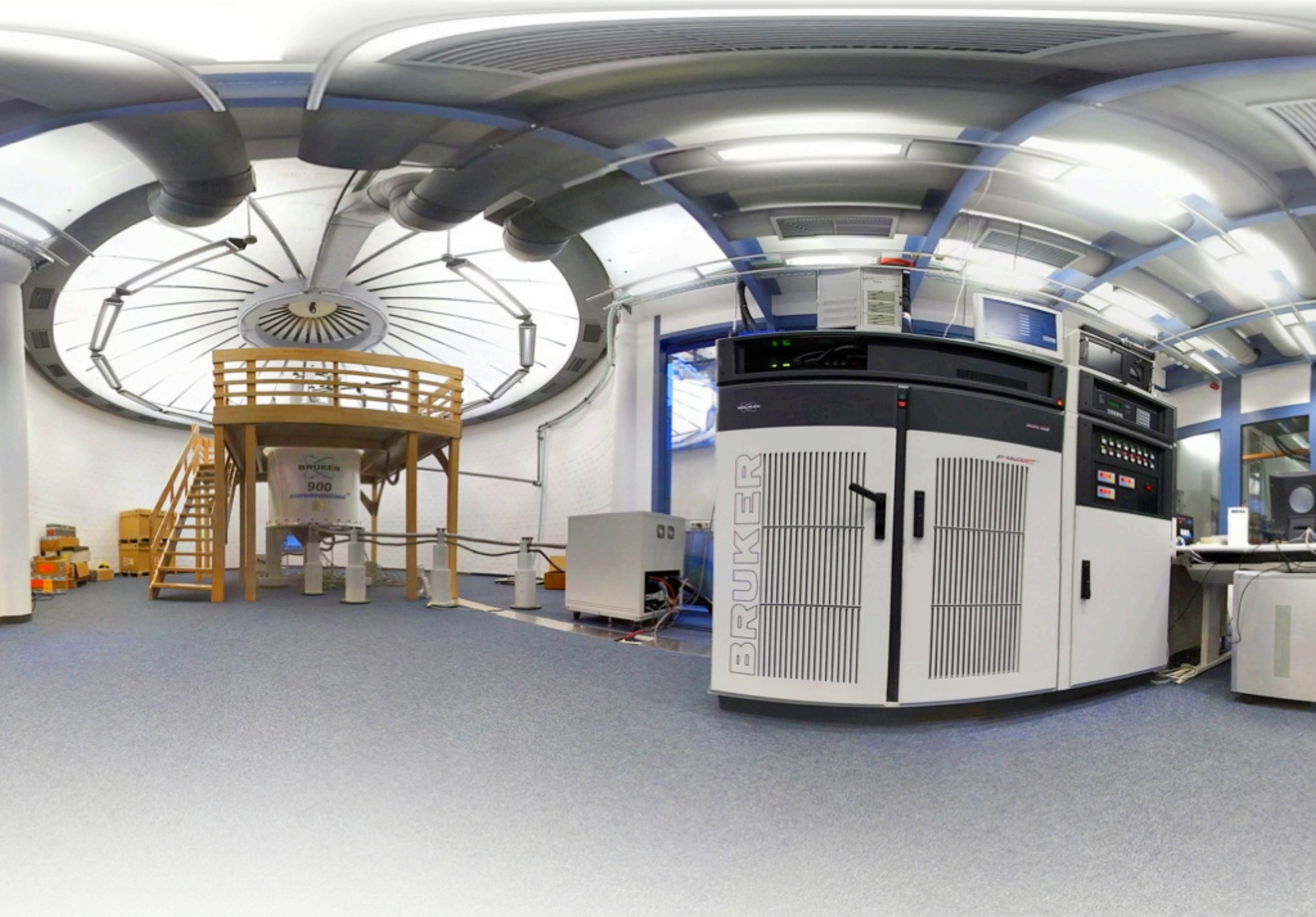
spectroscopy

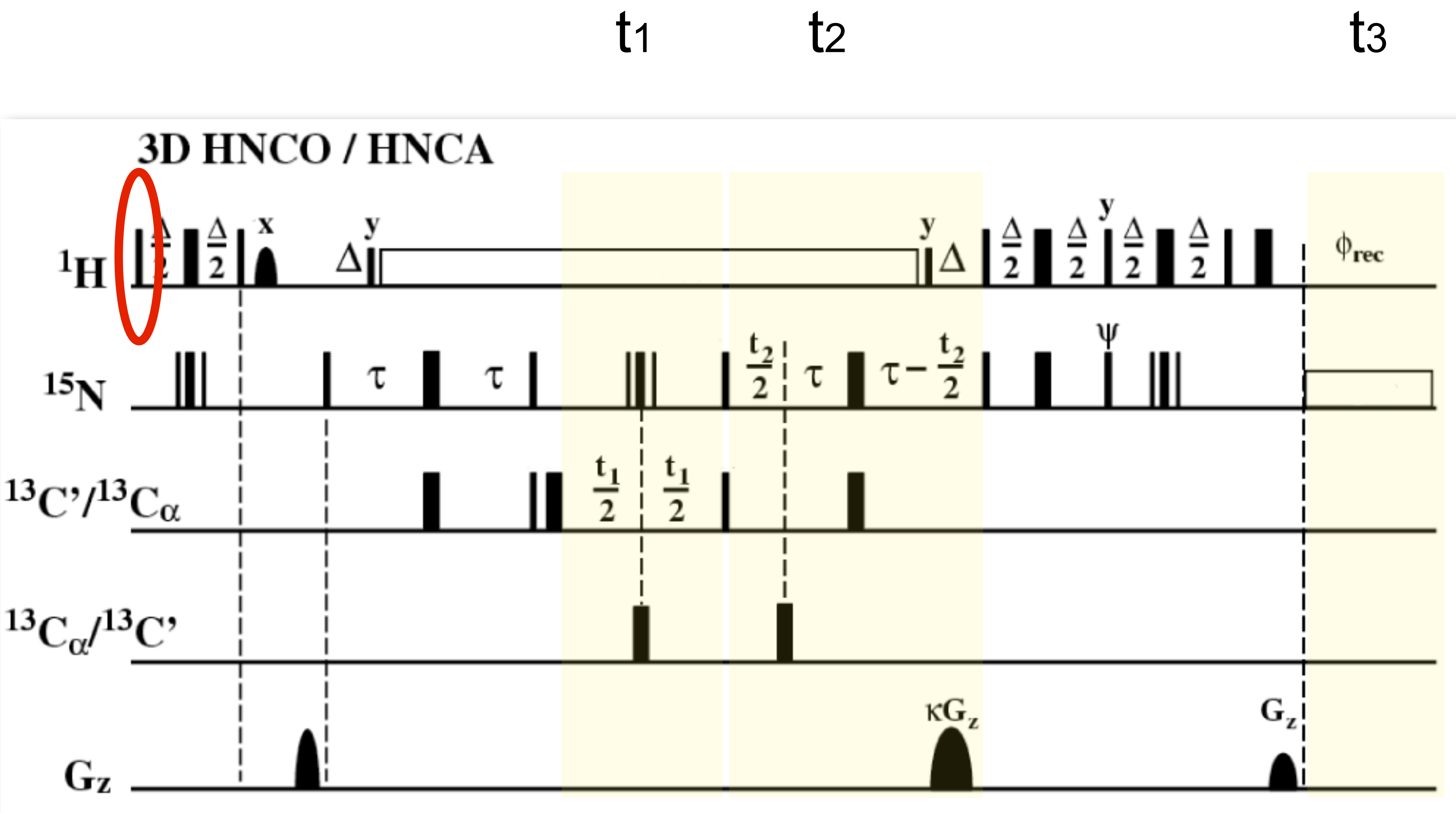


hyperpolarization

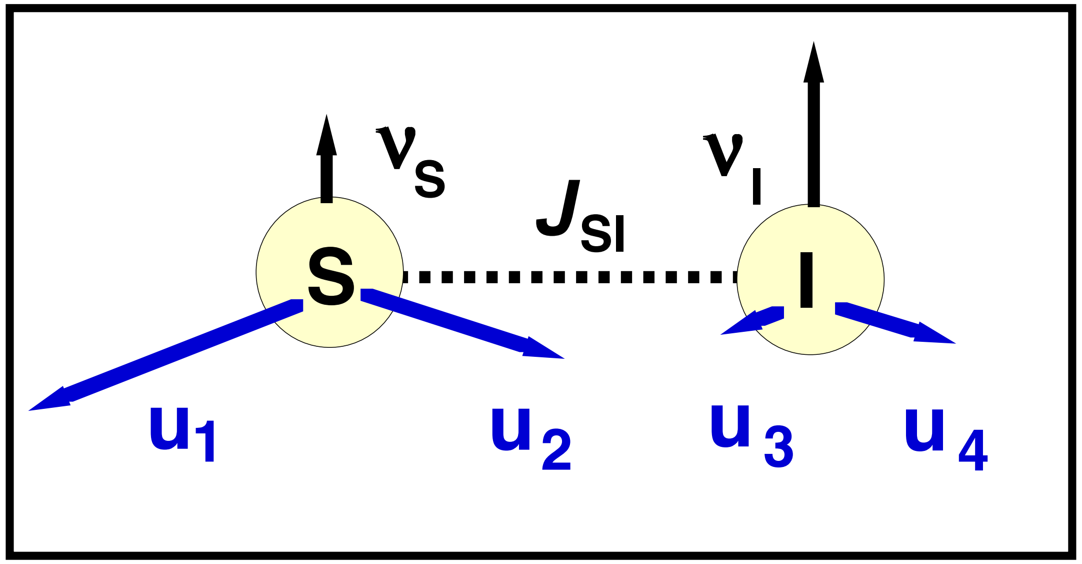
local spin manipulation and imaging

low power decoupling


BRUKER
900
BRUKER


t1
t2
t3
3D HNCO / HNCA
1H
15N
13C'/13Cα
13Cα/13C'
Gz
x
y
y
y
Δ
τ
τ − t2/2
ψ
φrec
κGz
Gz

# 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

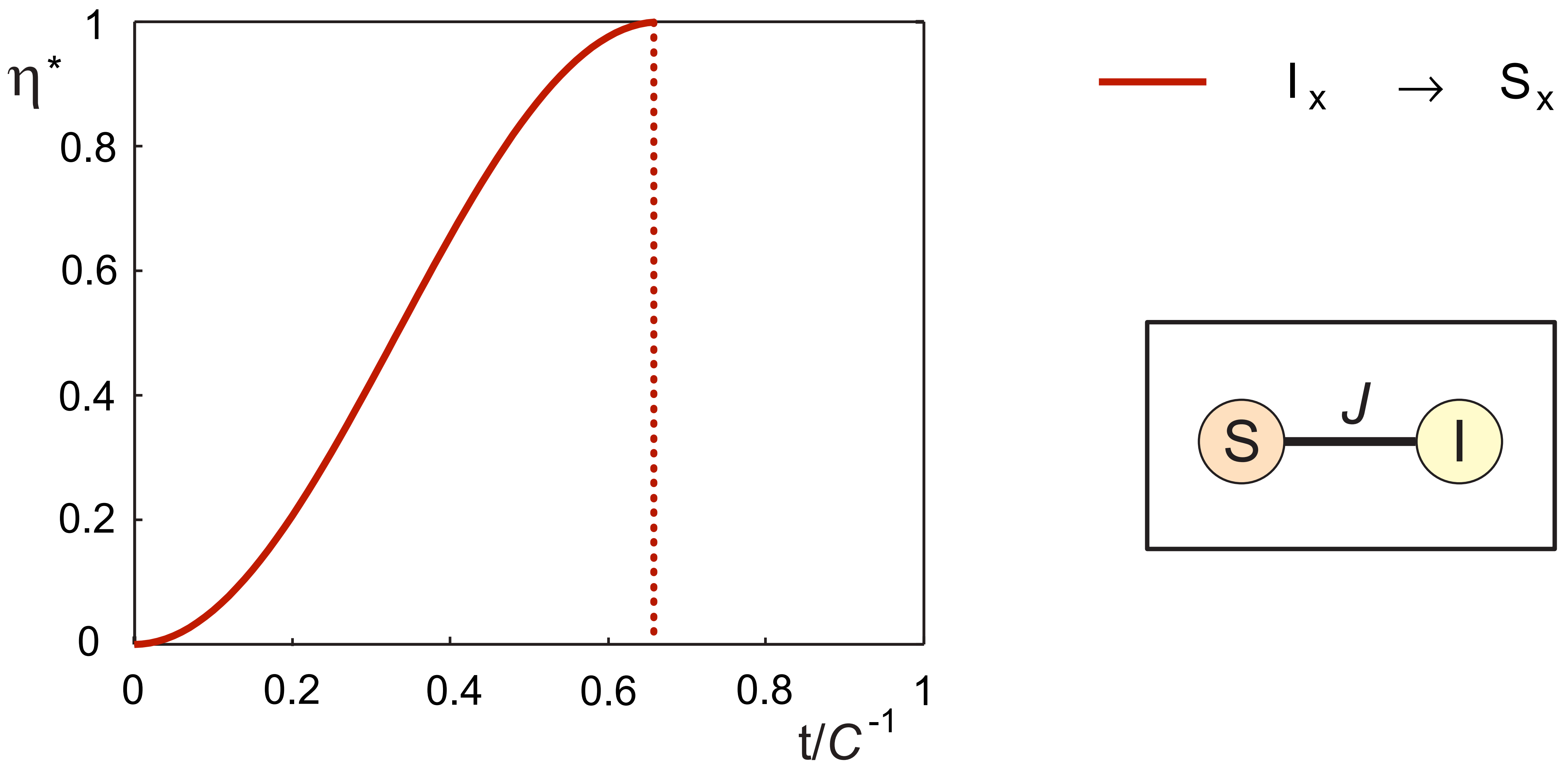
Characterization of ALL unitary operators
that can be created in time T

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

*Khaneja, Brockett, Glaser (2001)*

*Khaneja, Kramer, Glaser (2005)*

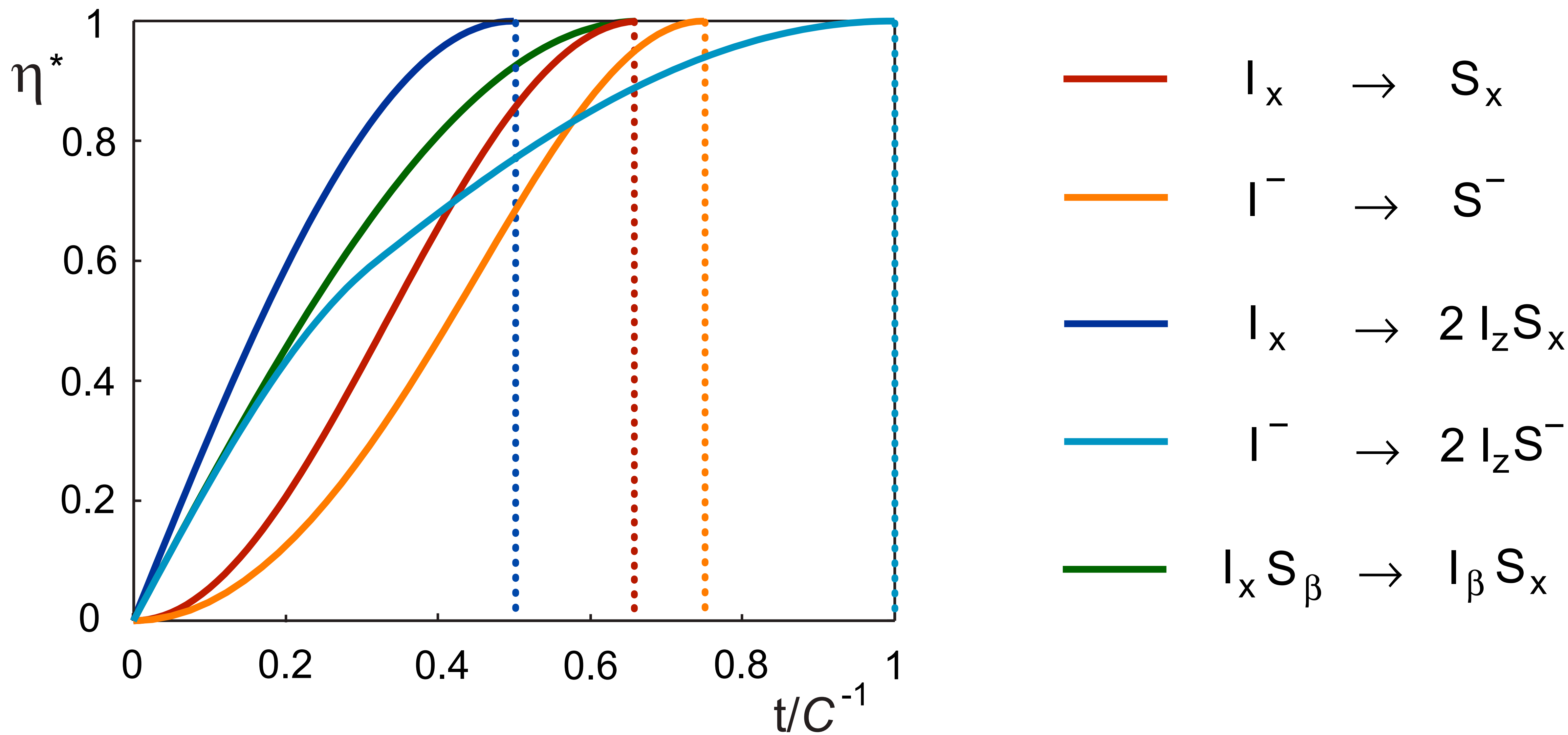
# TOP (time-optimal pulse) curves for dipolar coupling




Khaneja, Kramer, Glaser (2005)

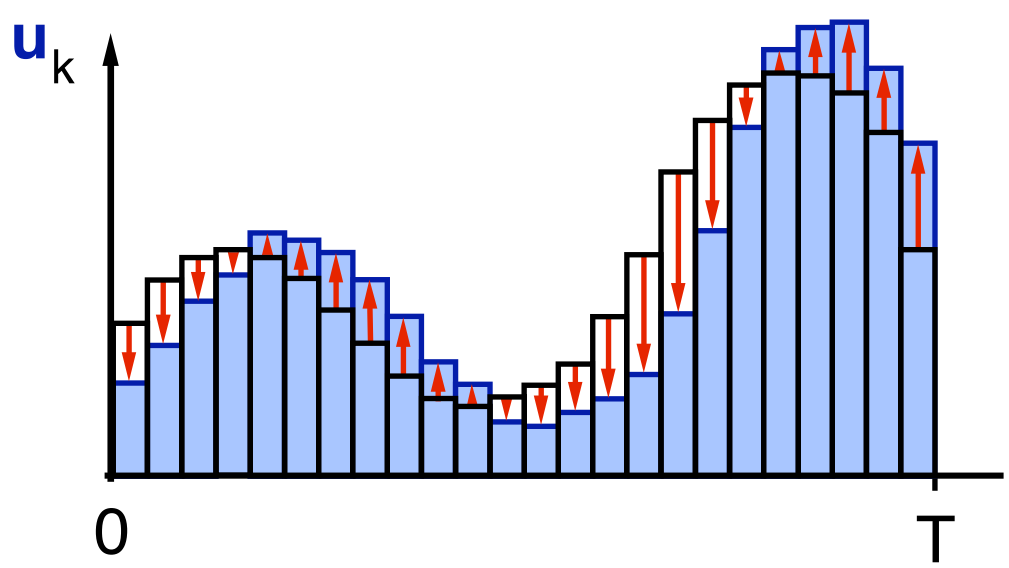
# TOP (time-optimal pulse) curves for dipolar coupling

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




Khaneja, Kramer, Glaser (2005)

# GRAPE (Gradient Ascent Pulse Engineering)




desired transfer: A ⟶ C

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

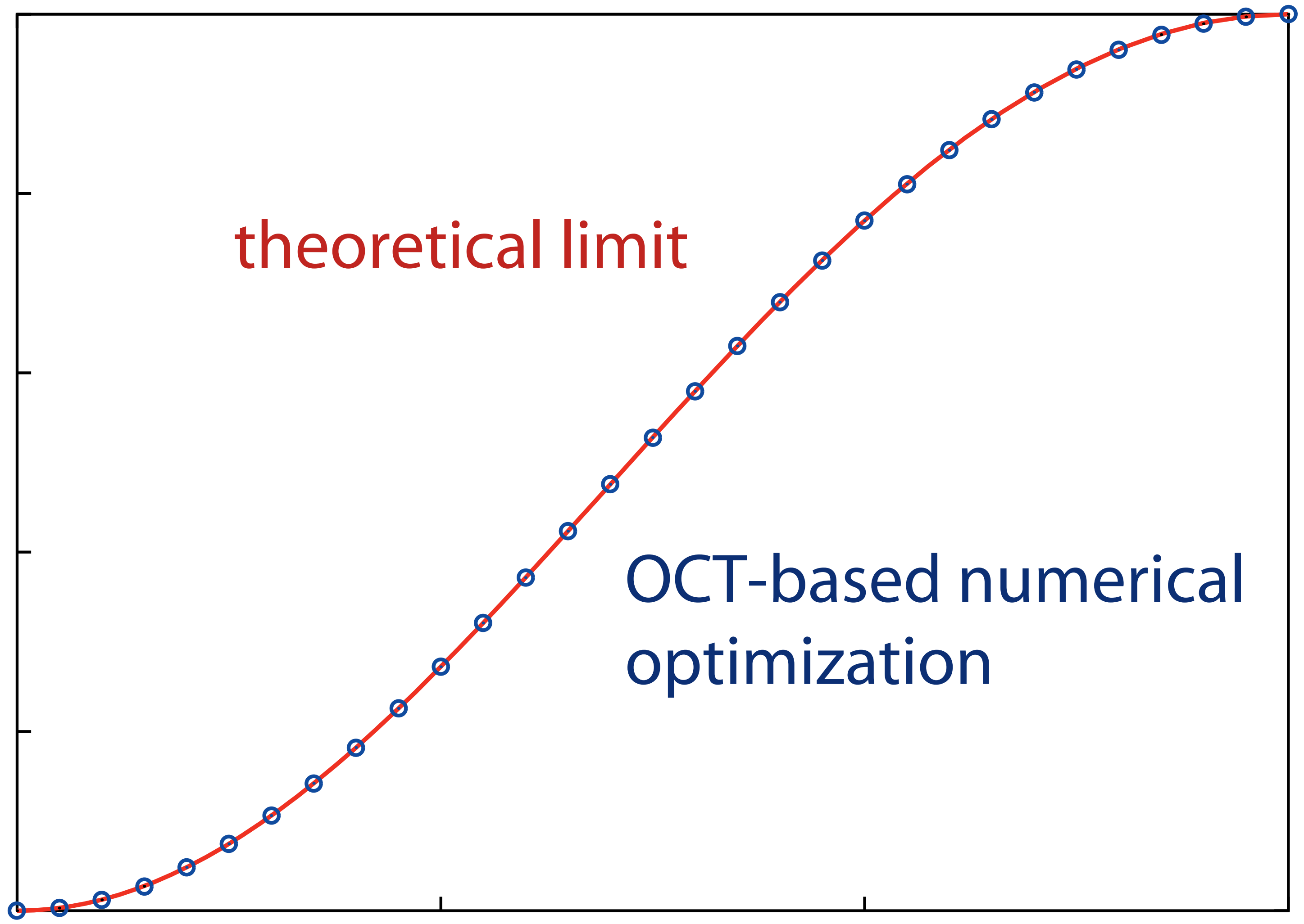
$\rho(0) = A$

$\lambda(T) = C$

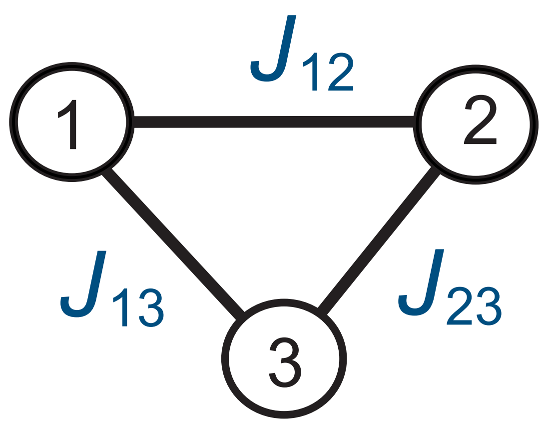
$$u_k(t) \longrightarrow u_k(t) + \varepsilon \langle \lambda(t) \,|\, [-i H_k, \rho(t)] \rangle$$

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

# Numerical OCT-based Algorithm finds theoretical limits



# Polarization transfer in homonuclear three spin systems



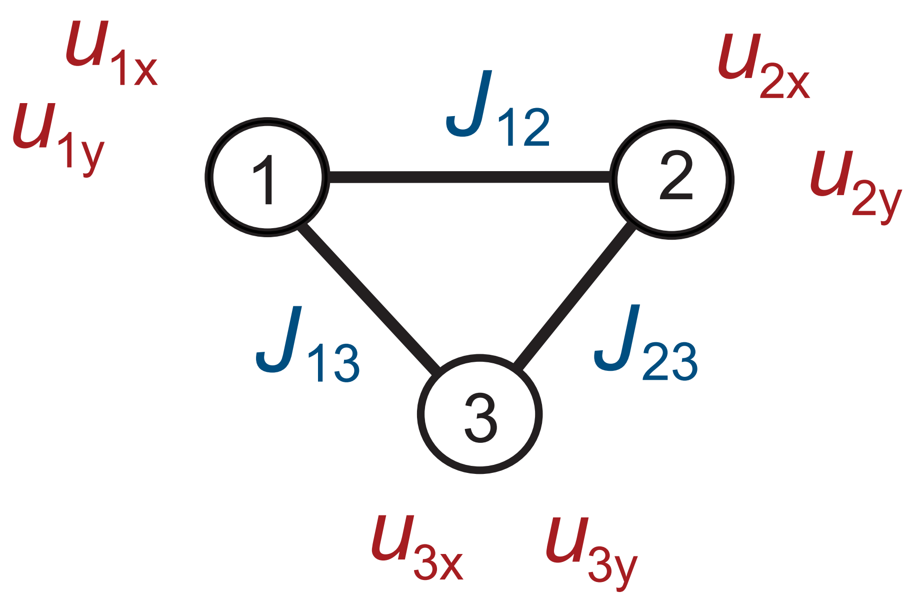

$$I_{1z} \longrightarrow I_{2z}$$

isotropic (Heisenberg) couplings

$$\sum_{m<n} 2\pi J_{mn}(I_{mx}I_{nx} + I_{my}I_{ny} + I_{mz}I_{nz})$$

J. Neves

# Polarization transfer in homonuclear three spin systems




$$I_{1z} \longrightarrow I_{2z}$$

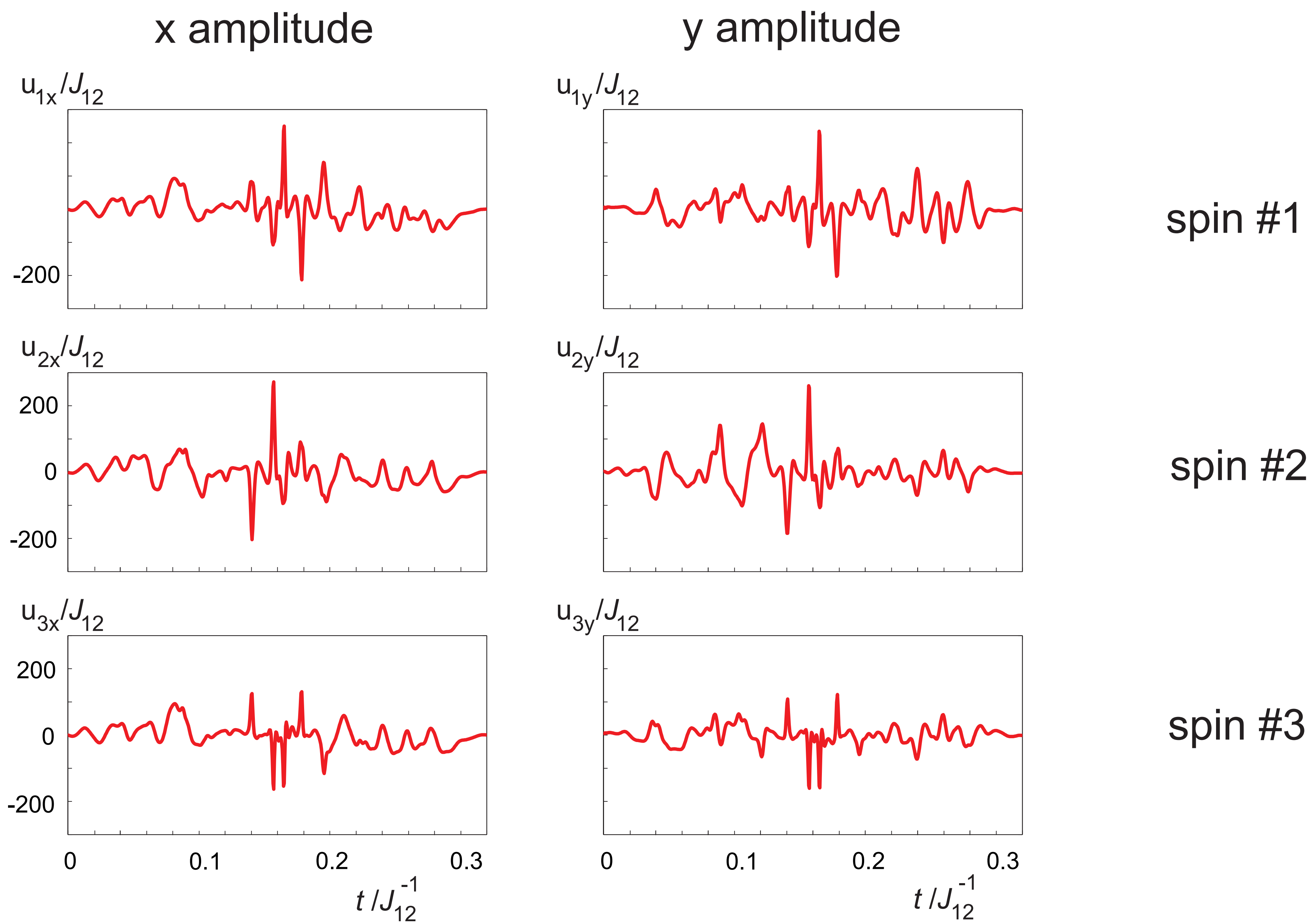
isotropic (Heisenberg) couplings

$$\sum_{m<n} 2\pi J_{mn}(I_{mx}I_{nx} + I_{my}I_{ny} + I_{mz}I_{nz})$$

idealized setting: fast, selective pulses (six control amplitudes)

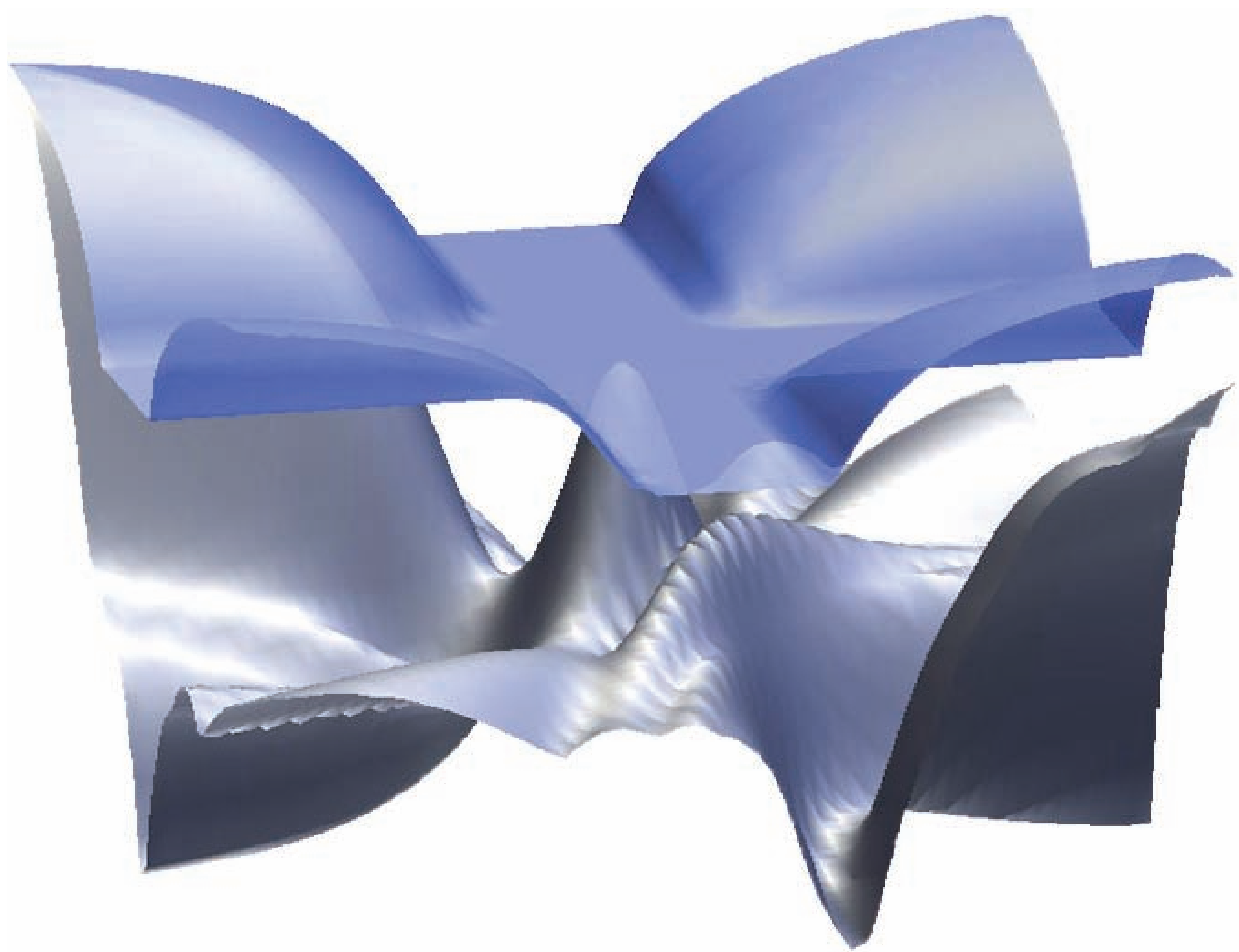
$$2\pi \sum_{m=1}^{3} \{u_{mx}(t)\, I_{mx} + u_{my}(t)\, I_{my}\}$$

# Optimized controls (radio frequency amplitudes)

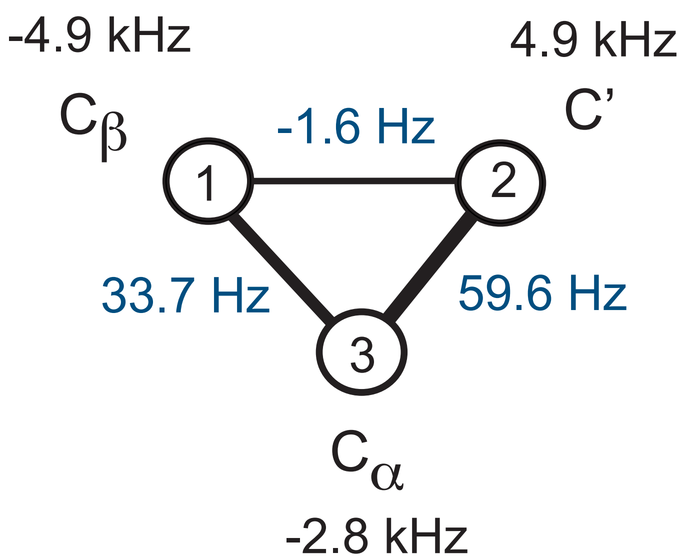


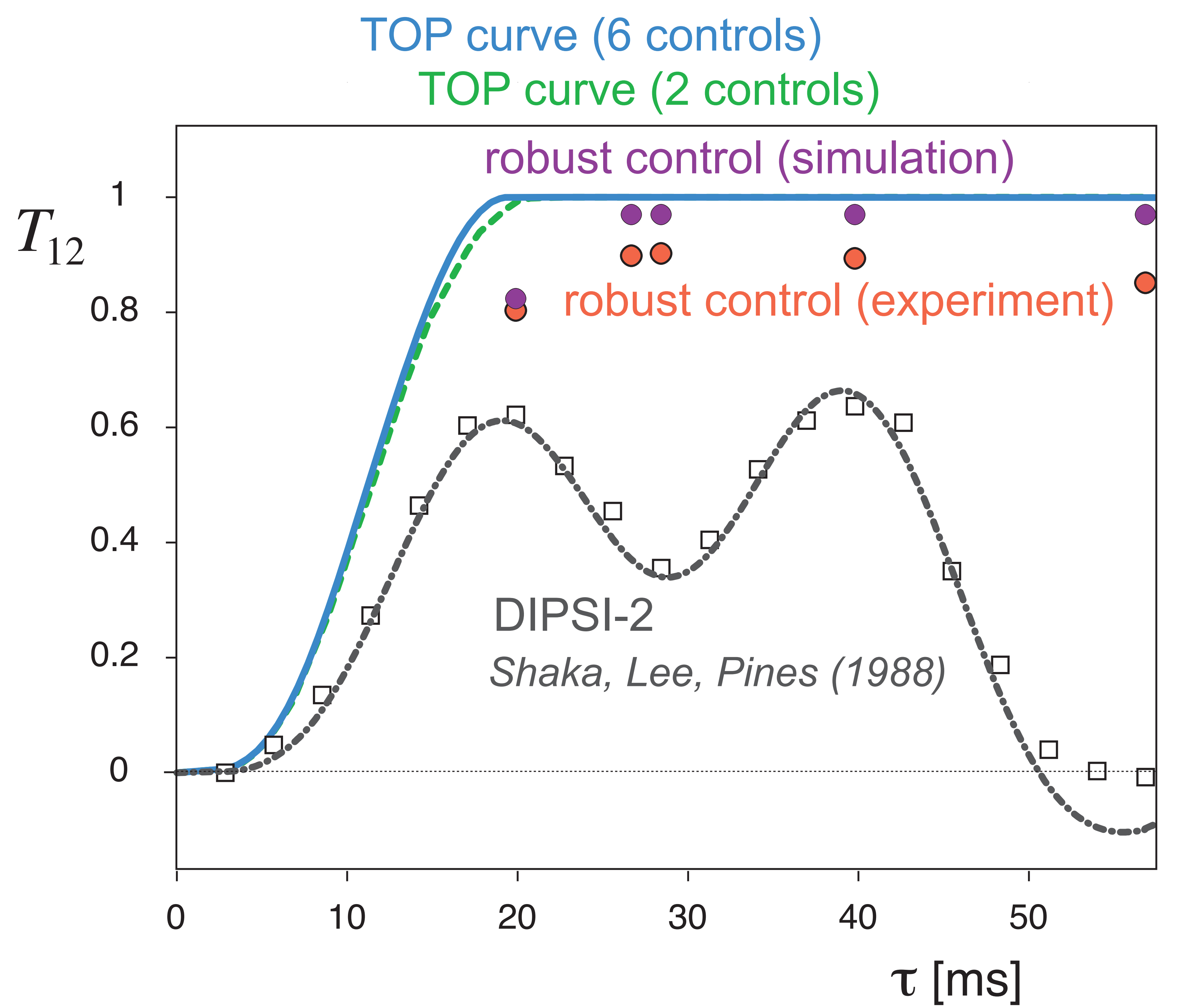

*Neves et al. (2006)*

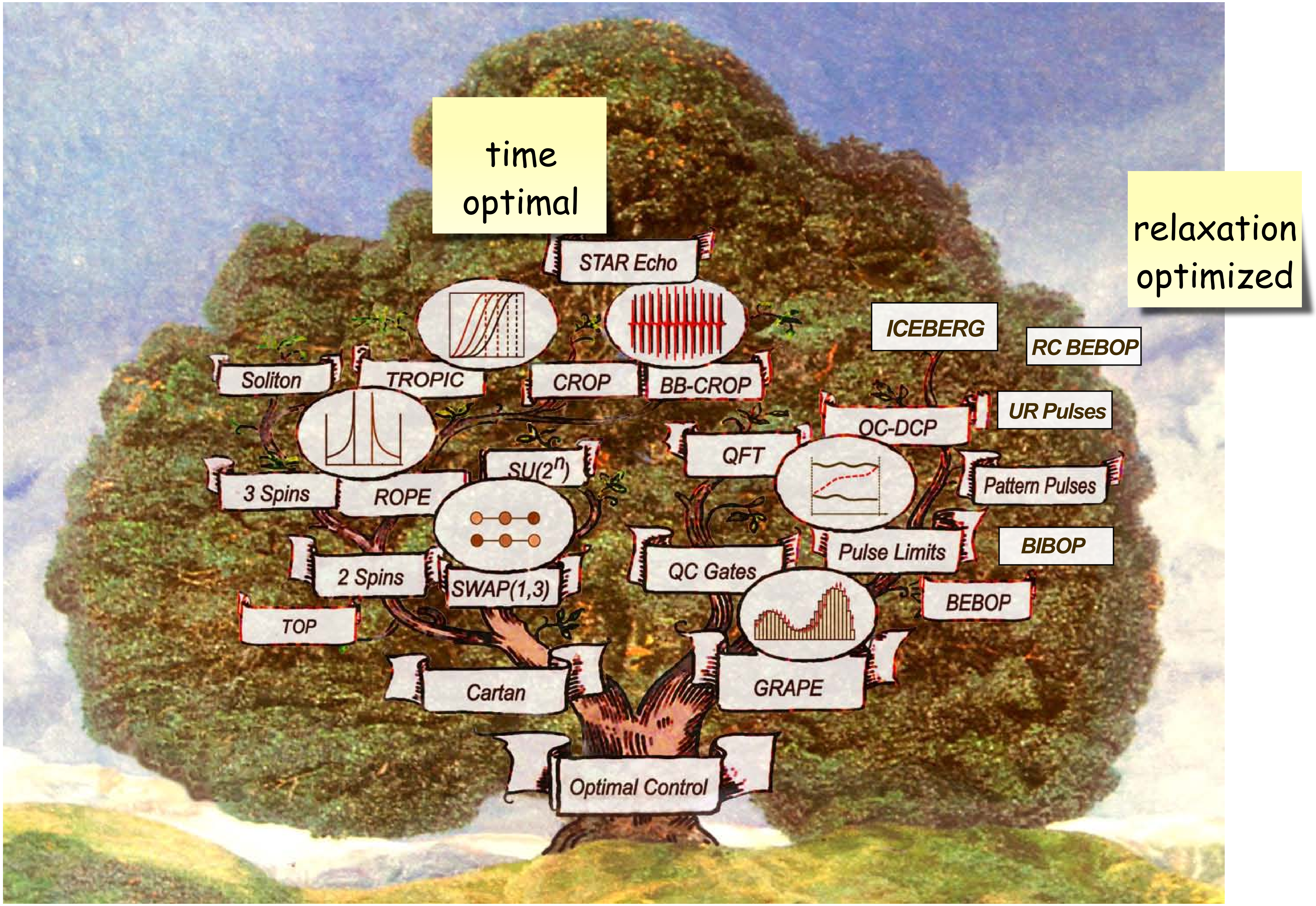
Transfer efficiency as a function of relative coupling constants $J_{13}/J_{12}$ and $J_{23}/J_{12}$



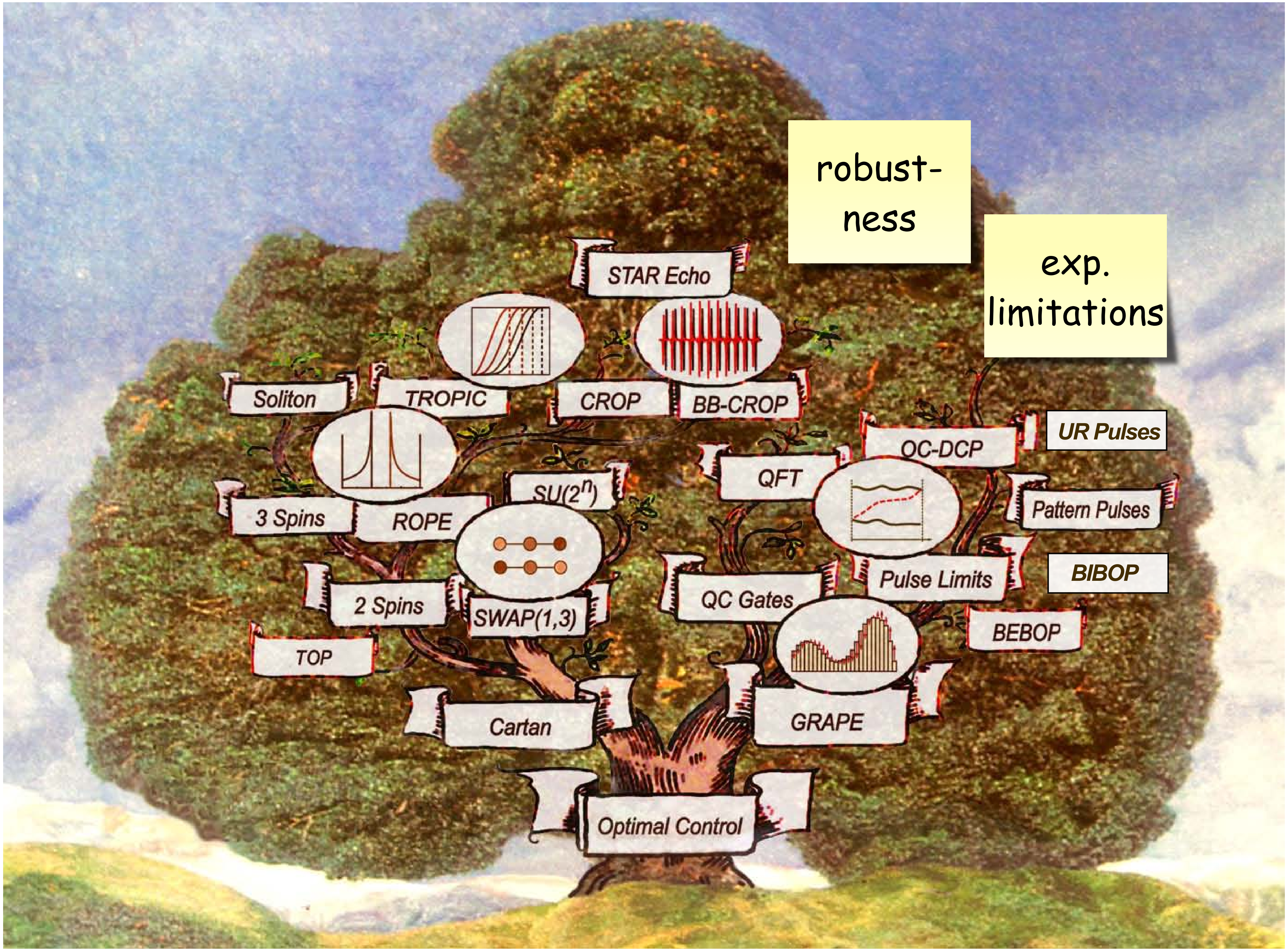
# Homonuclear three spin model system: $^{13}$C labelled alanine





time optimal
relaxation optimized
STAR Echo
ICEBERG
RC BEBOP
Soliton
TROPIC
CROP
BB-CROP
UR Pulses
OC-DCP
QFT
$SU(2^n)$
3 Spins
ROPE
Pattern Pulses
Pulse Limits
BIBOP
2 Spins
SWAP(1,3)
QC Gates
BEBOP
TOP
Cartan
GRAPE
Optimal Control



robust-
ness
exp.
limitations
STAR Echo
Soliton
TROPIC
CROP
BB-CROP
UR Pulses
OC-DCP
QFT
SU(2^n)
Pattern Pulses
3 Spins
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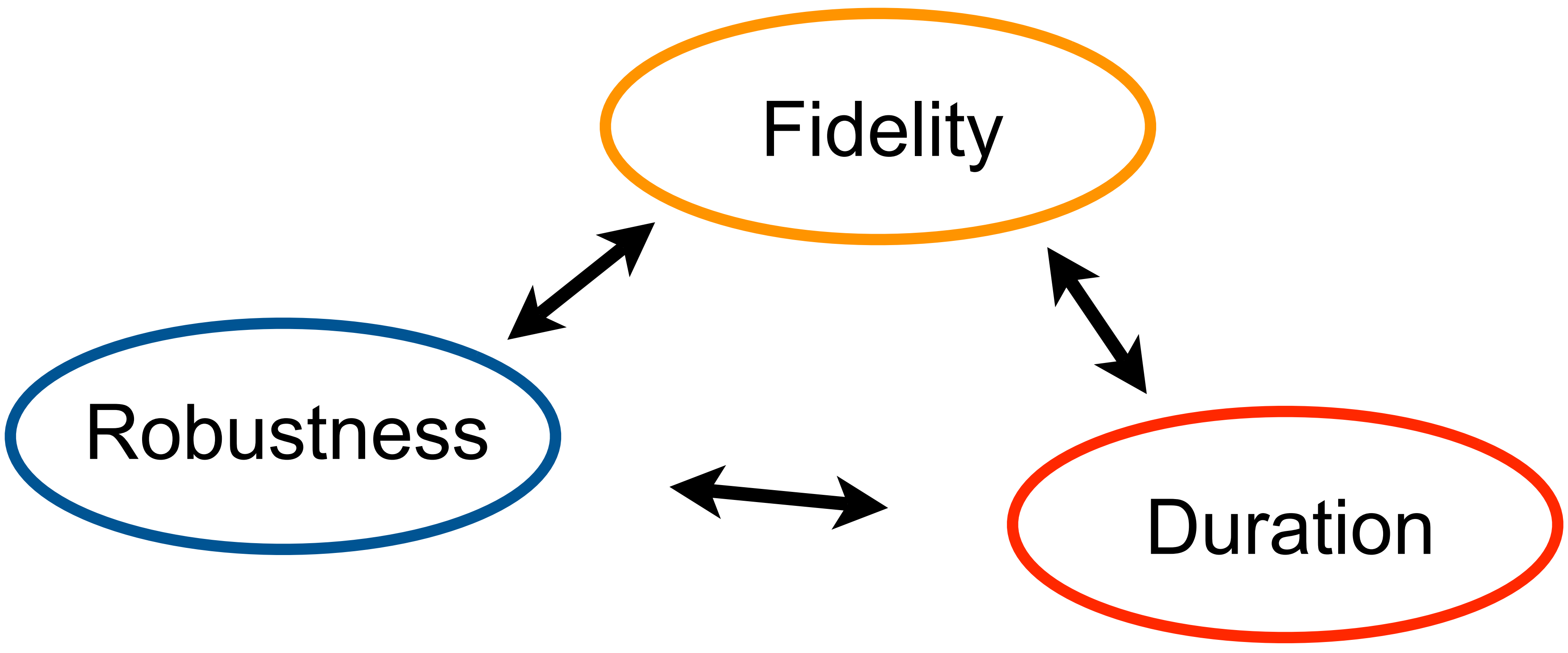
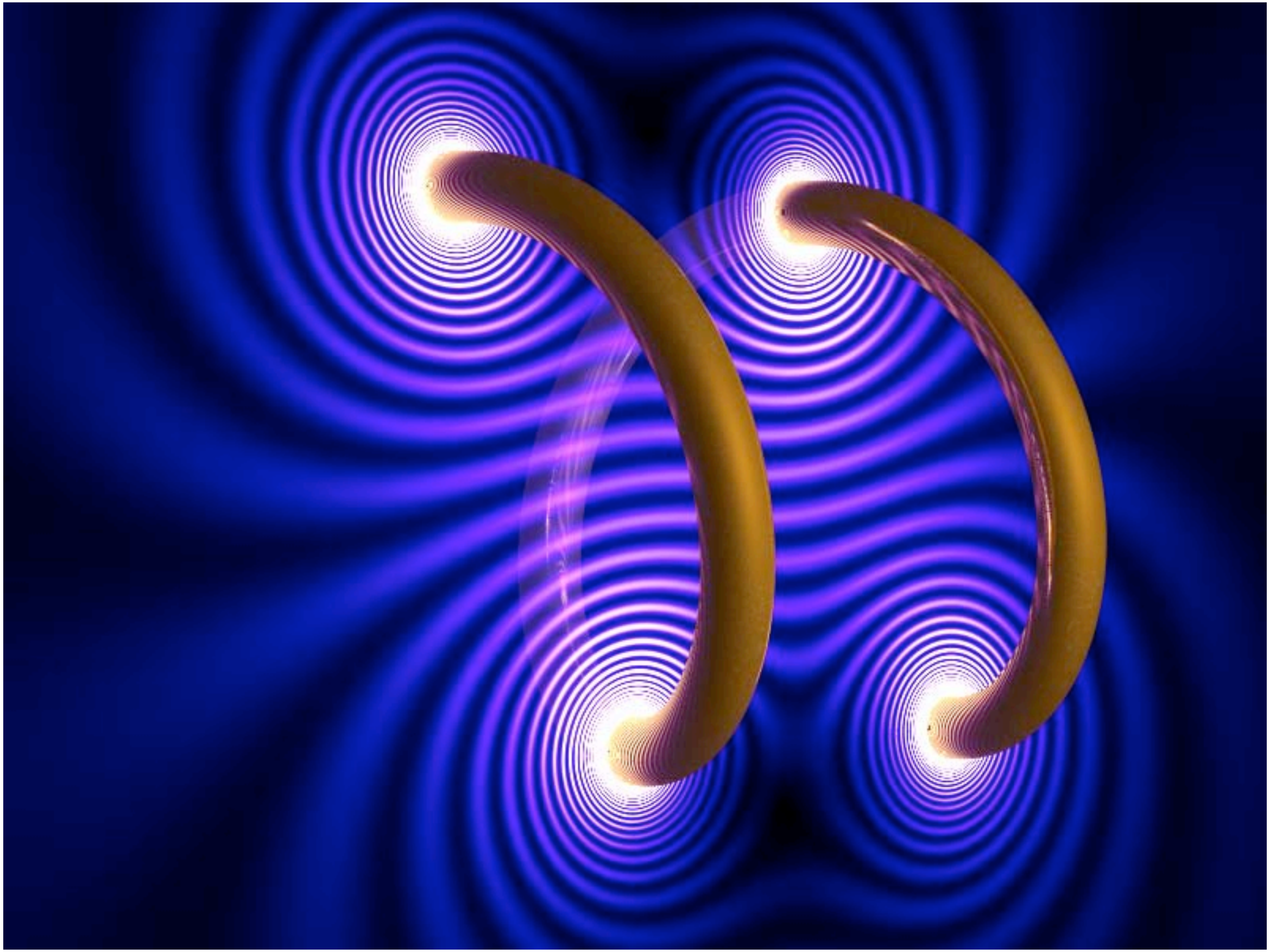
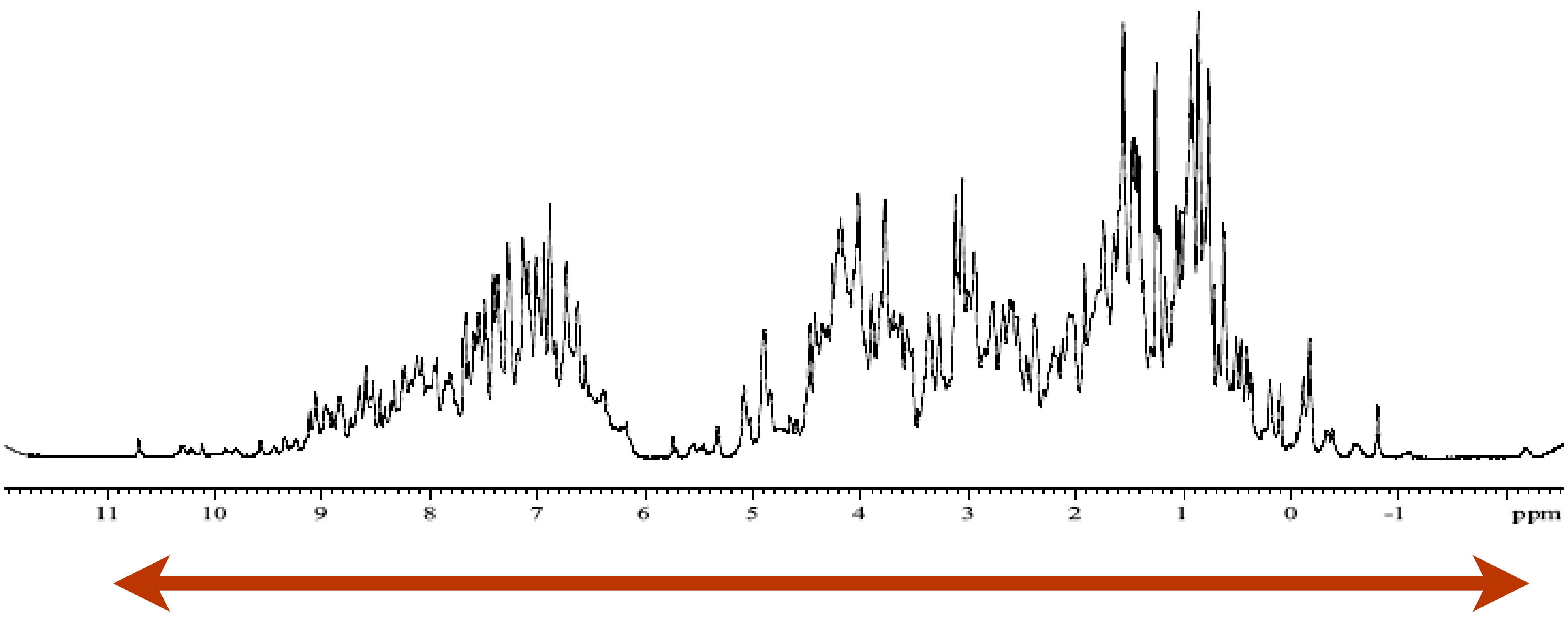
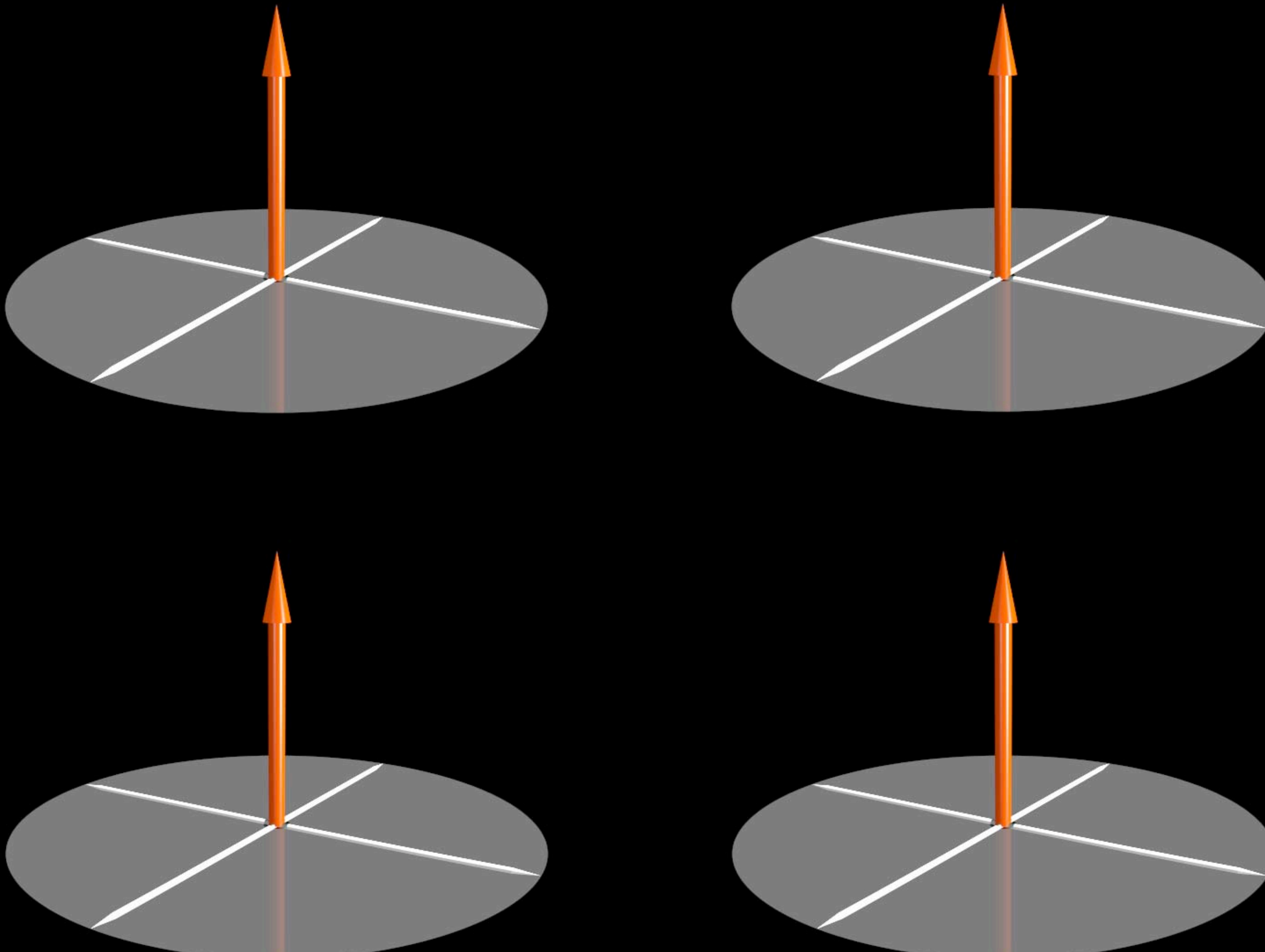
Optimal Control

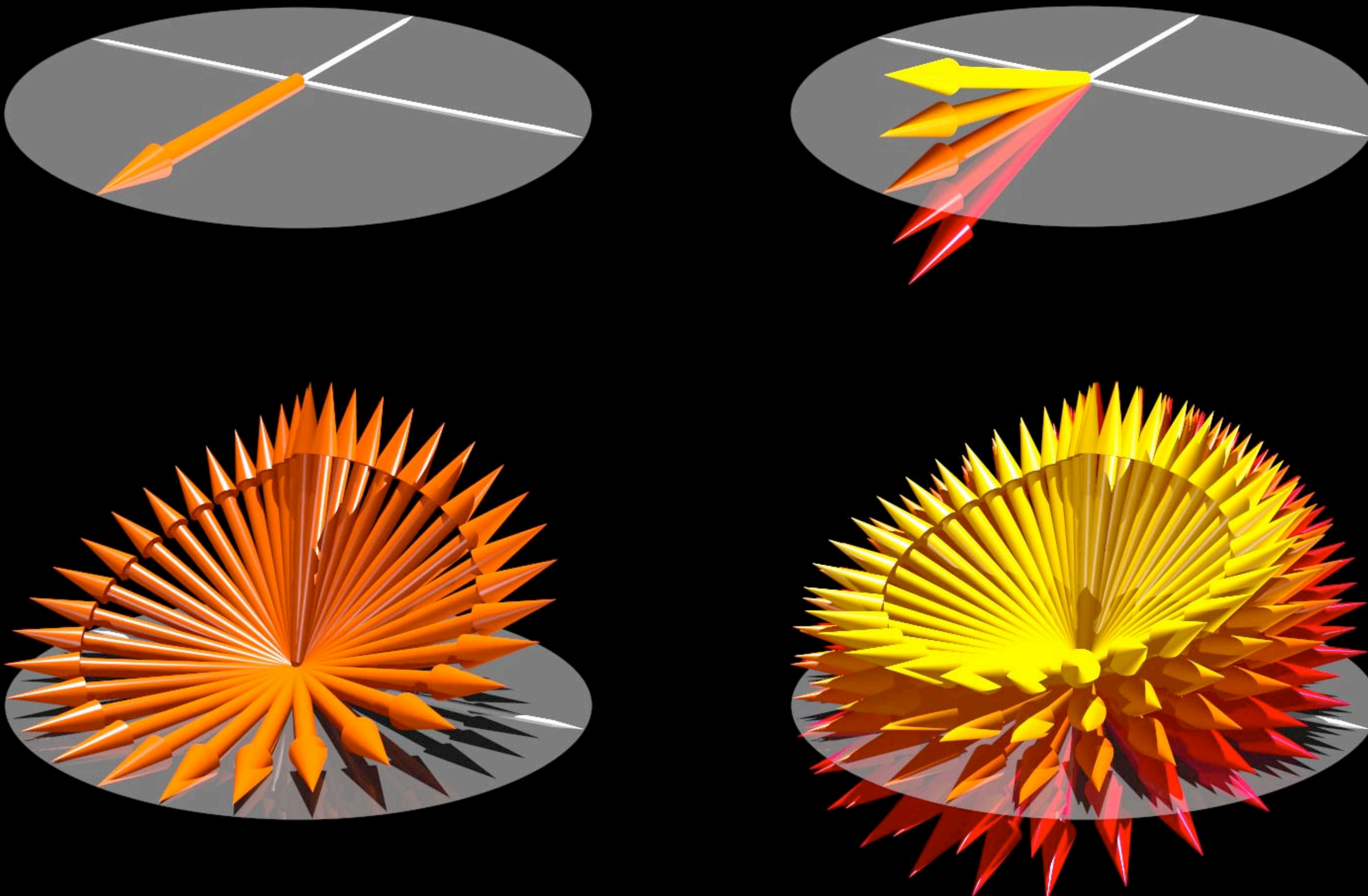

Fidelity
Robustness
Duration

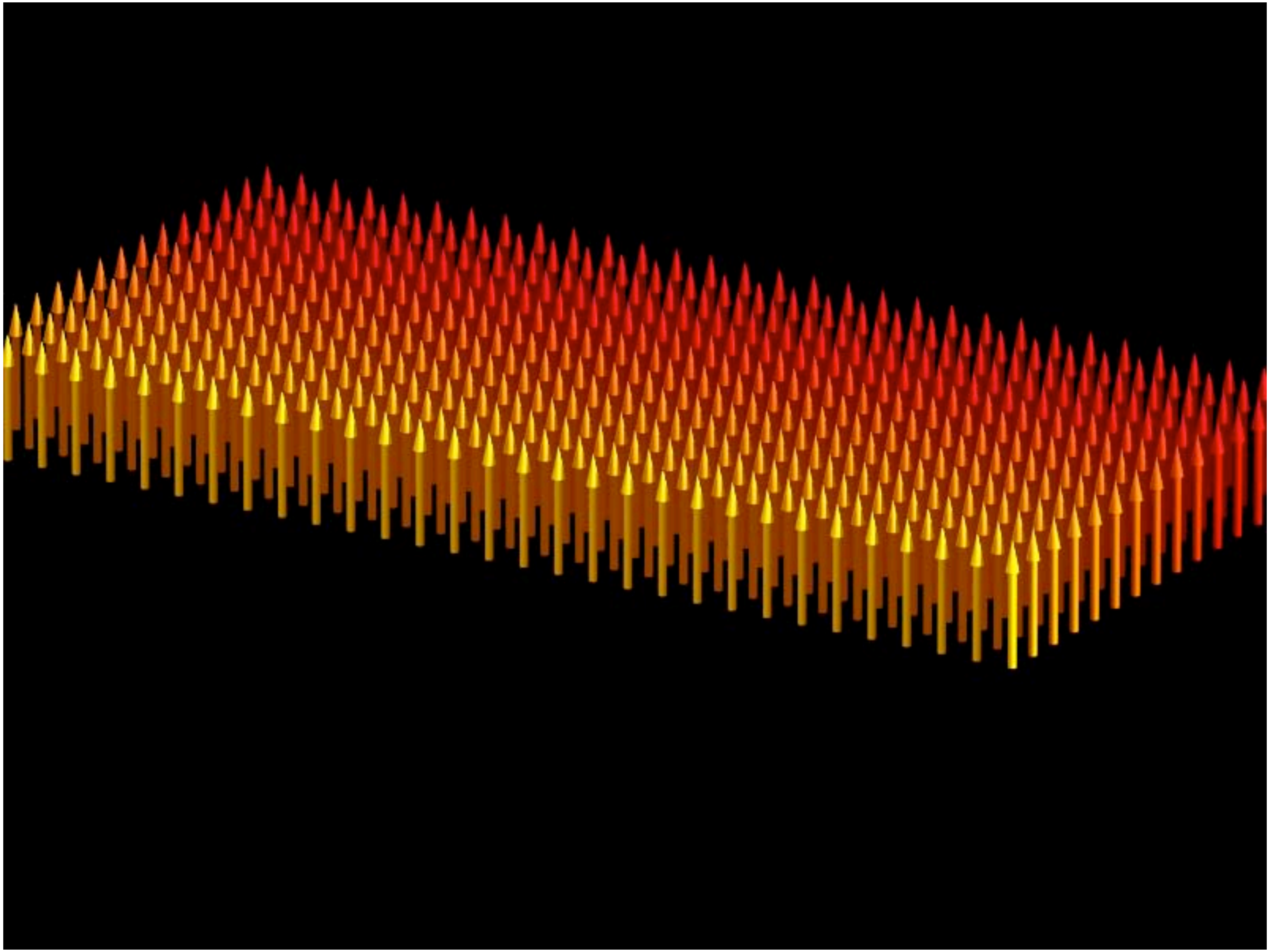


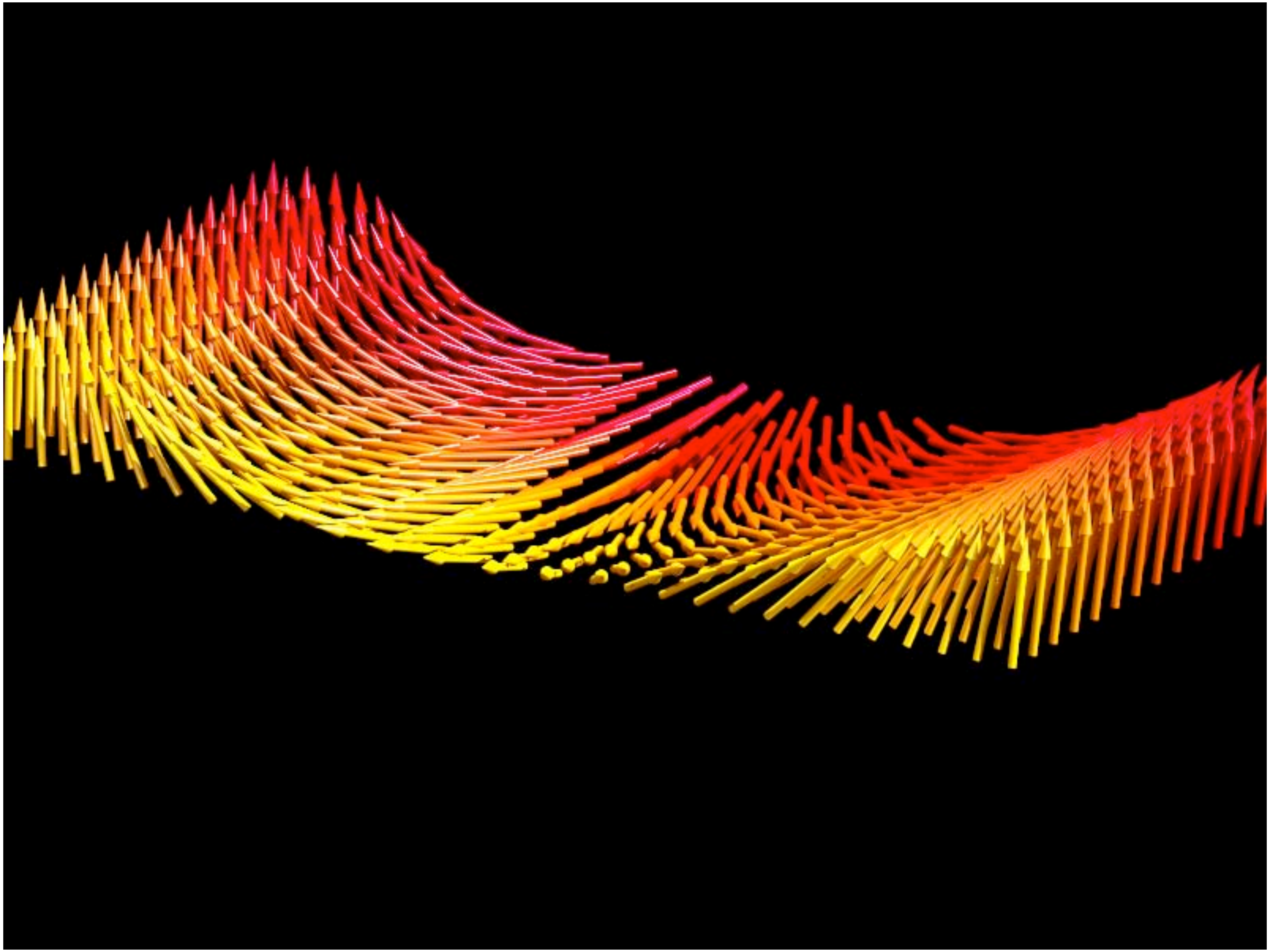



frequency dispersion

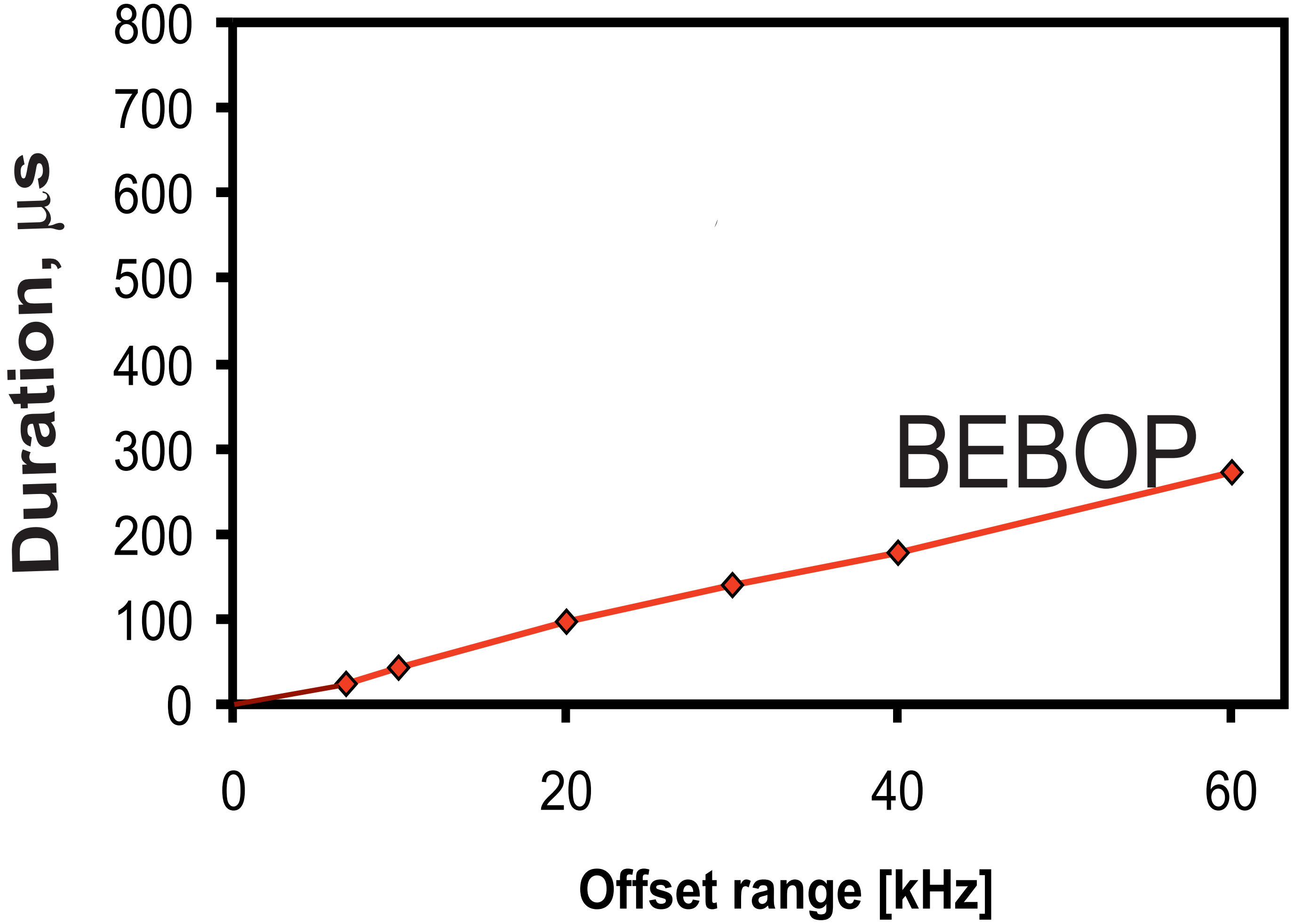








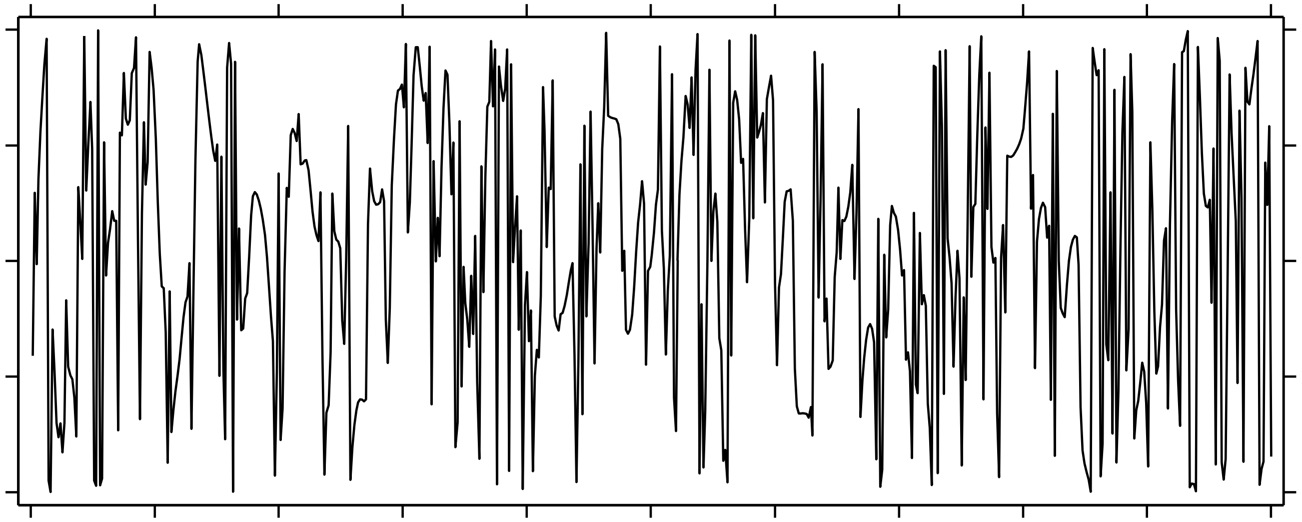
# Pulse duration as a function of offset range

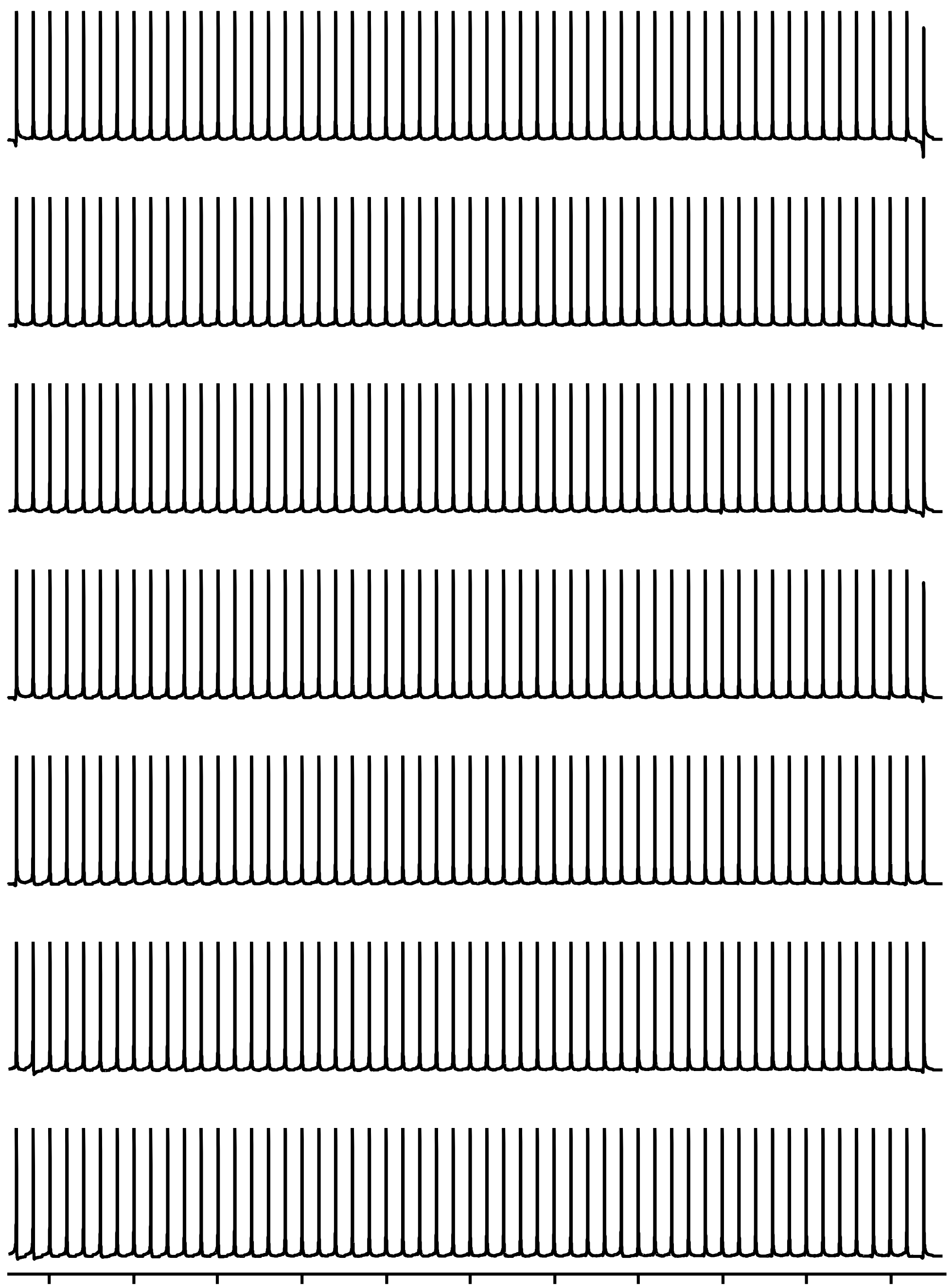



(excitation efficiency: 98%, max. rf amplitude: 10 kHz, no rf inhomogeneity)

# Robust broadband excitation pulse

PM-BEBOP

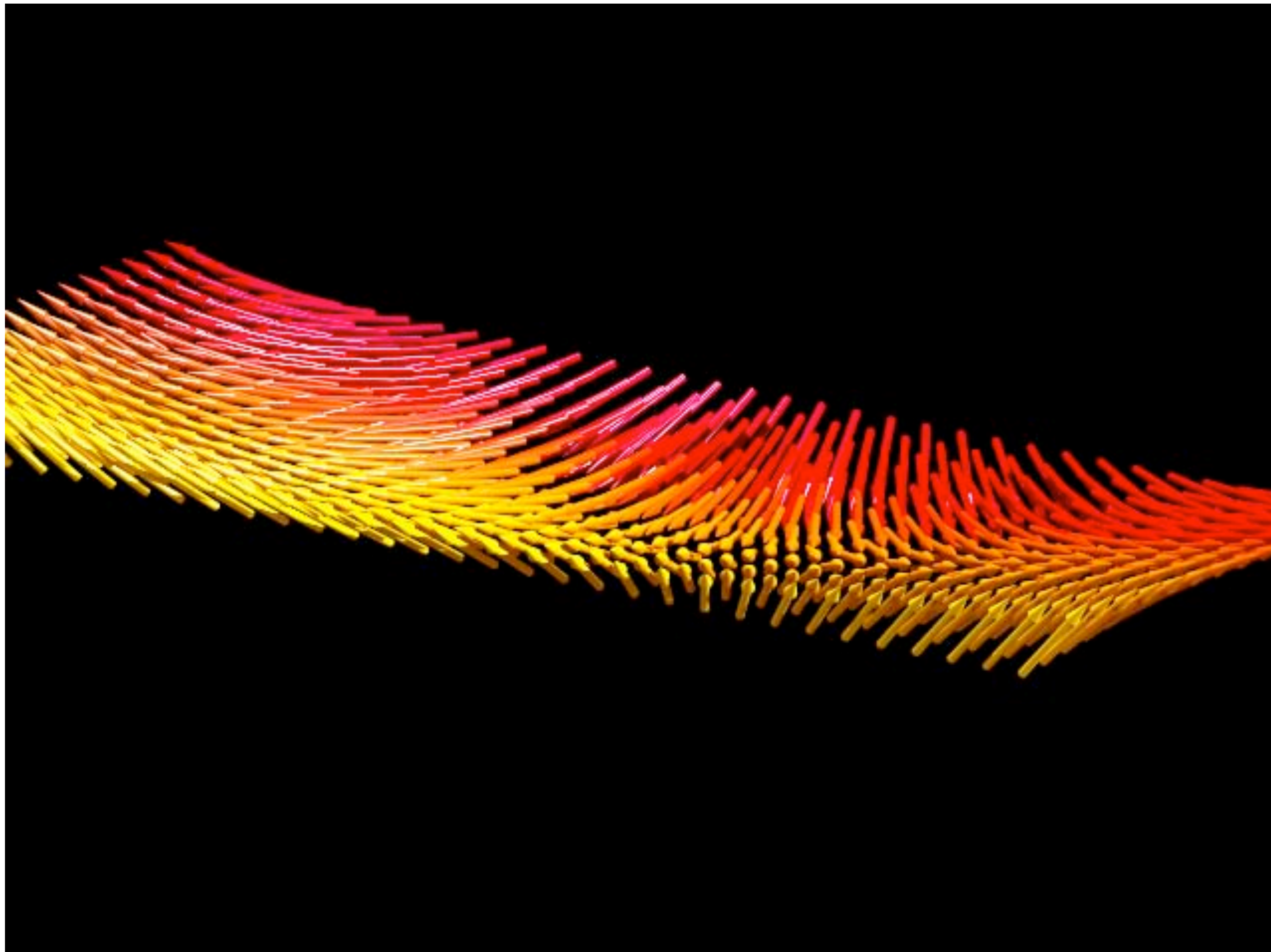


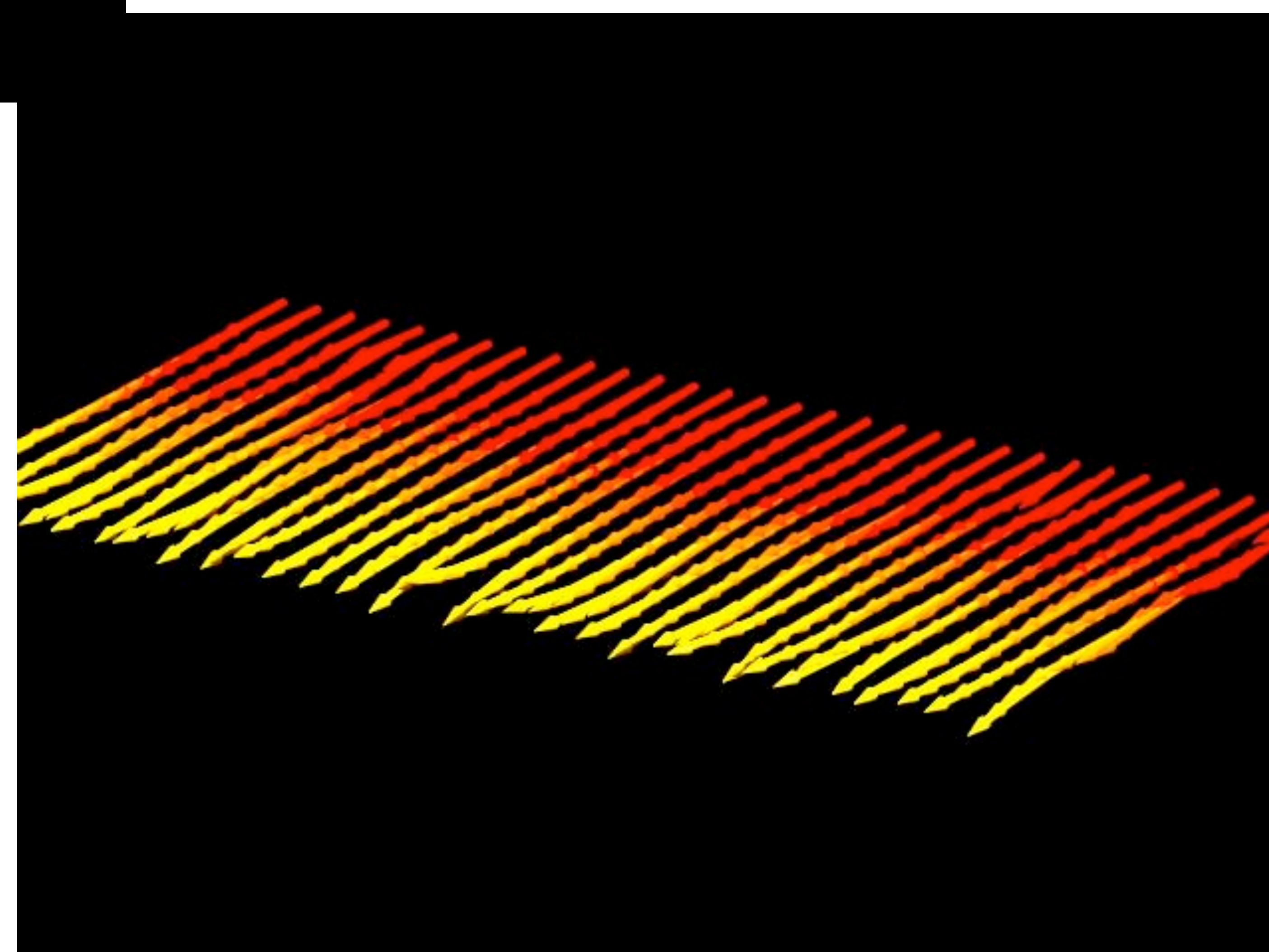


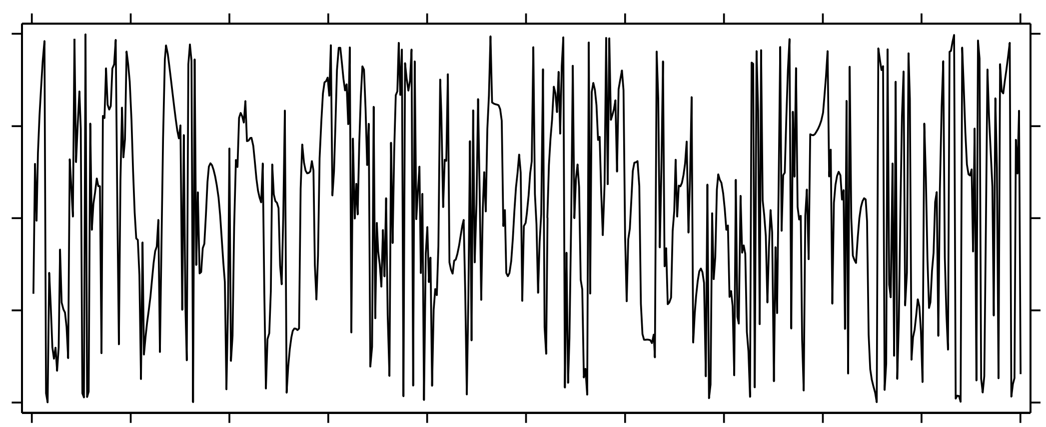
bandwidth: 50 kHz

rf amplitude: 15 kHz

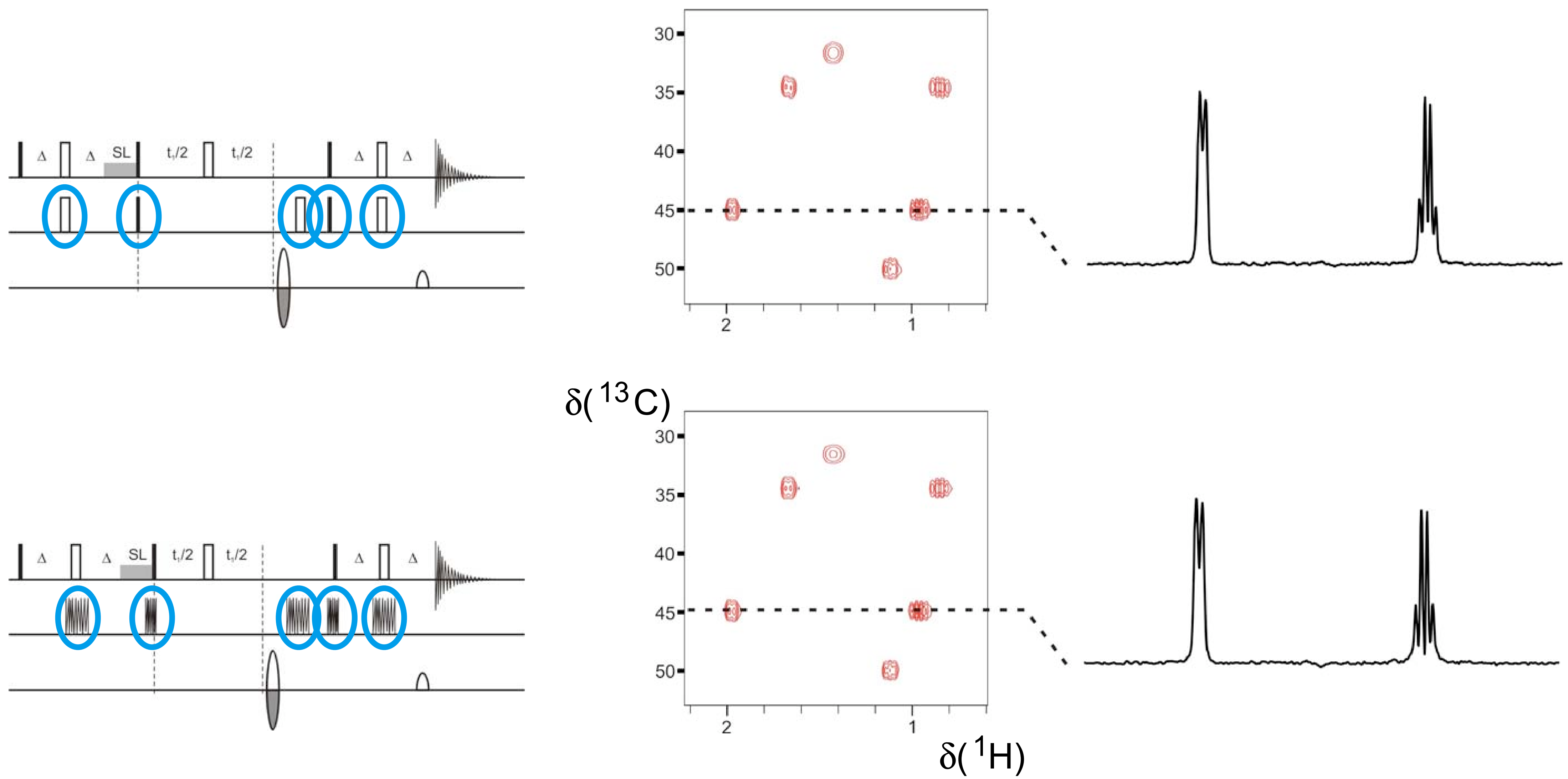
*Skinner et al. (2006)*







# Robust 90° and 180° BEBOP $^{13}C$ pulses applied to HSQC

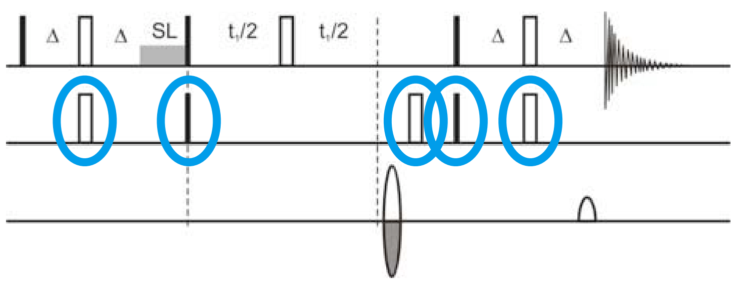


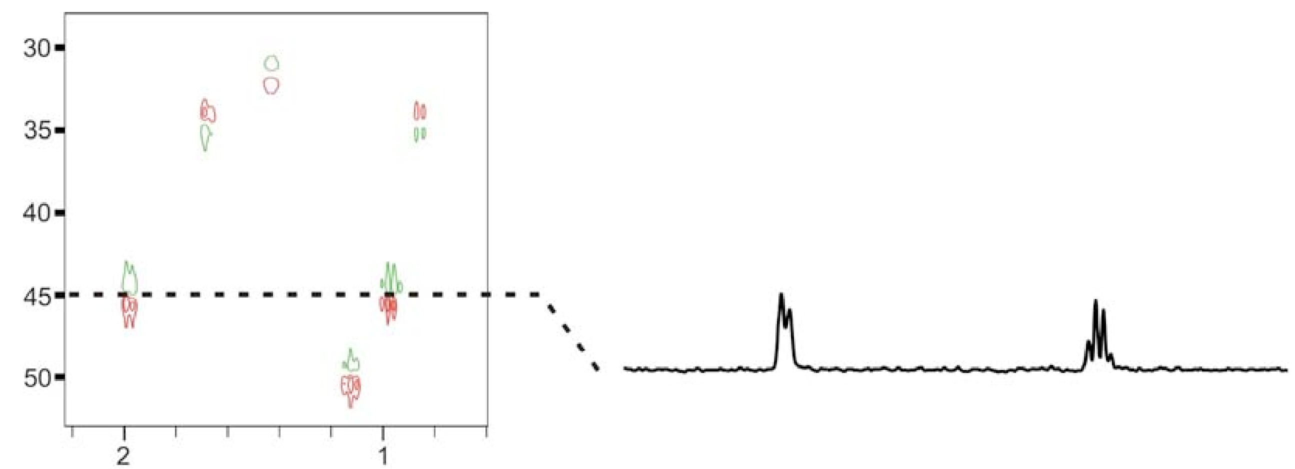

calibrated, no offset

*Skinner, Kobzar, Luy, Bendall, Bermel, Khaneja, Glaser, JMR 179, 241(2006)*

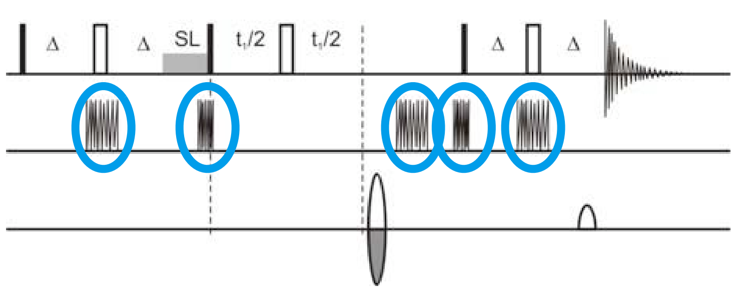
# Robust 90° and 180° BEBOP $^{13}$C pulses applied to HSQC

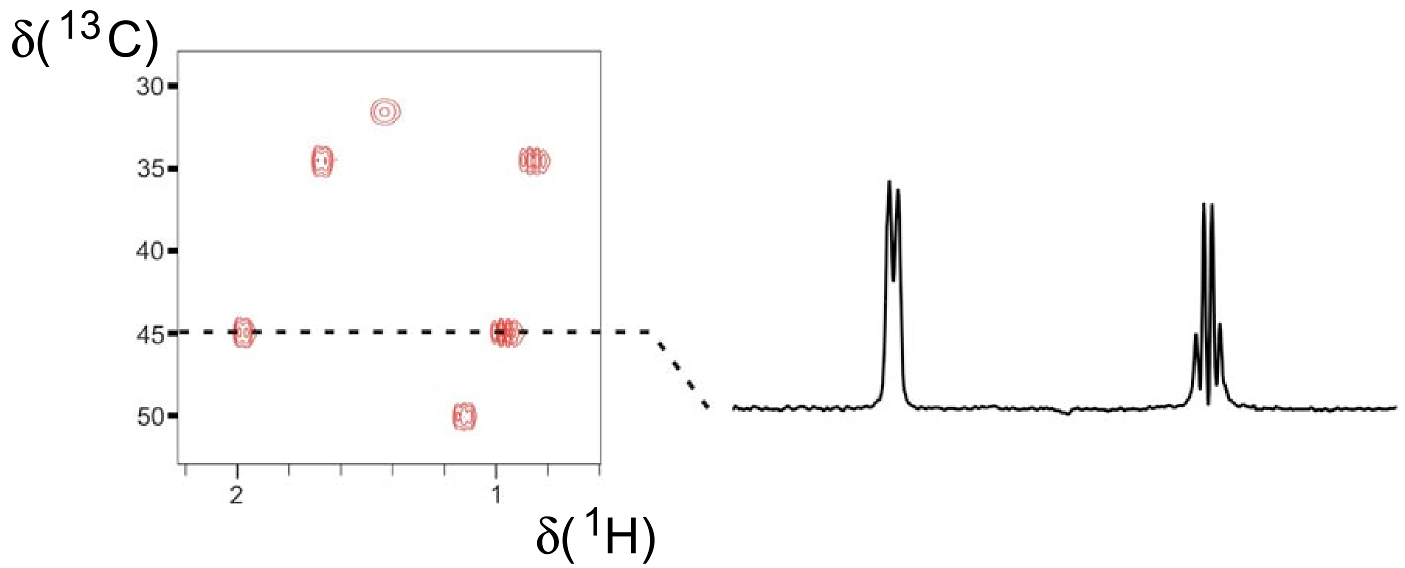
conventional HSQC




$^{13}$C-BEBOP HSQC

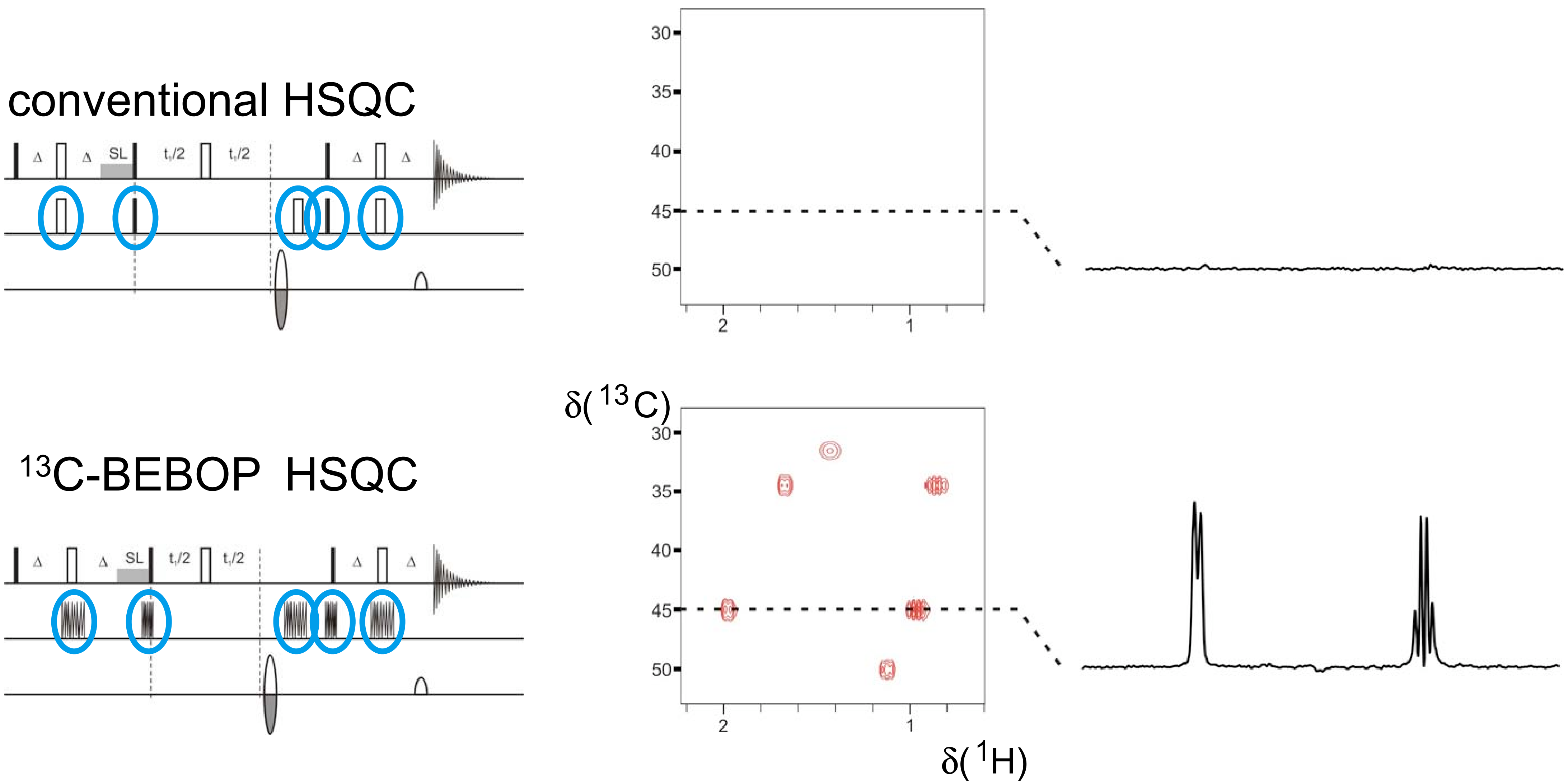



miscalibrated by 3dB, 8 kHz offset

*Skinner, Kobzar, Luy, Bendall, Bermel, Khaneja, Glaser, JMR 179, 241(2006)*

# Robust 90° and 180° BEBOP $^{13}C$ pulses applied to HSQC




miscalibrated by 3dB, 16 kHz offset

*Skinner, Kobzar, Luy, Bendall, Bermel, Khaneja, Glaser, JMR 179, 241(2006)*