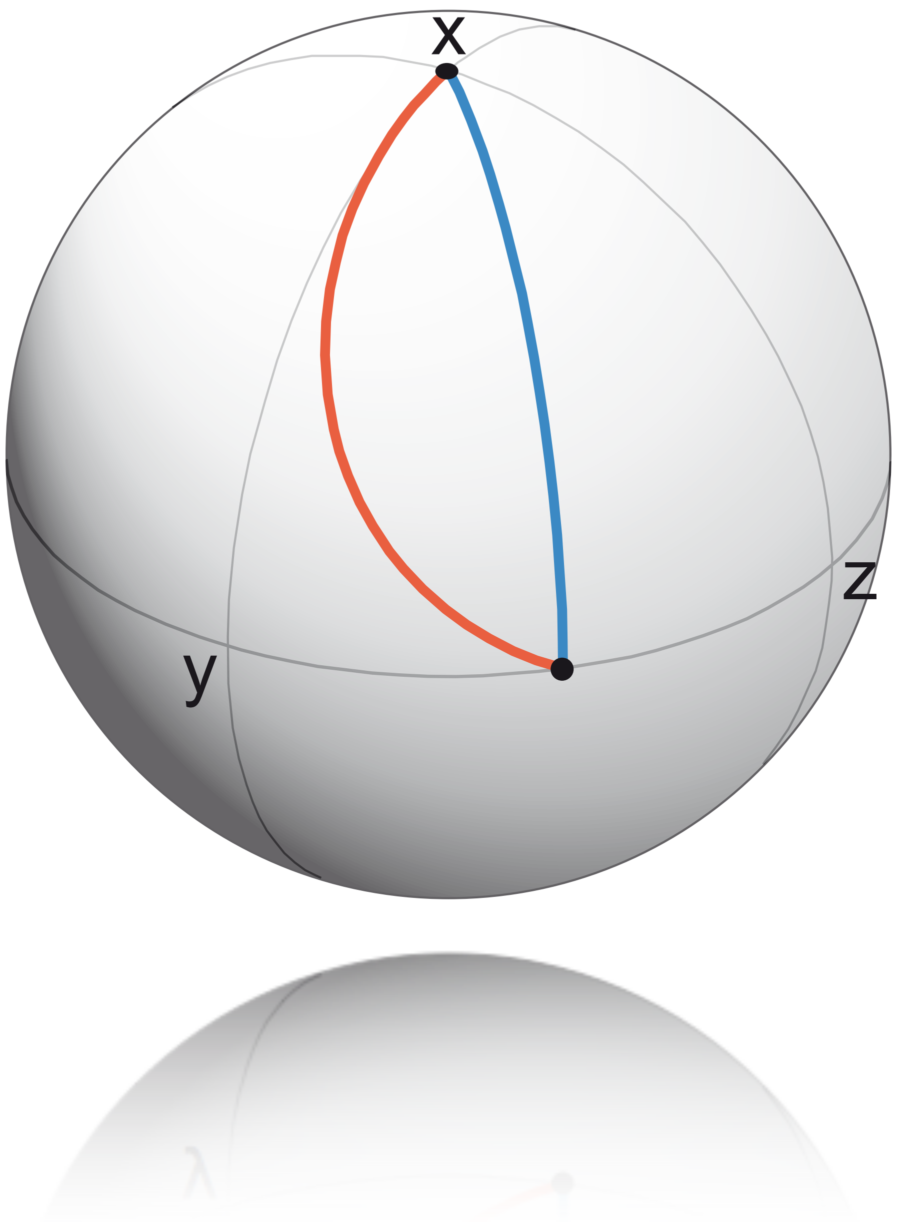
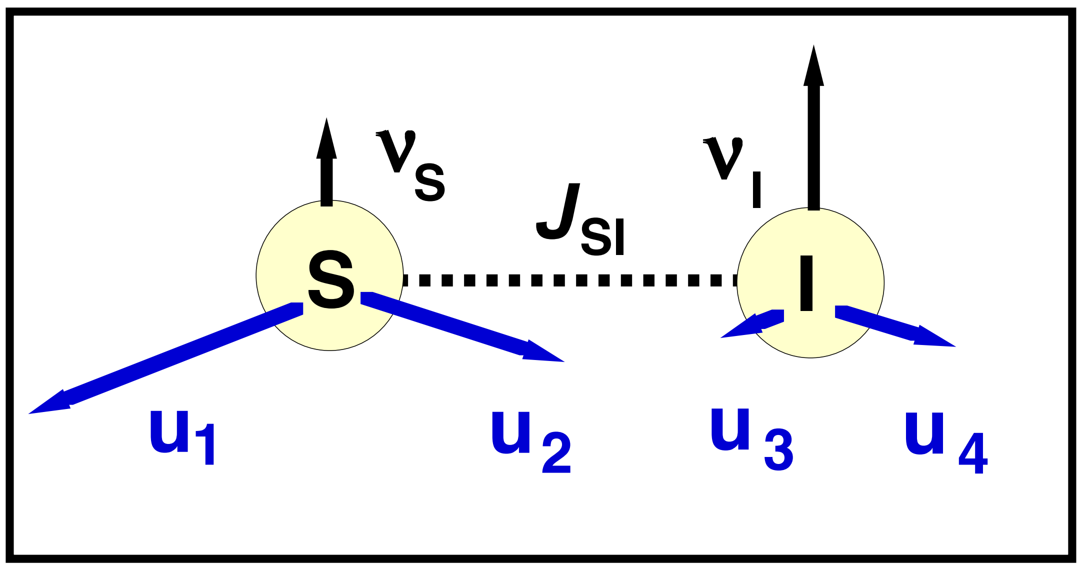


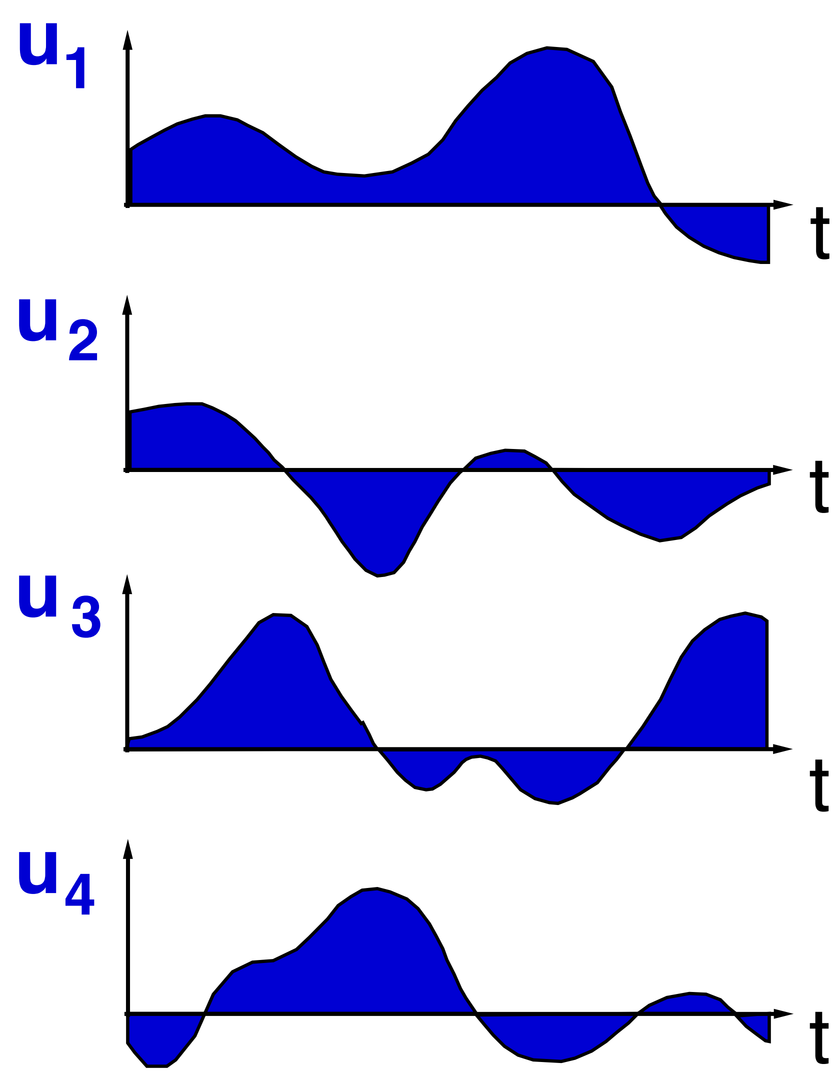
GRAPE,
Robust Control and
Quantum Gate Design Metric

Steffen Glaser, *TU München*

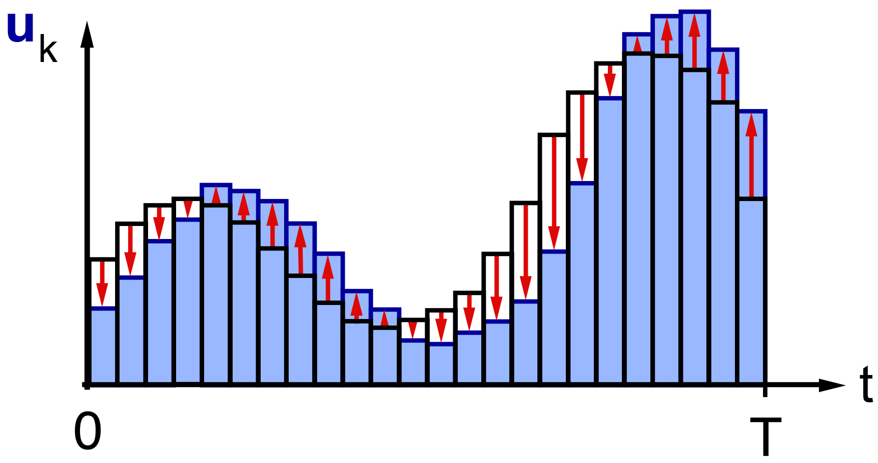
Control Parameters u_k (t)



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



GRAPE (Gradient Ascent Pulse Engineering)



desired transfer: $A \longrightarrow C$

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

$\rho(0) = A$

$\lambda(T) = C$

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

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

Robust control using GRAPE algorithm: single qubit examples

References:

N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, S. J. Glaser, "Optimal Control of Coupled Spin Dynamics: Design of NMR Pulse Sequences by Gradient Ascent Algorithms", J. Magn. Reson. 172, 296-305 (2005).

T. E. Skinner, T. O. Reiss, B. Luy, N. Khaneja, S. J. Glaser, "Application of Optimal Control Theory to the Design of Broadband Excitation Pulses for High Resolution NMR", J. Magn. Reson. 163, 8-15 (2003).

T. E. Skinner, T. O. Reiss, B. Luy, N. Khaneja, S. J. Glaser, "Reducing the Duration of Broadband Excitation Pulses Using Optimal Control with Limited RF Amplitude", J. Magn. Reson. 167, 68-74 (2004).

K. Kobzar, T. E. Skinner, N. Khaneja, S. J. Glaser, B. Luy, "Exploring the Limits of Broadband Excitation and Inversion Pulses", J. Magn. Reson. 170, 236-243 (2004).

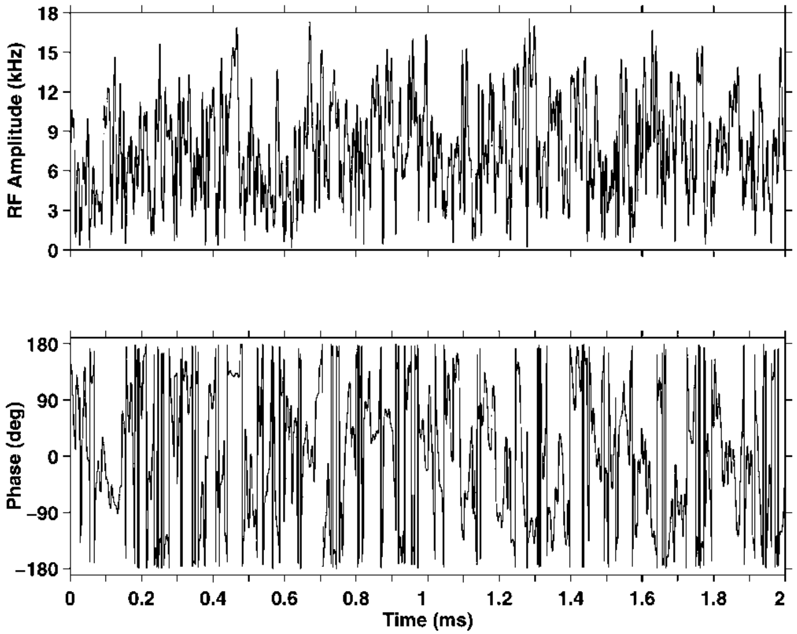
T. E. Skinner, T. O. Reiss, B. Luy, N. Khaneja, S. J. Glaser, "Tailoring the Optimal Control Cost Function to a Desired Output: Application to Minimizing Phase Errors in Short Broadband Excitation Pulses", J. Magn. Reson., 172, 17-23 (2005).

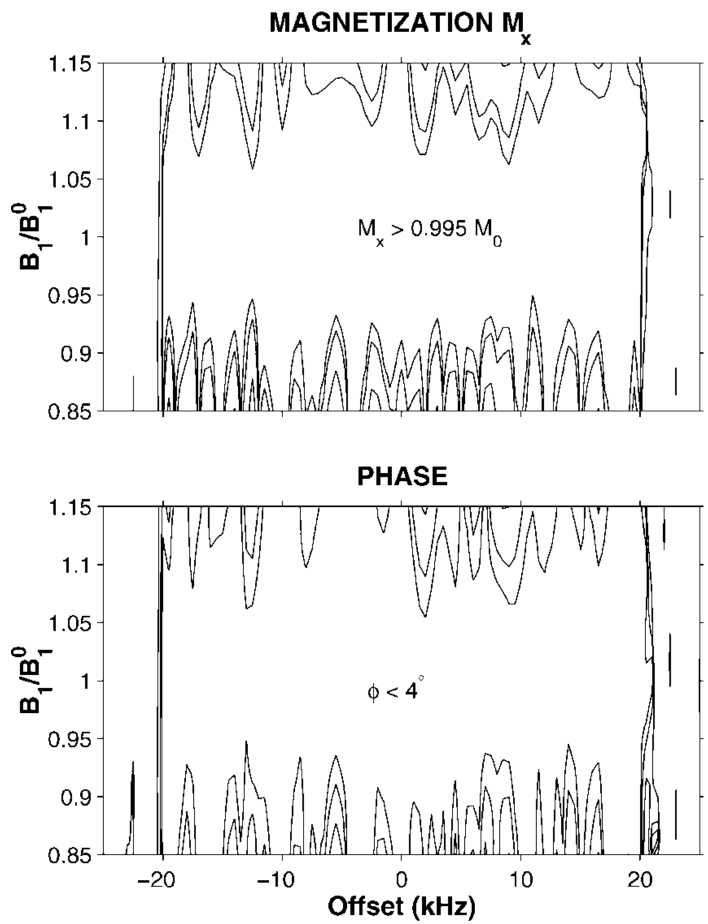
T. E. Skinner, K. Kobzar, B. Luy, R. Bendall, W. Bermel, N. Khaneja, S. J. Glaser, "Optimal Control Design of Constant Amplitude Phase-Modulated Pulses: Application to Calibration-Free Broadband Excitation", J. Magn. Reson. 179, 241-249 (2006).

B. Luy, K. Kobzar, T. E. Skinner, N. Khaneja, S. J. Glaser, "Construction of Universal Rotations from Point to Point Transformations", J. Magn. Reson. 176, 179-186 (2005).

Robust control of a single spin

Control fields

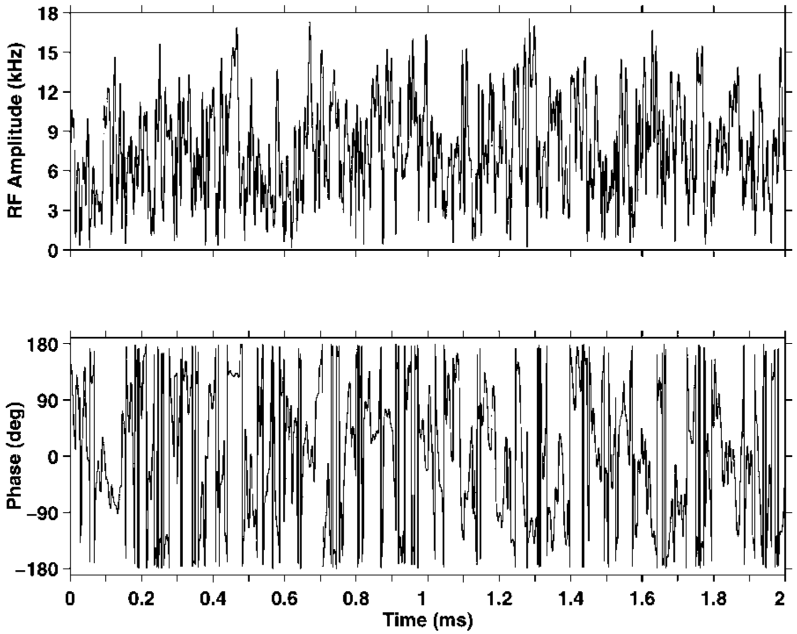


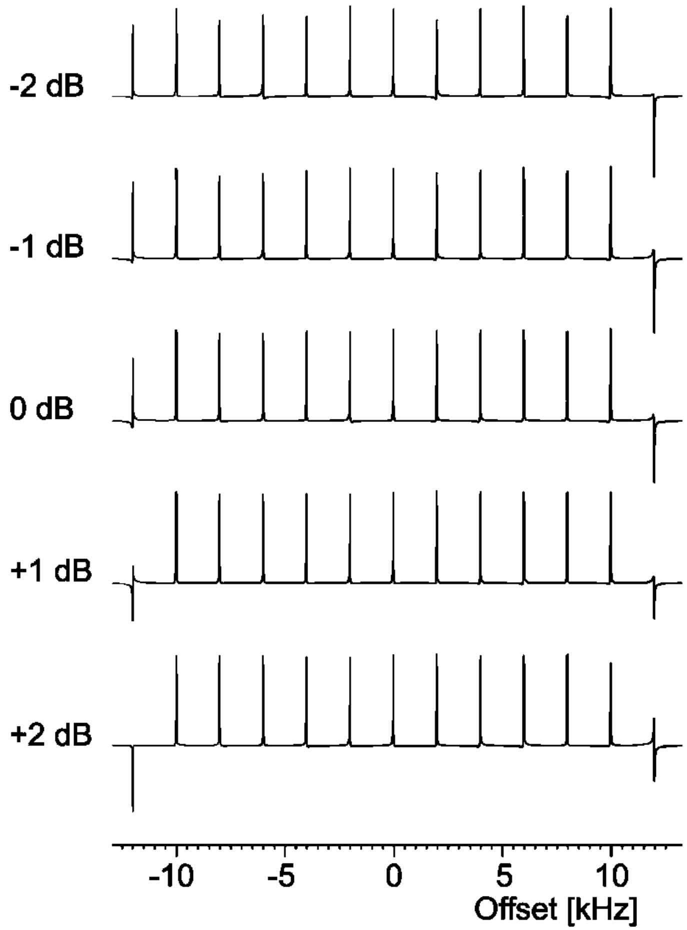


Skinner, Reiss, Khaneja, Luy, Glaser (2003)

Robust control of a single qubit

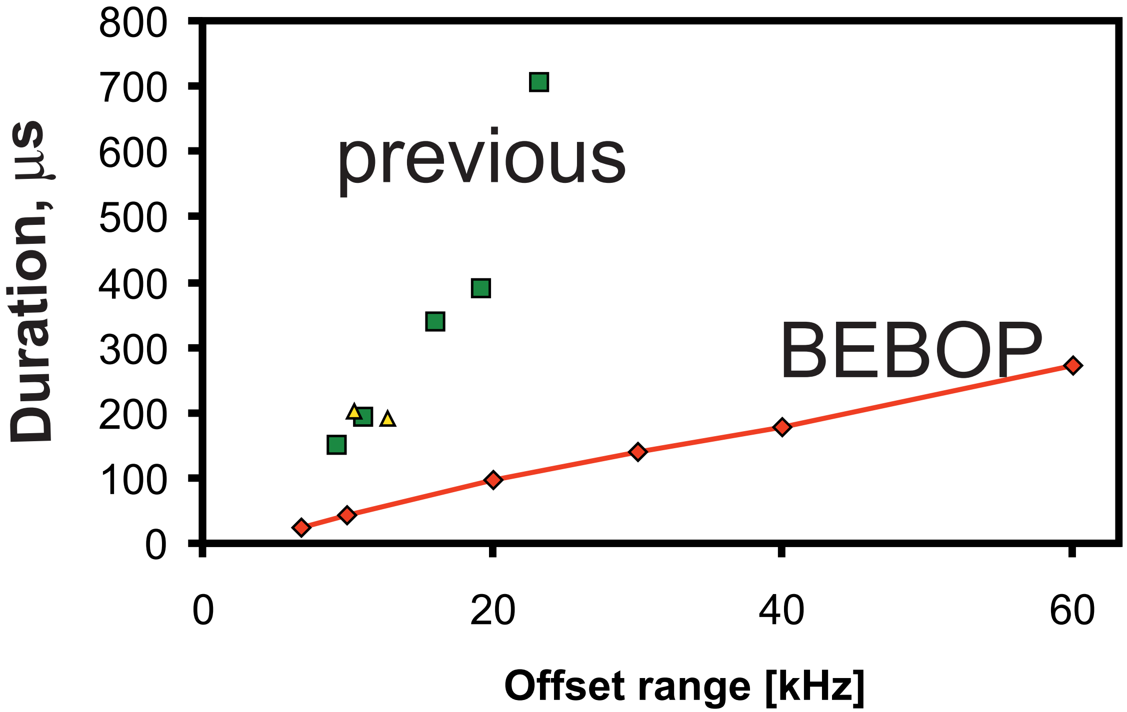
Control fields





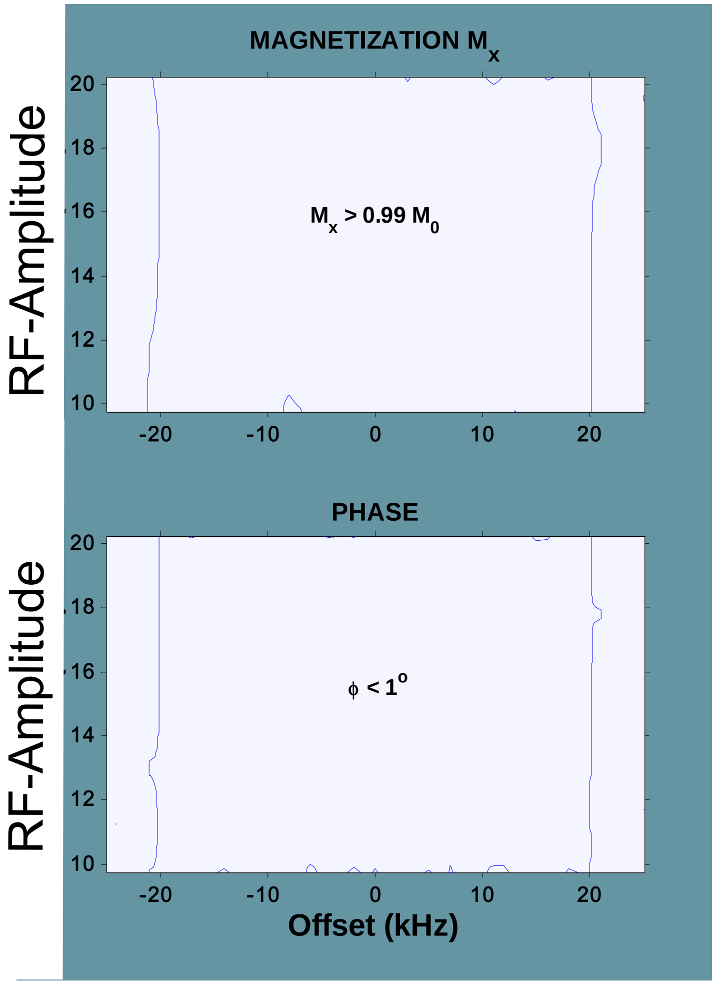
Skinner, Reiss, Khaneja, Luy, Glaser (2003)

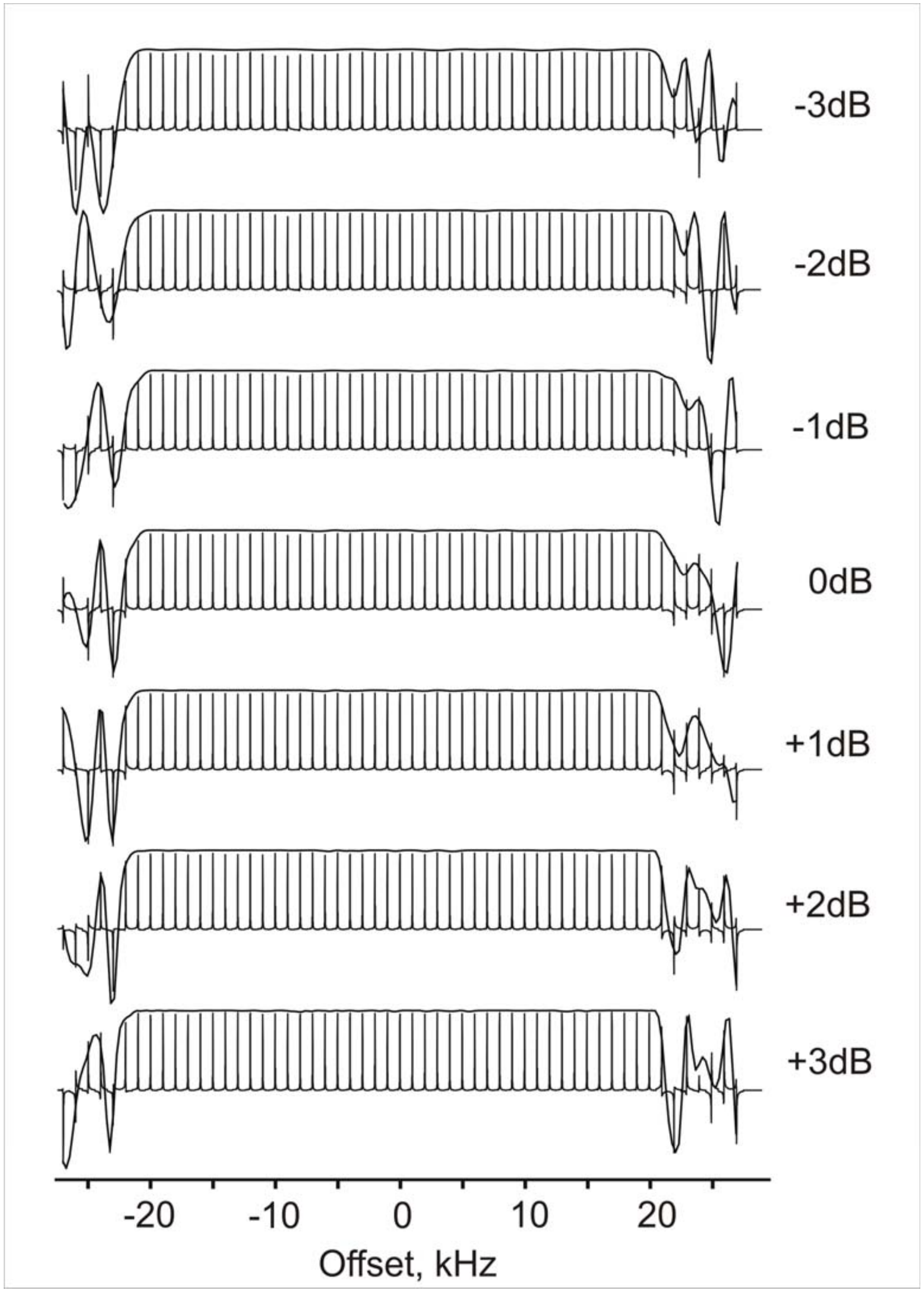
Previous excitation pulses with the same performance are significantly longer than optimized pulses (BEBOP)



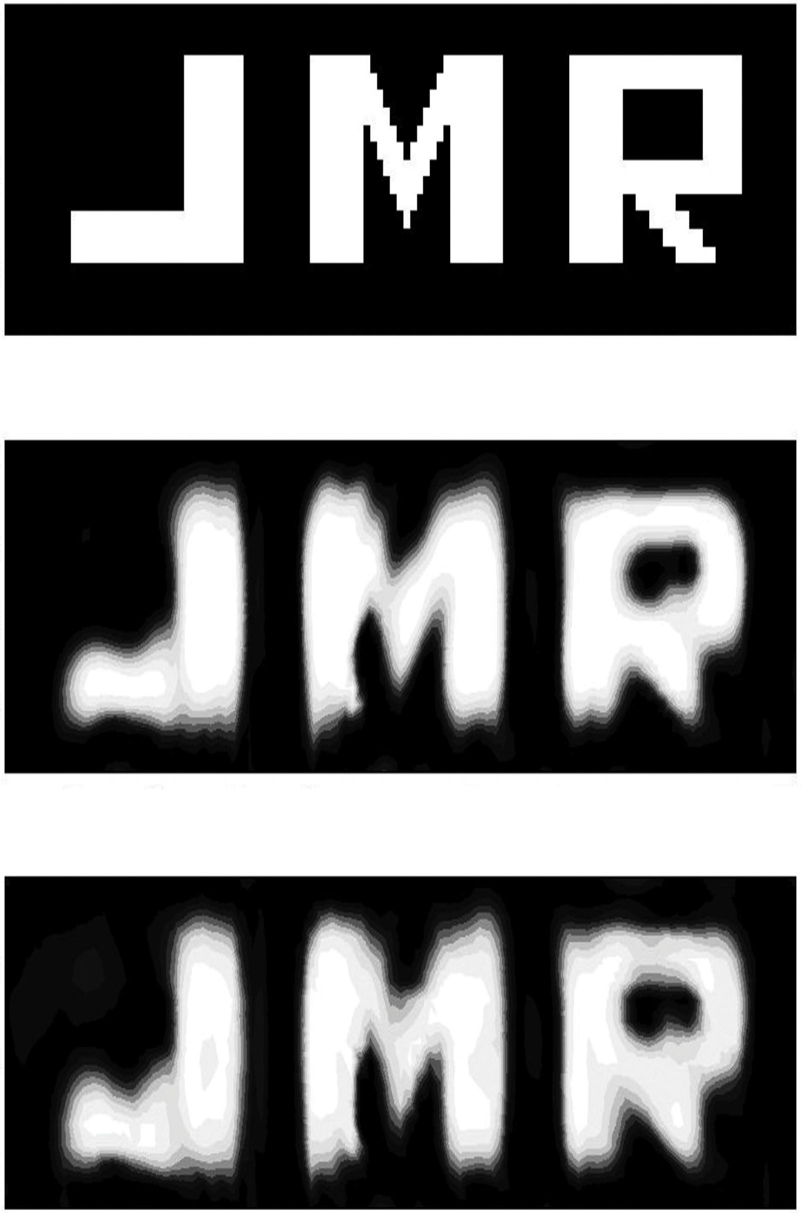
(excitation efficiency: 98%, max. rf amplitude: 10 kHz, no rf inhomogeneity)

robust, broadband excitation pulse

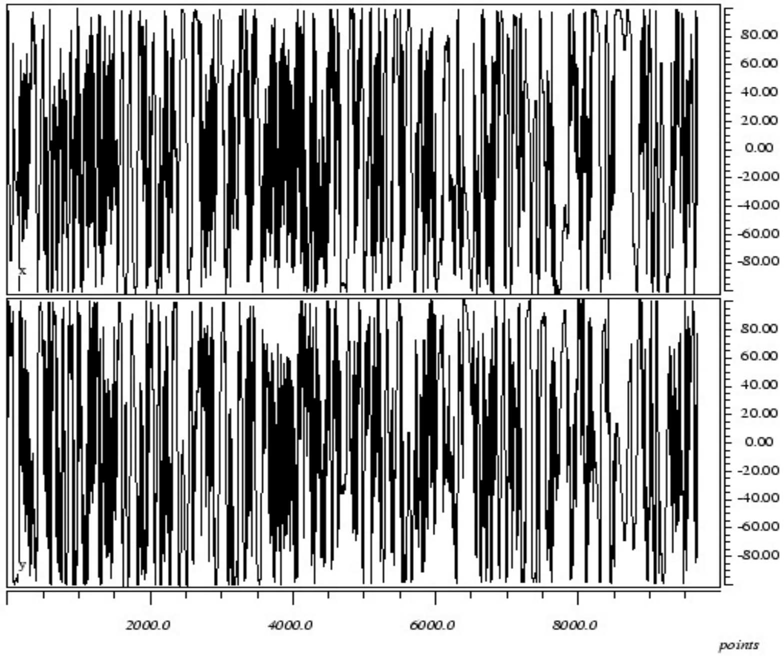




Pattern Pulses

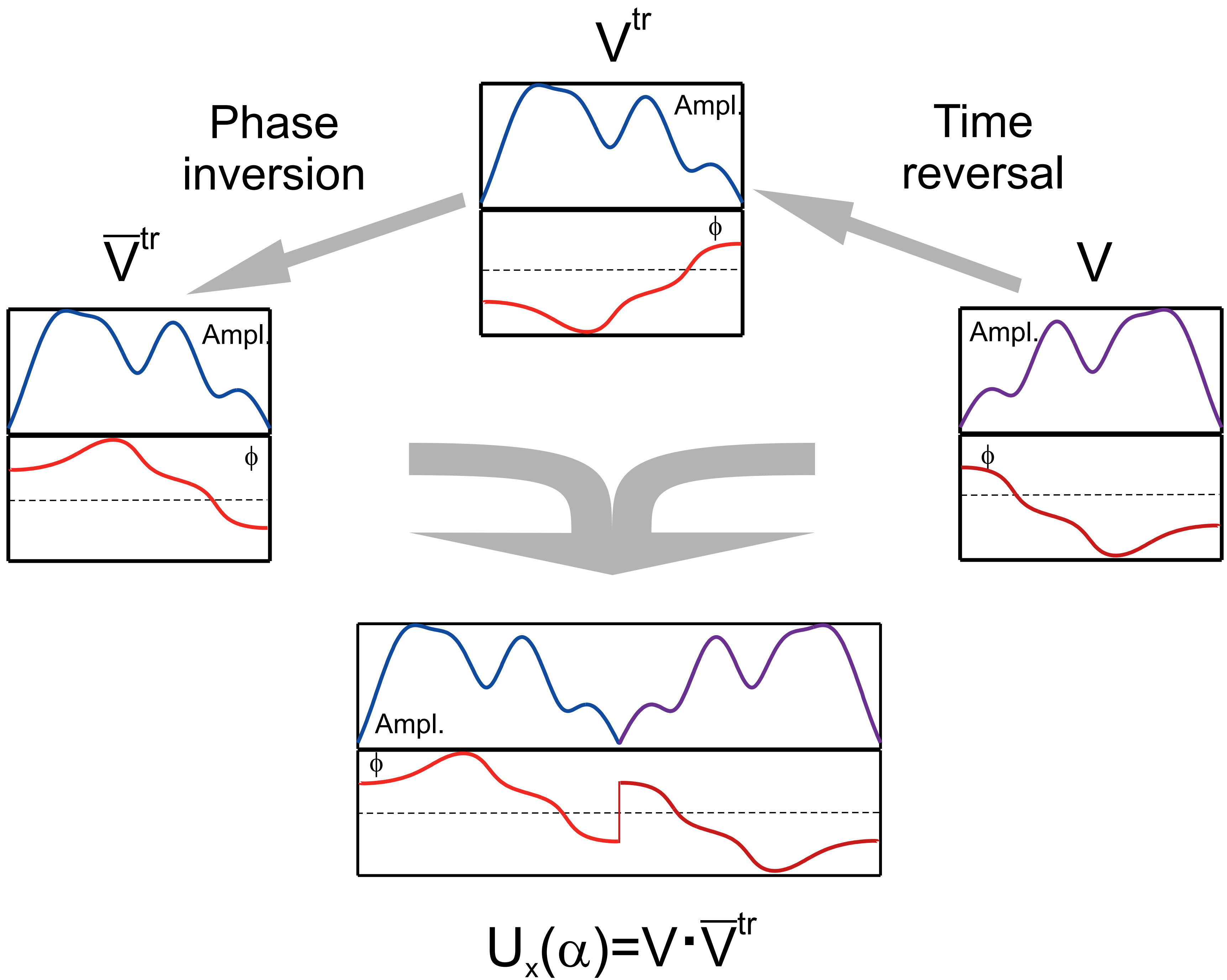


rf amplitude (x)



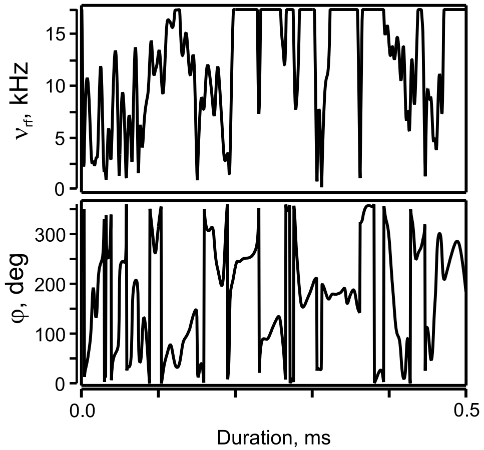
rf amplitude (y)

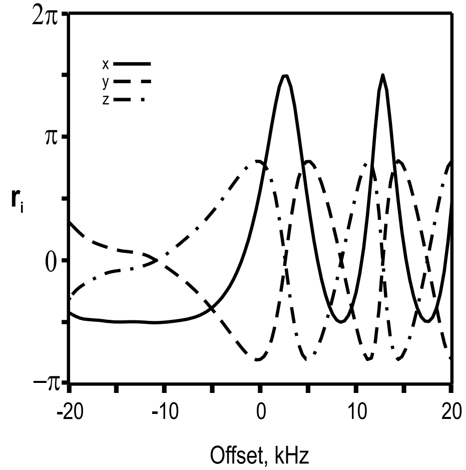
Kobzar et al., J. Magn. Reson. (2005)

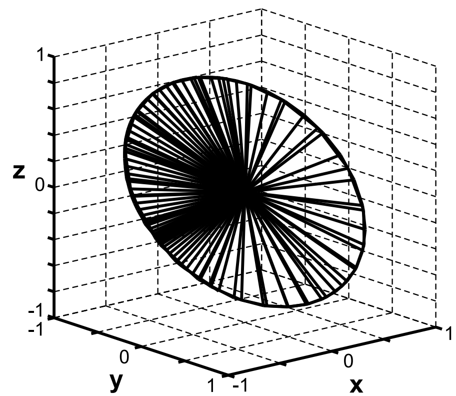


V^{tr}
Phase inversion
Time reversal
$\overline{V}^{tr}$
V
Ampl.
ϕ
Ampl.
ϕ
Ampl.
ϕ
Ampl.
ϕ
$U_x(\alpha)=V\cdot\overline{V}^{tr}$

From excitation to refocussing pulse



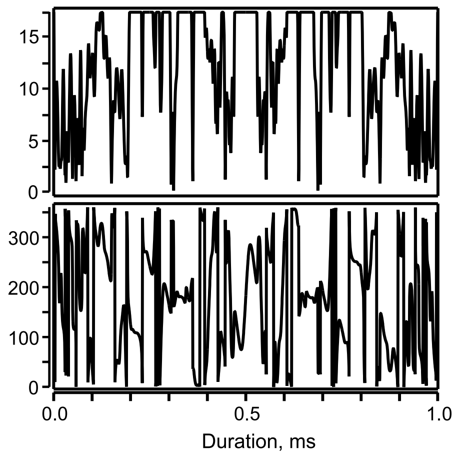


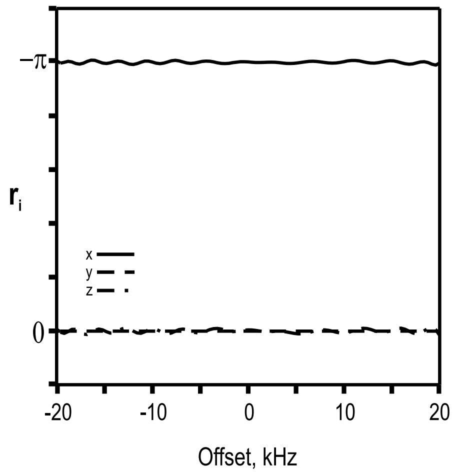


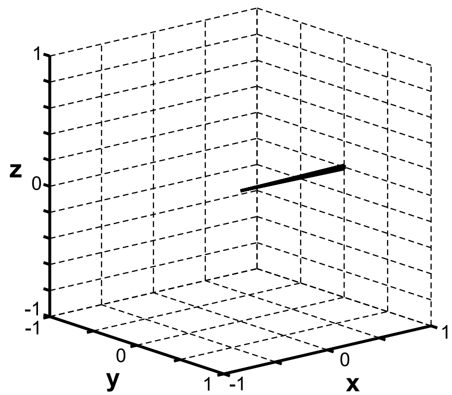
amplitude and phase of pulse sequence

components of rotation vector

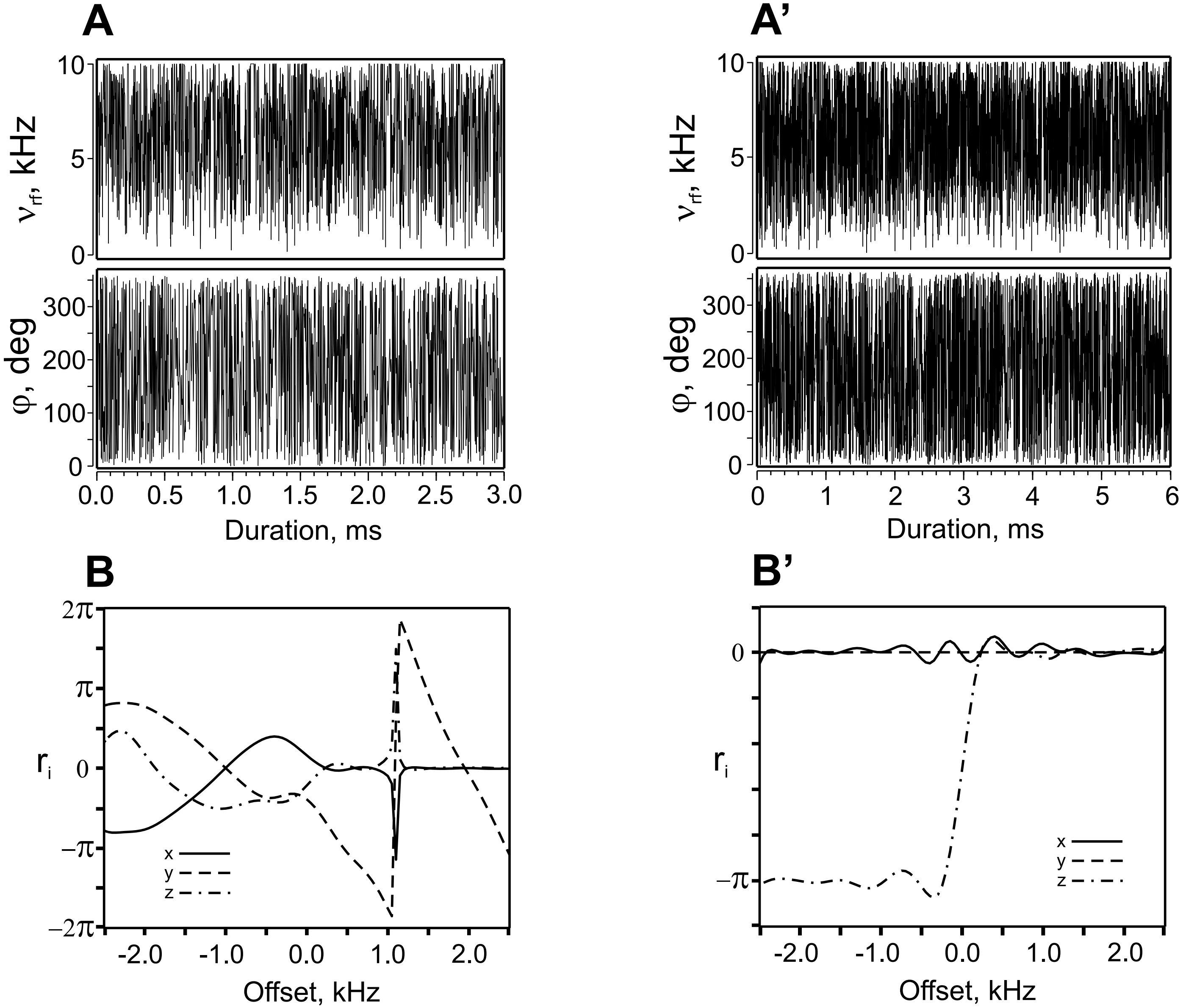
orientation of rotation vector



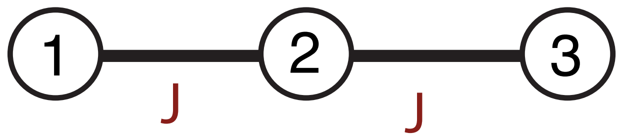




Construction of a band-selective 180°_z rotation



Time-Optimal Simulation of Trilinear Coupling Terms



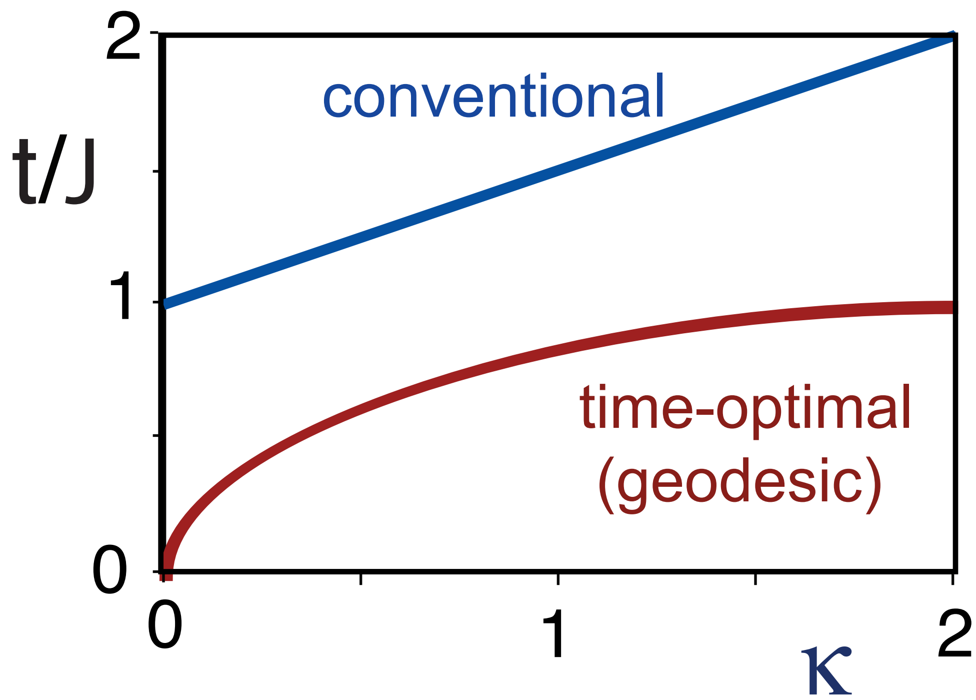
given:

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

desired:

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

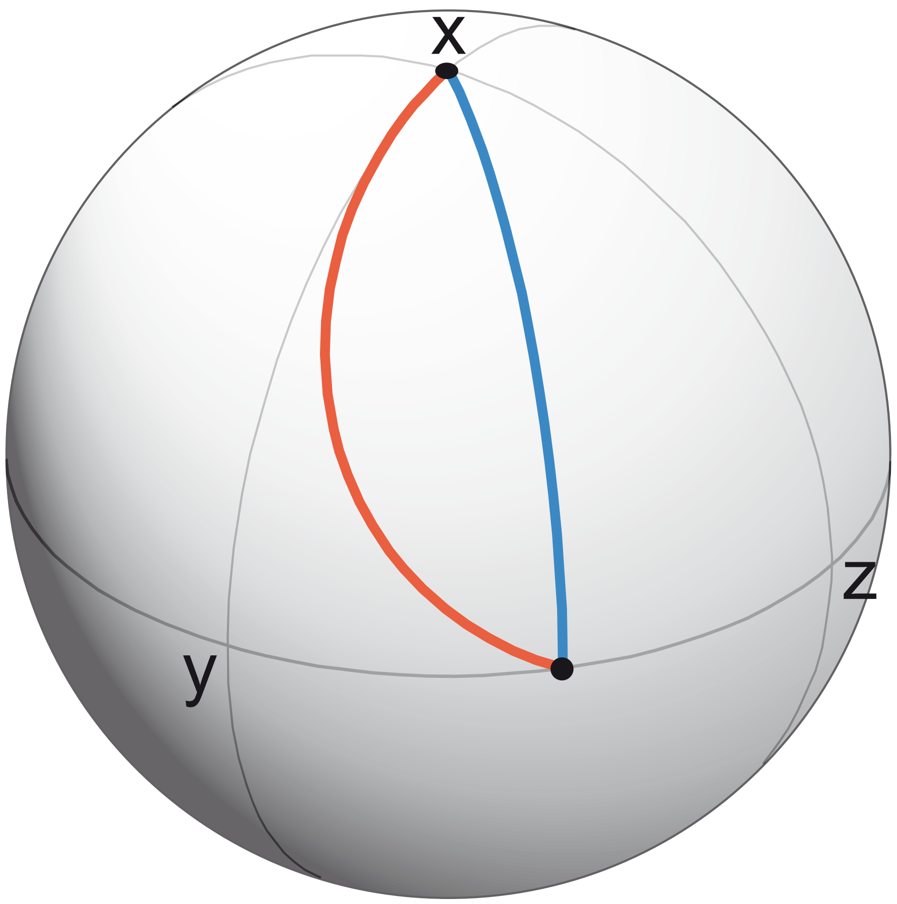
$$U = \exp\{-i\,\kappa\, 2\pi\, I_{1z} I_{2z} I_{3z}\}$$



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

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

Geodesics on a sphere



Euklidian metric

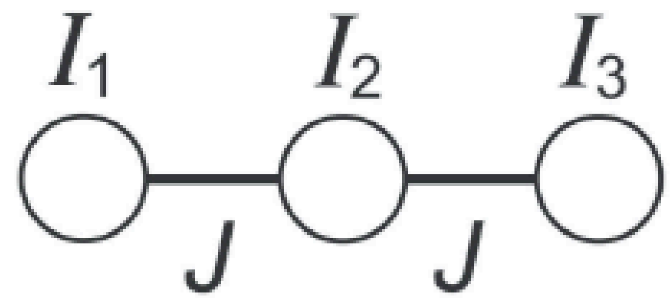
$$(dx)^2 + (dy)^2 + (dz)^2$$

“quantum gate design metric”

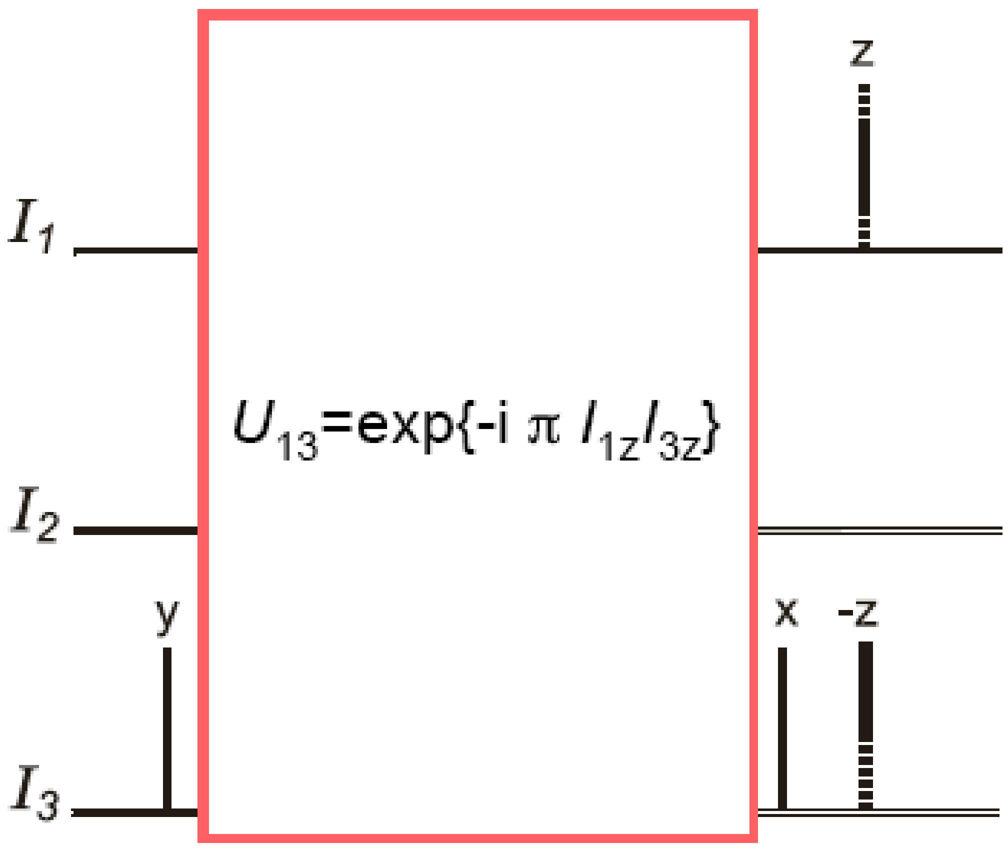
$$\frac{(dx)^2 + (dz)^2}{y^2}$$

Khaneja et al., Phys. Rev. A 75, 012322 (2007).

Generating CNOT(1,3)



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



$$\mathcal{U}_{13} = \exp\left\{-i\frac{\pi}{2}2I_{1z}I_{3z}\right\}$$

$$x = (x_1, x_2, x_3, x_4, x_5, x_6)$$

$$x_1 = \langle I_{1x} \rangle$$
$$x_2 = \langle 2 I_{1y} I_{2z} \rangle$$
$$x_3 = \langle 2 I_{1y} I_{2x} \rangle$$
$$x_4 = \langle 4 I_{1y} I_{2y} I_{3z} \rangle$$
$$x_5 = \langle 4 I_{1y} I_{2z} I_{3z} \rangle$$
$$x_6 = -\langle 2 I_{1x} I_{3z} \rangle$$

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

$$\mathcal{H}_A = u_A(t) \pi J I_{2y}$$

$$\mathcal{H}_B = u_B(t) \pi J I_{2x}$$

$$x_A = (x_1, x_2, x_3, x_4)^t$$

$$x_B = (x_3, x_4, x_5, x_6)^t$$

$$\frac{dx_{A,B}}{dt} = \pi J \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -u_{A,B} & 0 \\ 0 & u_{A,B} & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} x_{A,B}$$

$$\frac{dx_{A,B}}{dt} = \pi J \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -u_{A,B} & 0 \\ 0 & u_{A,B} & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} x_{A,B}$$

$(1,0,0,0)$ $\left(0, x_2', x_3', \frac{1}{\sqrt{2}}\right)$ $\left(0, 0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$

$x(t)=x_1(t),\ y(t)=\sqrt{x_2^2(t)+x_3^2(t)}$ and $z(t)=x_4(t)$ $\tan\,\theta(t)=\frac{x_2(t)}{x_3(t)}$

$$\frac{d}{dt}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \pi J \begin{bmatrix} 0 & -\sin\,\theta(t) & 0 \\ \sin\,\theta(t) & 0 & -\cos\,\theta(t) \\ 0 & \cos\,\theta(t) & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

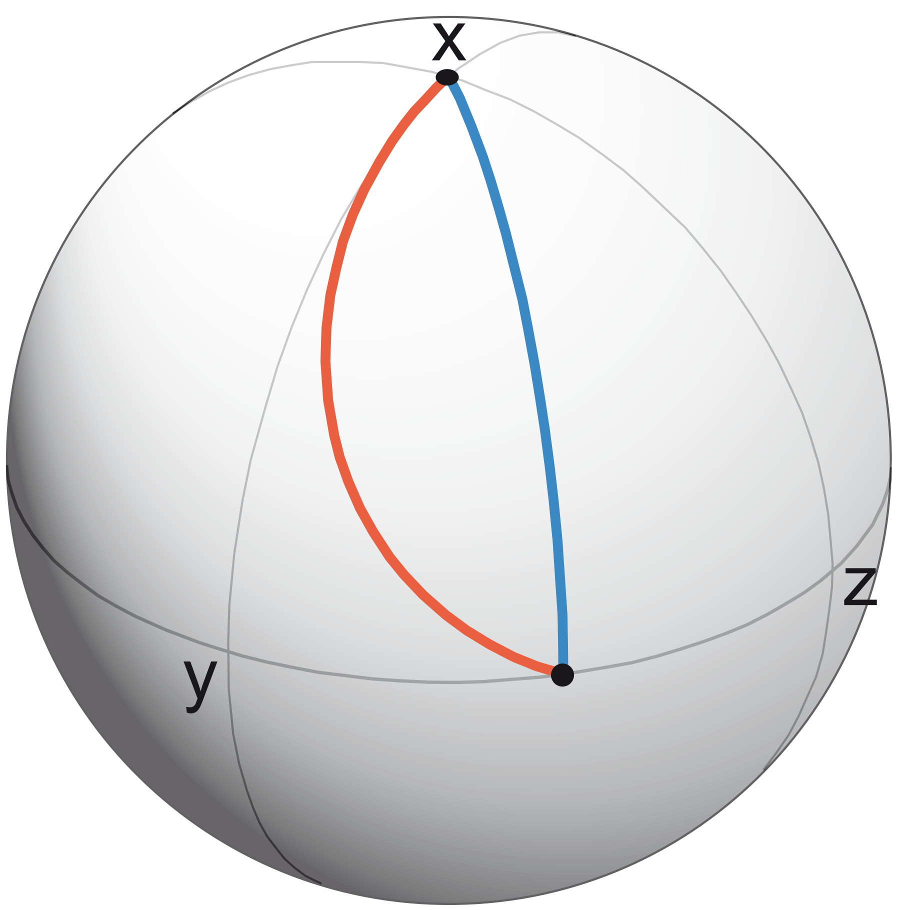
$$\frac{dx_{A,B}}{dt} = \pi J \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -u_{A,B} & 0 \\ 0 & u_{A,B} & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} x_{A,B}$$

transfer time: $\frac{1}{\pi J} \int \underbrace{\sqrt{\frac{(\dot{x})^2 + (\dot{z})^2}{y^2}}}_{L} dt$ $\qquad y^2 = 1 - x^2 - z^2$

Euler-Lagrange equations for the geodesic

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x}; \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{z}}\right) = \frac{\partial L}{\partial z}$$

Geodesics on a sphere



Euklidian metric

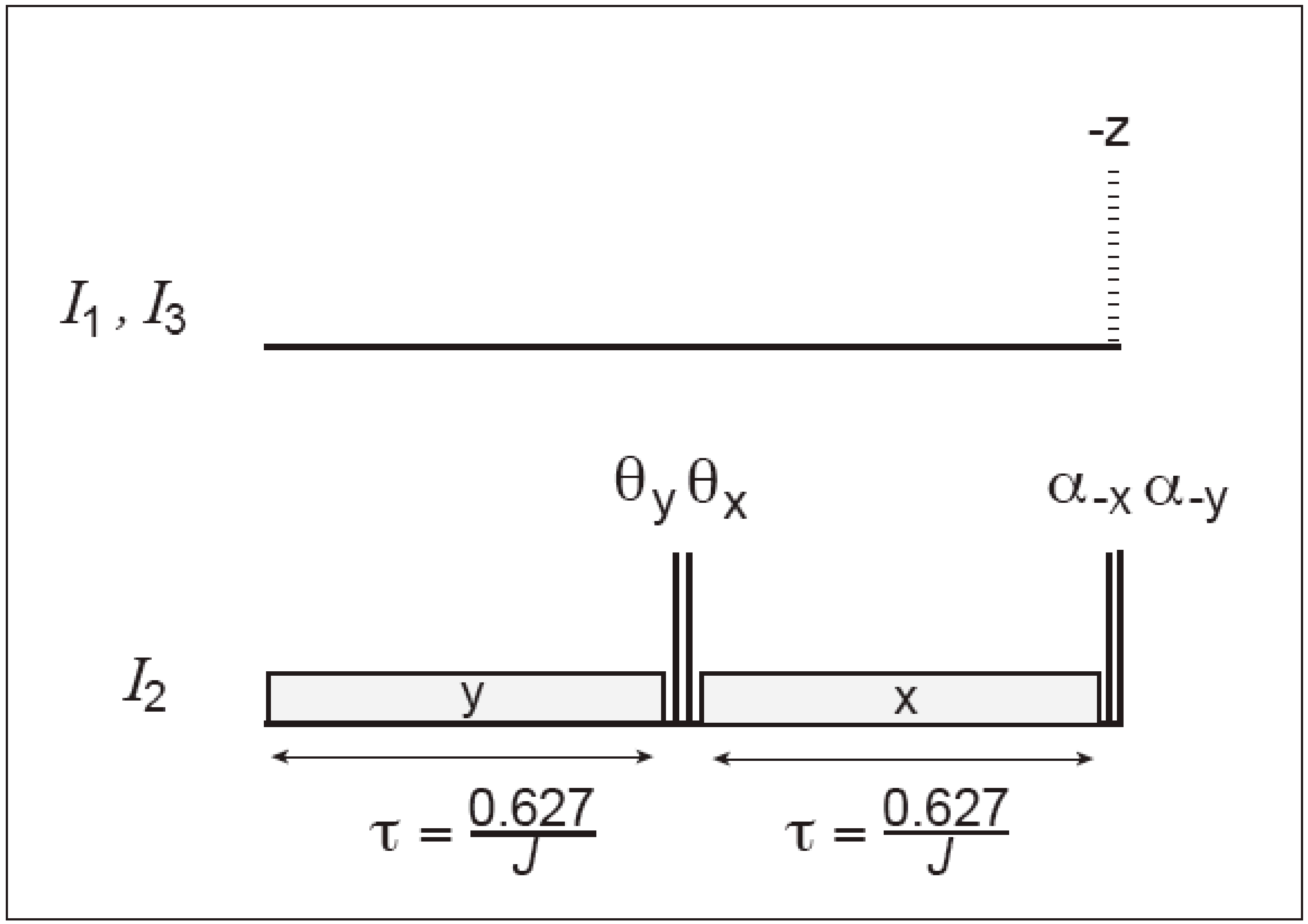
$$(dx)^2 + (dy)^2 + (dz)^2$$

"quantum gate design metric"

$$\frac{(dx)^2 + (dz)^2}{y^2}$$

Khaneja et al., Phys. Rev. A 75, 012322 (2007).

Pulse sequence for creating $U_{13}=\exp\{-i\,\pi\, I_{1z}I_{3z}\}$



$\theta=180^\circ-\alpha=31.4^\circ$, weak pulse amplitude: 0.52 J

Khaneja et al., Phys. Rev. A 75, 012322 (2007)

TABLE I. Duration τ_C of various implementations of the CNOT(1,3) gate.

Pulse sequence	τ_C (units of J^{-1})	Relative duration (%)
Sequence 1 (C1)	3.5	100
Sequence 2 (C2)	2.5	71.4
Sequence 3 (C3)	2.0	57.1
Sequence 4 (C4)	1.866	53.3
Sequence 5 (C5)	1.253	38.8

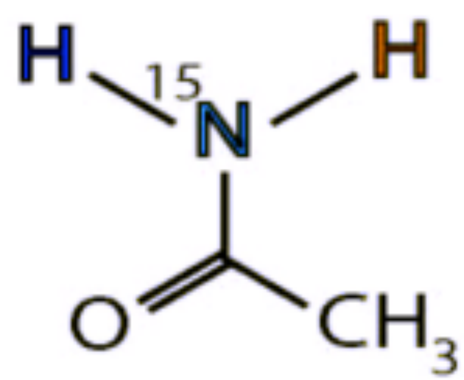
(C1, C2) D. Collins, K. W. Kim, W. C. Holton, H. Sierzputowska-Gracz, and E. O. Stejskal, Phys. Rev. A **62**, 022304 (2000).

(C3, C4, C5) *Khaneja et al., Phys. Rev. A 75, 012322 (2007)*

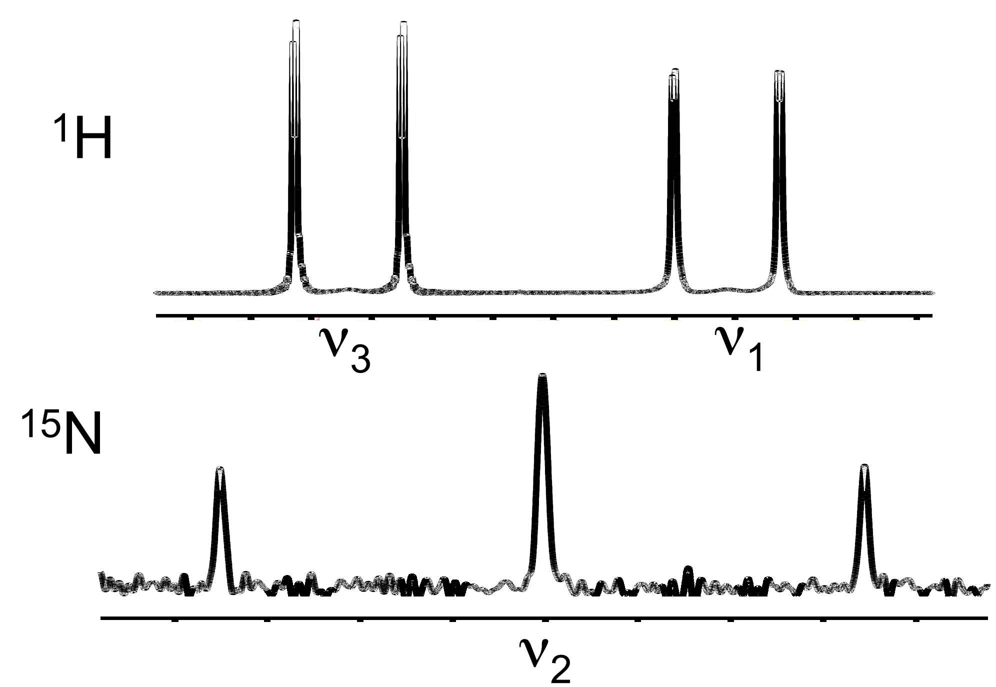
Experimental Demonstration

Solvent: DMSO-d_6
Temp.: 295 K
Bruker 500 Avance Spectrometer

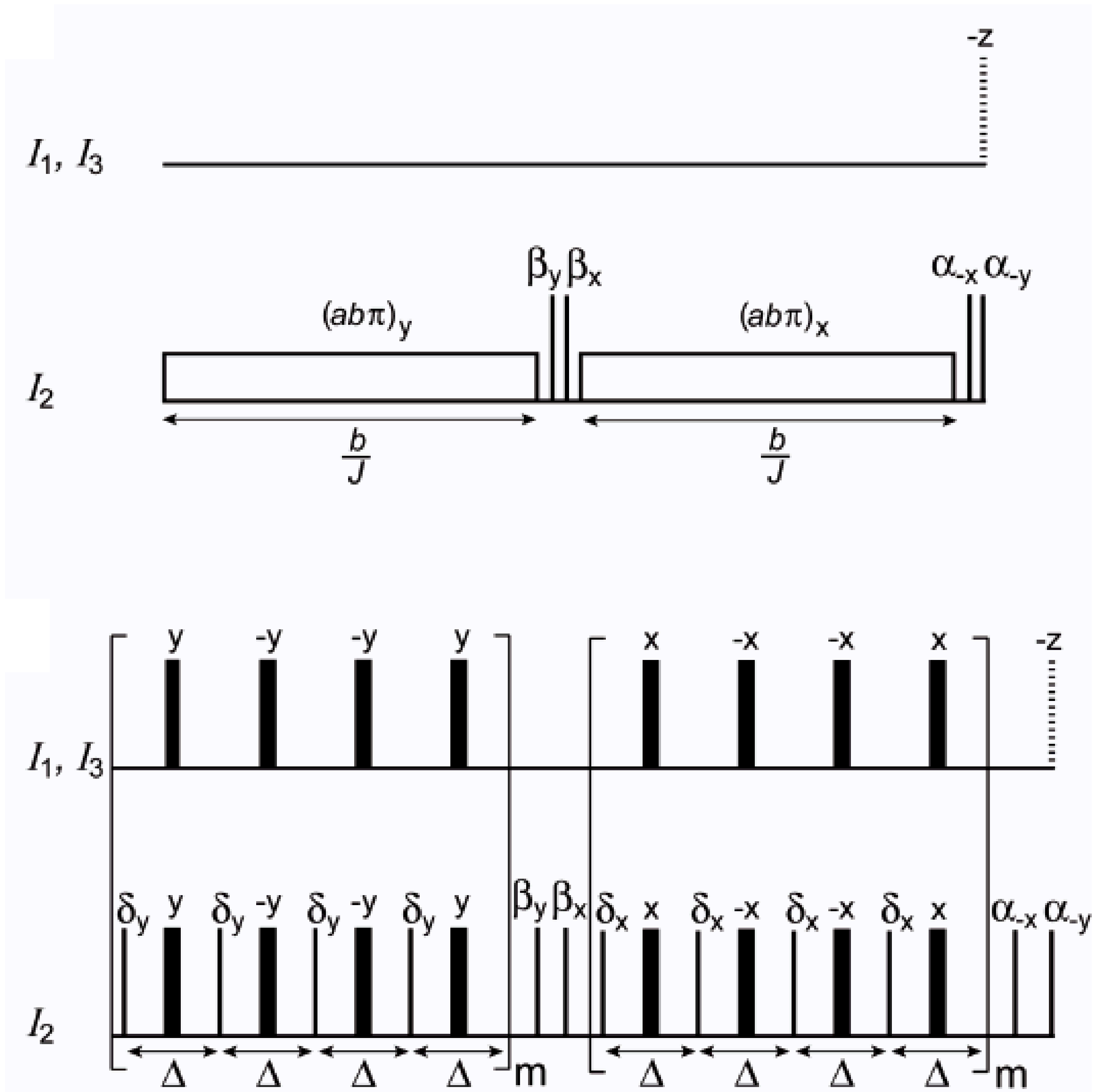
J_{12} = - 87.3 Hz $\approx$ J_{23} = - 88.8 Hz » J_{13}= 2.9 Hz
$\Delta\nu_{13}$ = 310 Hz



^{15}N - acetamide



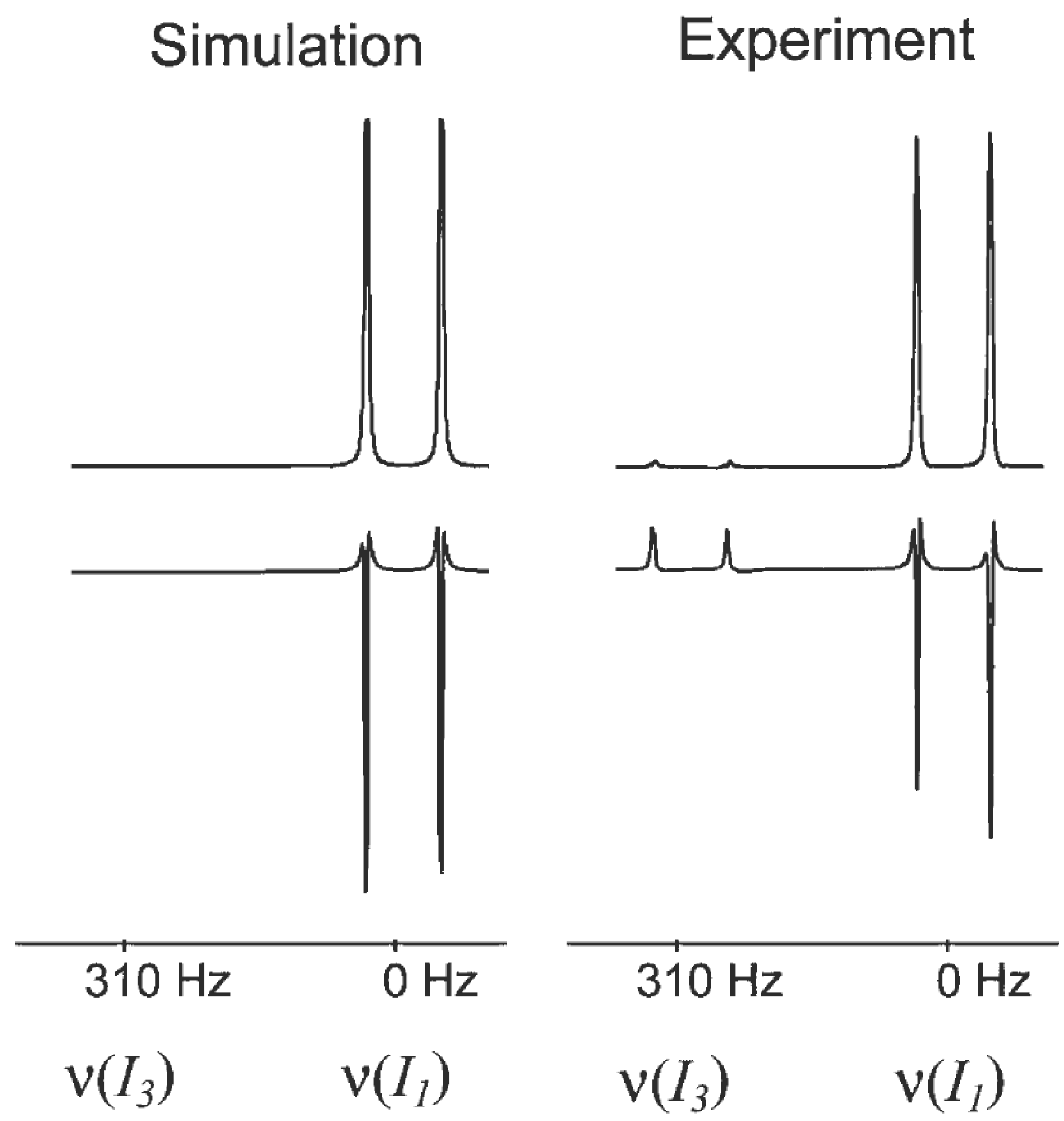
Experimental Demonstration U_{13}



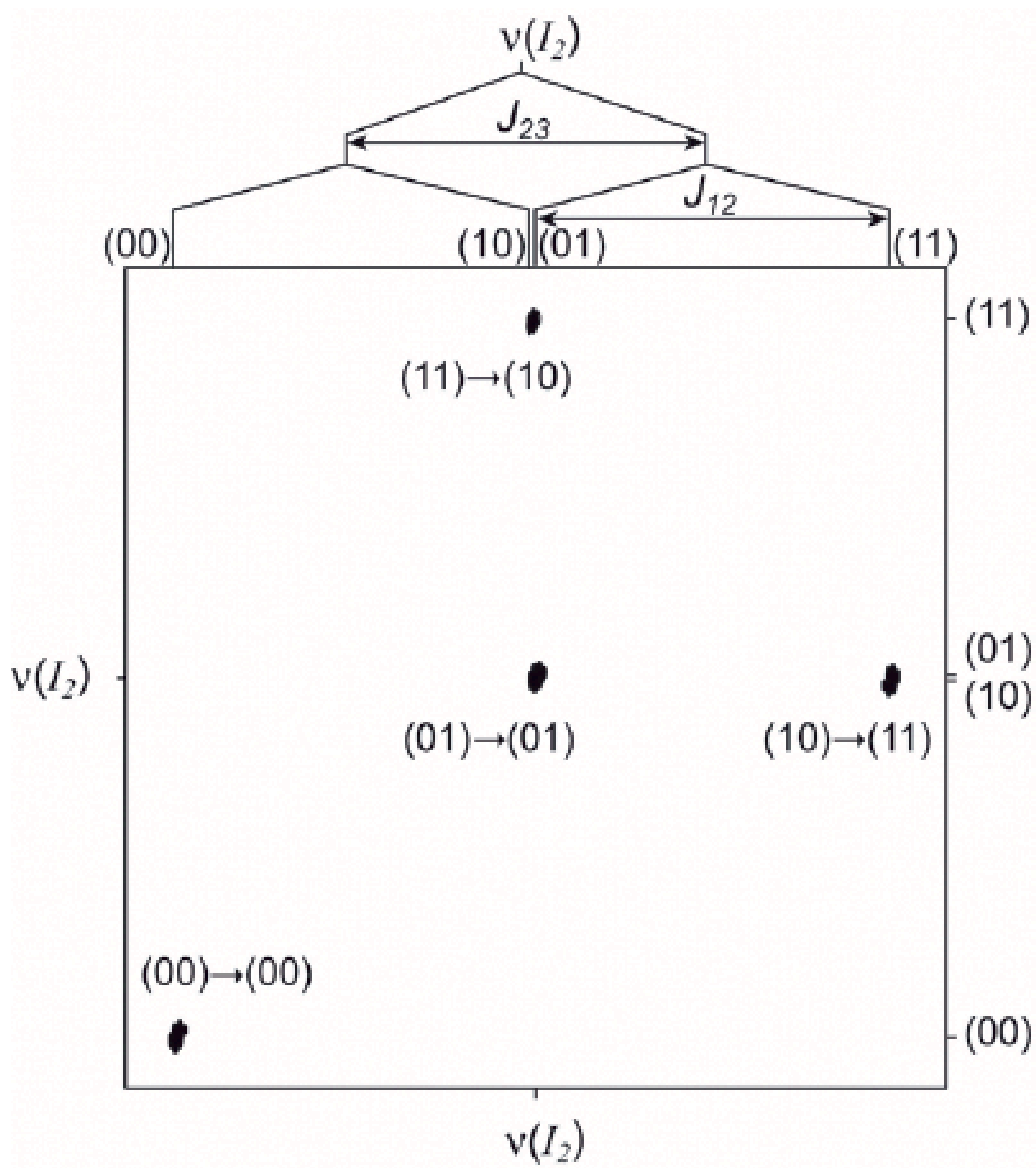
$$\mathcal{U}_{13} = \exp\{-i\tfrac{\pi}{2} 2I_{1z}I_{3z}\}$$

$\rho_A = I_{1x}$

$\rho_B = 2I_{1y}I_{3z}$

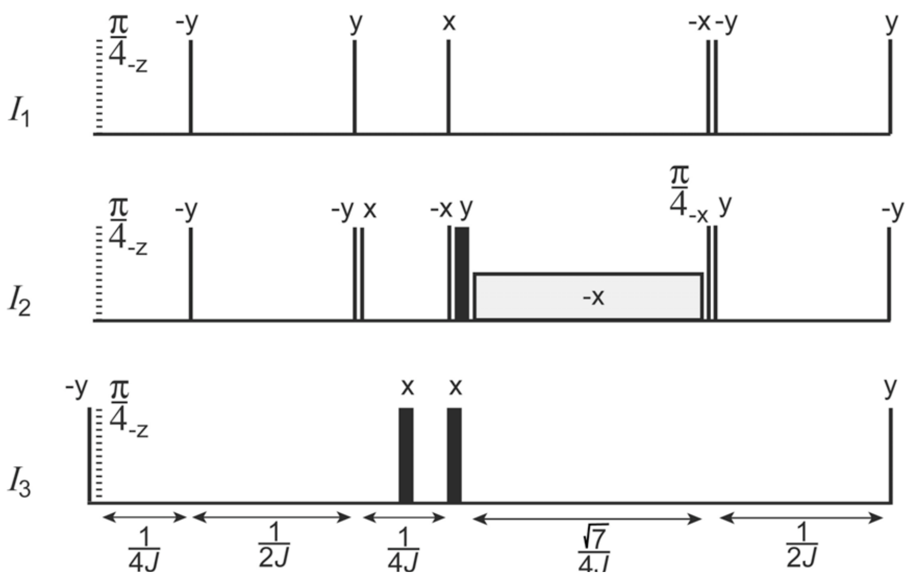


Experimental demonstration of CNOT(1,3)

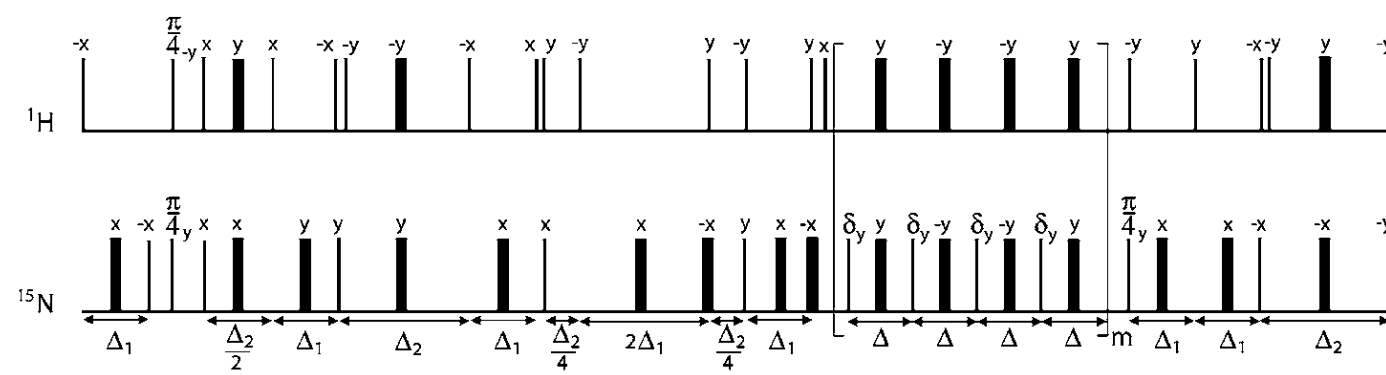


Toffoli gate

ideal sequence

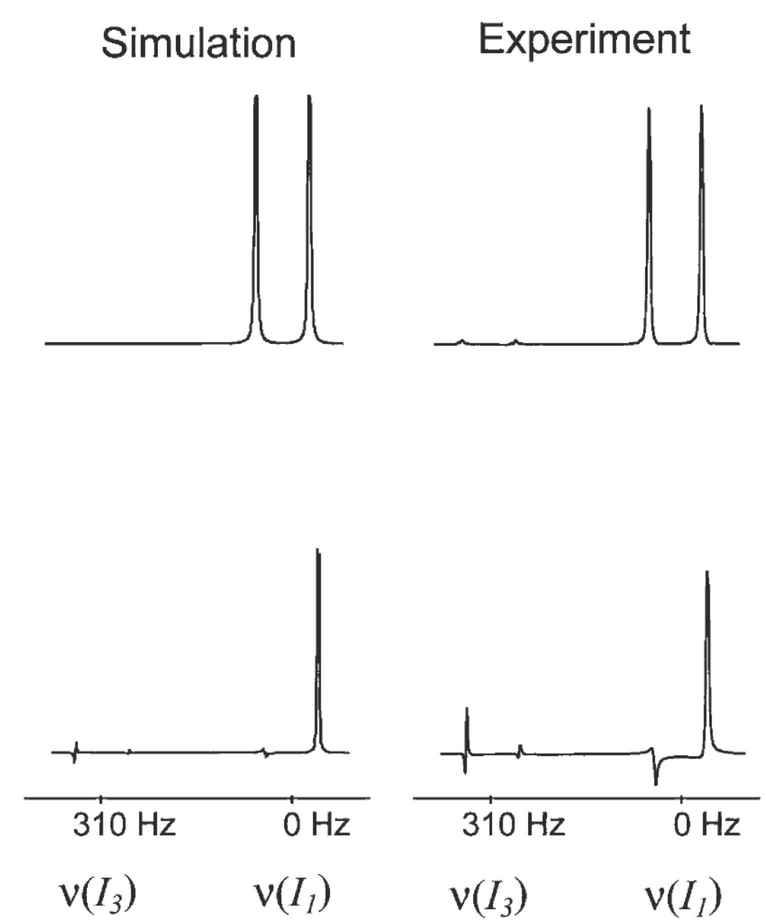


experimental sequence



$$\rho_A = I_{1x}$$

$$\rho_D = \frac{1}{\sqrt{2}}(I_{1x} + 2I_{1x}I_{2z} + 2I_{1x}I_{3x} - 4I_{1x}I_{2z}I_{3x})$$



Khaneja et al., Phys. Rev. A 75, 012322 (2007)

TABLE II. Duration τ_T of various implementations of the Toffoli gate.

Pulse sequence	τ_T (units of J^{-1})	Relative duration (%)
Sequence 1 (T1)	9.0	100
Sequence 2 (T2)	4.5	50
Sequence 3 (T3)	4.75	52.8
Sequence 4 (T4)	3.16	35.1
Sequence 5 (T5)	2.57	28.6
Sequence 6 (T6)	2.16	24.0

(T1) D. P. DiVincenzo, Proc. R. Soc. London, Ser. A **1969**, 261 (1998).

(T3) T. Sleator and H. Weinfurter, Phys. Rev. Lett. **74**, 4087 (1995).

Khaneja et al., Phys. Rev. A 75, 012322 (2007)

Acknowledgments

Harvard

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

R. Brockett

G. Wagner, D. Früh, T. Ito

A. Fahmy, J. Myers

University of Aarhus

N. C. Nielsen, A. C. Sivertsen, M. Bjerring

Wright State

T. Skinner

Bruker Biospin, Karlsruhe

W. Bermel, F. Engelke

Technische Universität München (TUM)

J. Neves, N. Pomplun, B. Heitmann,
R. Marx, T. Reiss, C. Kehlet, F. Kramer,
T. Schulte-Herbrüggen, A. Spörl, R. Fisher

B. Luy, K. Kobzar

H. Kessler, J. Klages, A. Frank

Funding

EU (QAP, BIO-DNP), DFG, DAAD, ENB