Time-Optimal Control of Quantum Dynamics and NMR Quantum Computing

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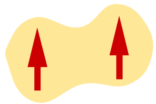
Quantum Computing



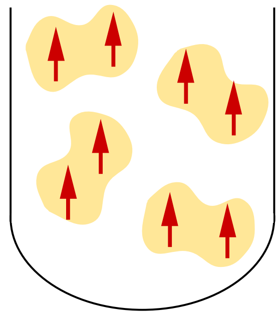
Pure state $|\Psi\rangle$

Measurement:

random *eigenvalue* of observable

(collapse of state function)

Ensemble quantum computing



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

Pseudo-pure state $\rho_{PPS} = \mathbf{1} + \alpha|\Psi_p\rangle\langle\Psi_p|$

Measurement:

expectation value of observable

(no collapse of state functions)

NMR-Quantum Computing Algorithms based on Pseudo-Pure States (PPS)

Scaling Problem!

Creation of PPS from ρ_{th} results in exponential signal loss

Possible Solutions:

- Preparation of pure states (para hydrogen)

  Hübler, Bargon, Glaser, Chem. Phys. Lett. 323, 377 (2000)

- Quantum algorithms based on ρ_{th}

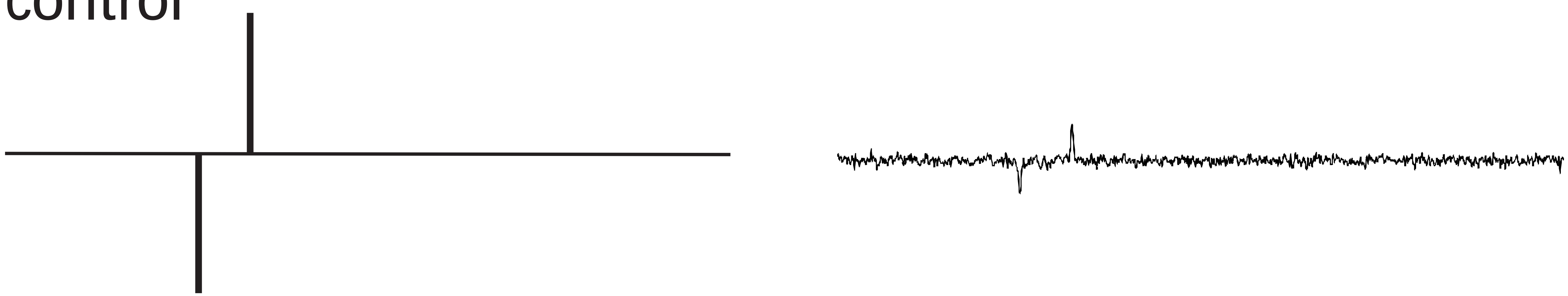
  Myers, Fahmy, Glaser, Marx, Phys. Rev. A 63, 032302 (2001)

Thermal Deutsch-Jozsa Algorithm

output for constant function

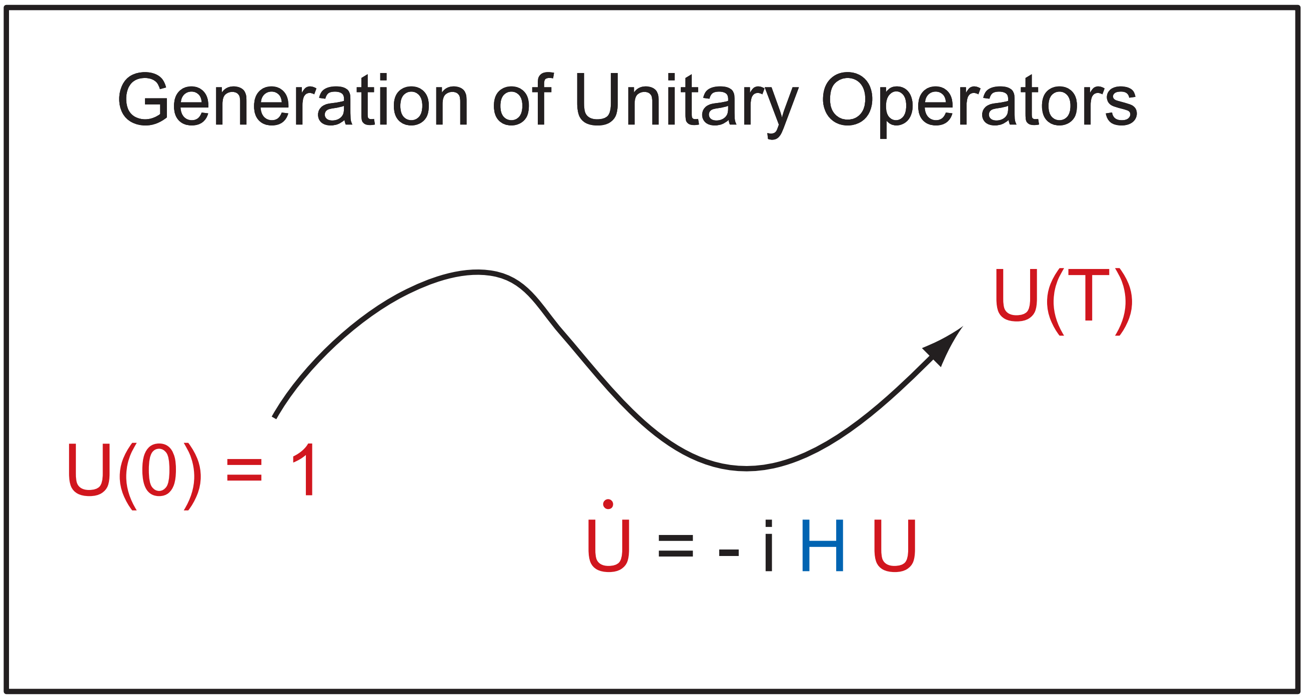
output for balanced function

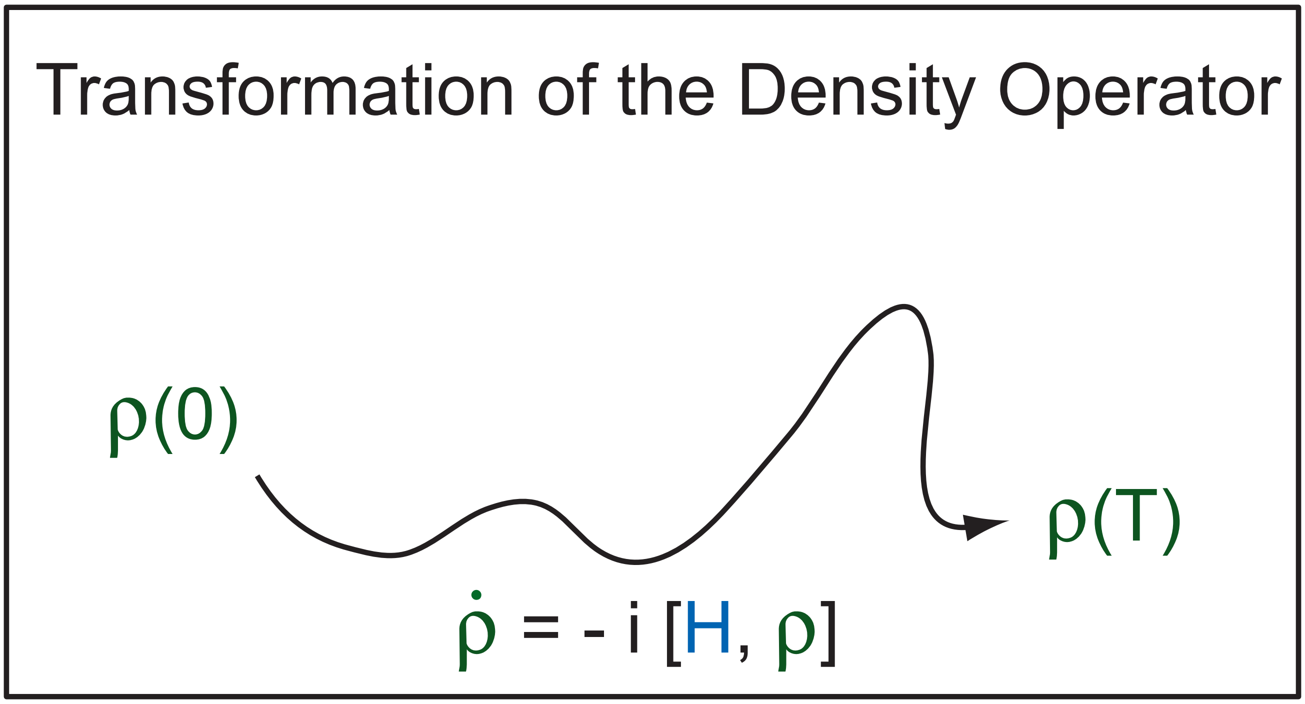
control



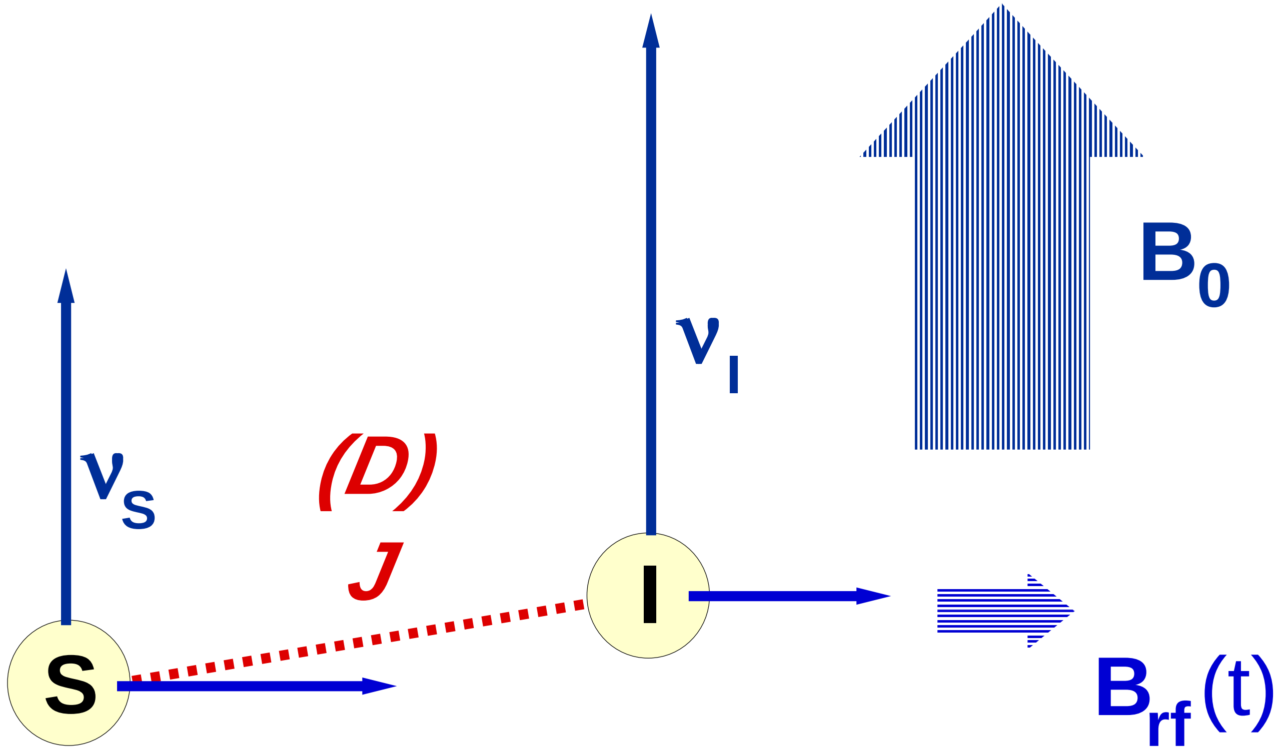
Time-Optimal Control of Quantum Systems

$$H = H_d + \sum u_k H_k$$





Interactions



Spin Hamiltonian: $\mathbf{H_0} + \mathbf{H_{rf}}(t)$

$$H = H_d + \sum u_k H_k$$

$$= H_c + H_{rf}$$

Strong-Pulse Limit: $H_{rf} >> H_c$

2 time scales: H_{rf} : fast

H_c : slow

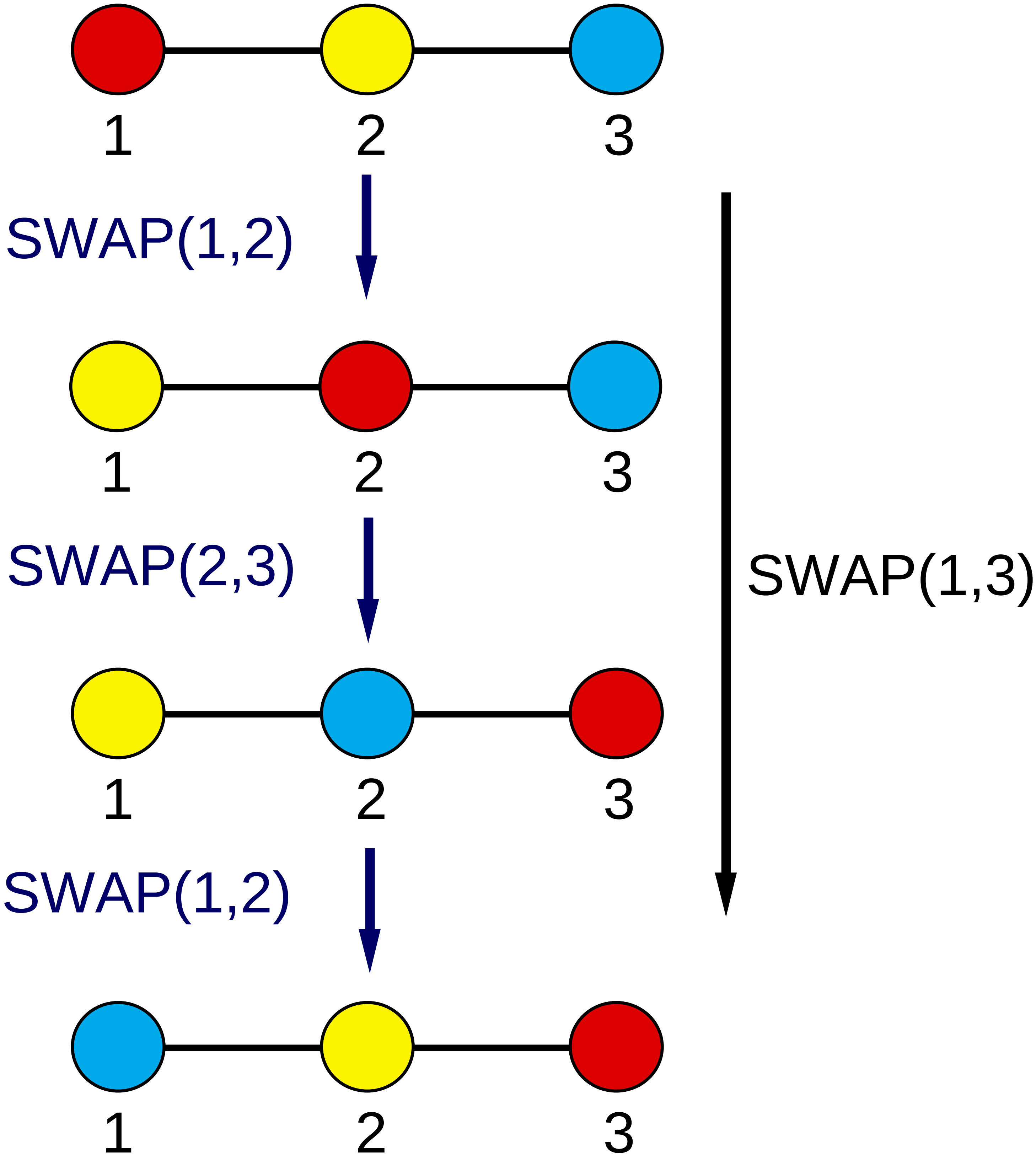
Adjoint Time-Optimal Control Problem:

Find shortest path in quotient space

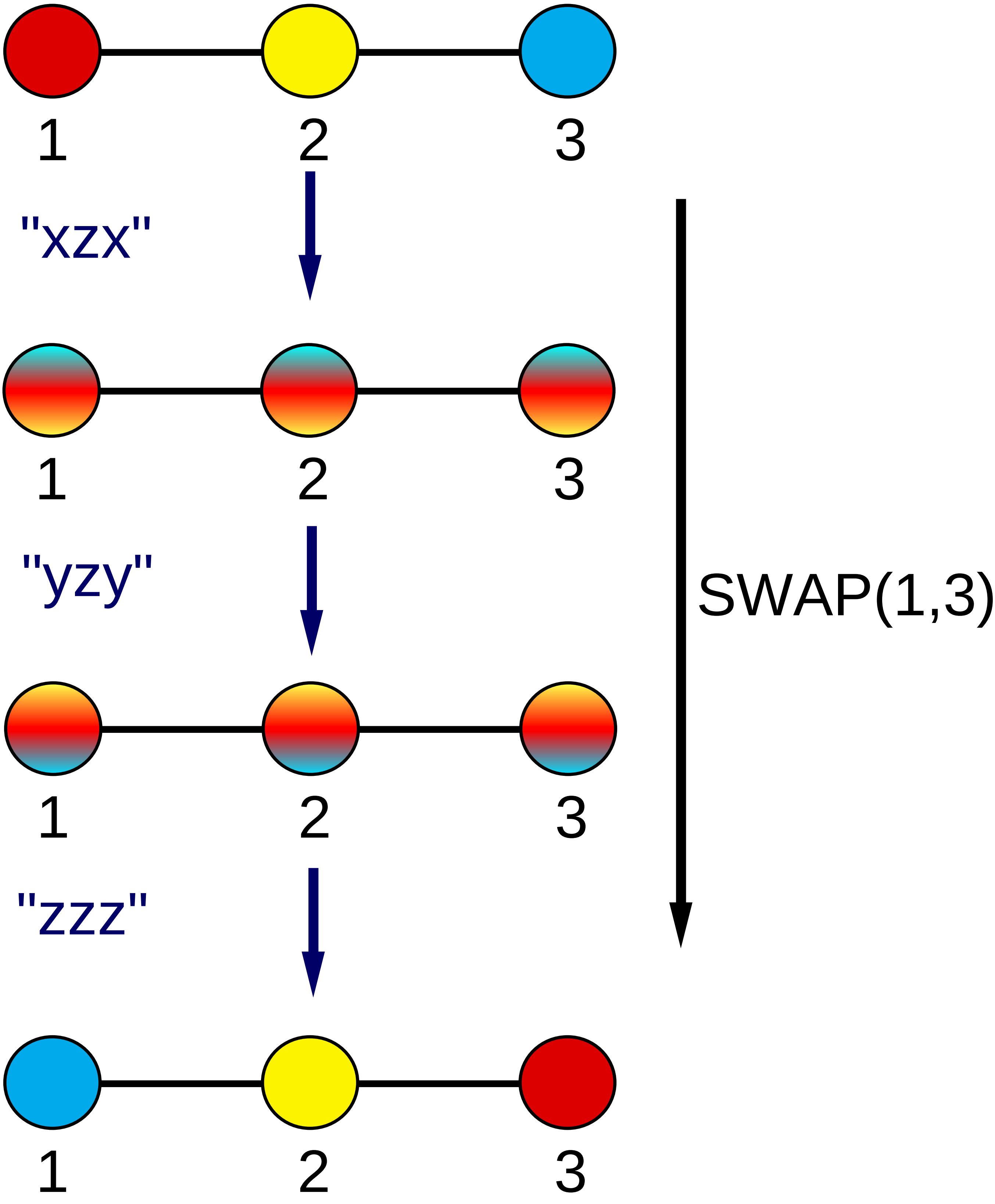
→ sub-Riemannian geodesics

Khaneja, Brockett, Glaser (2001)
Khaneja, Glaser, Brockett (2002)

Indirect SWAP-Operation

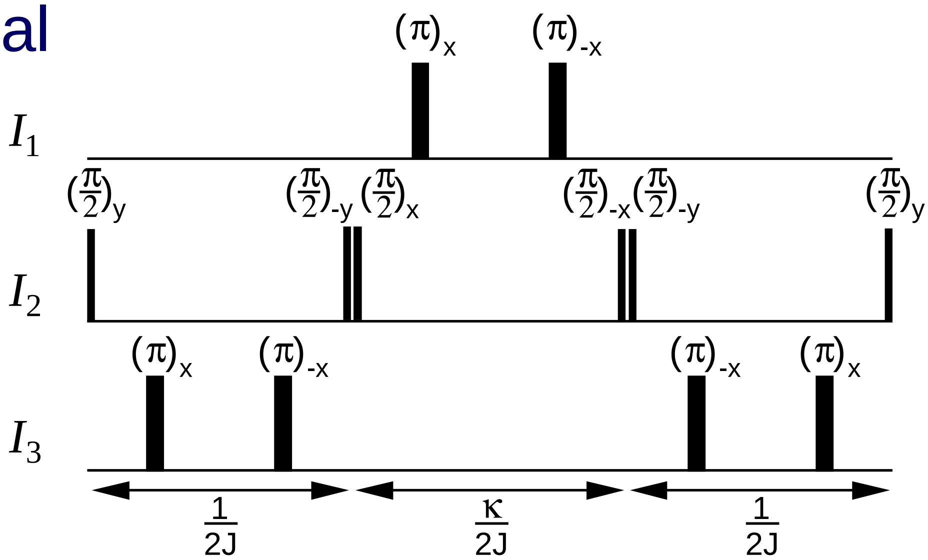


Indirect SWAP-Operation

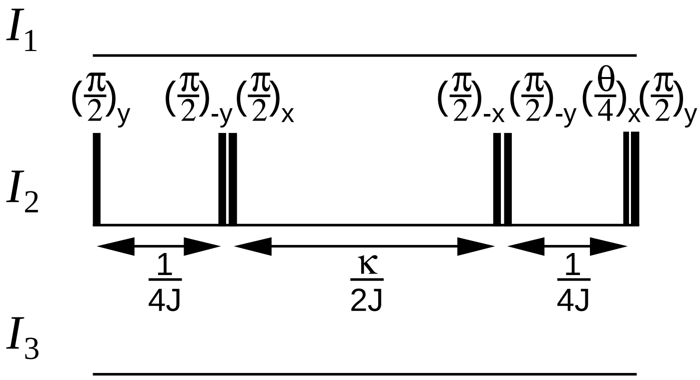


Basic Pulse Sequences ("zzz")

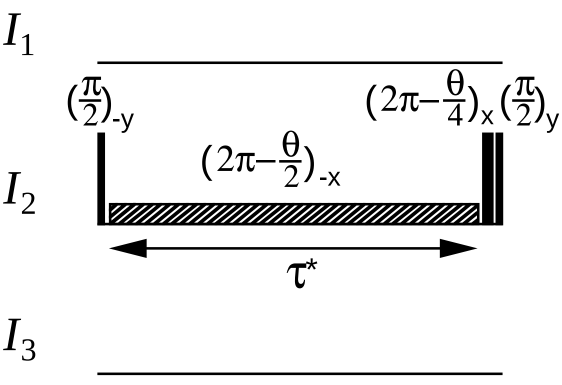
conventional

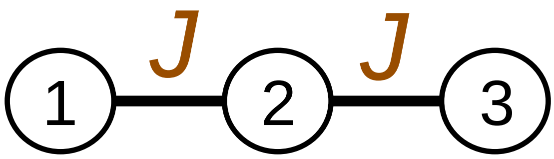


improved



geodesic





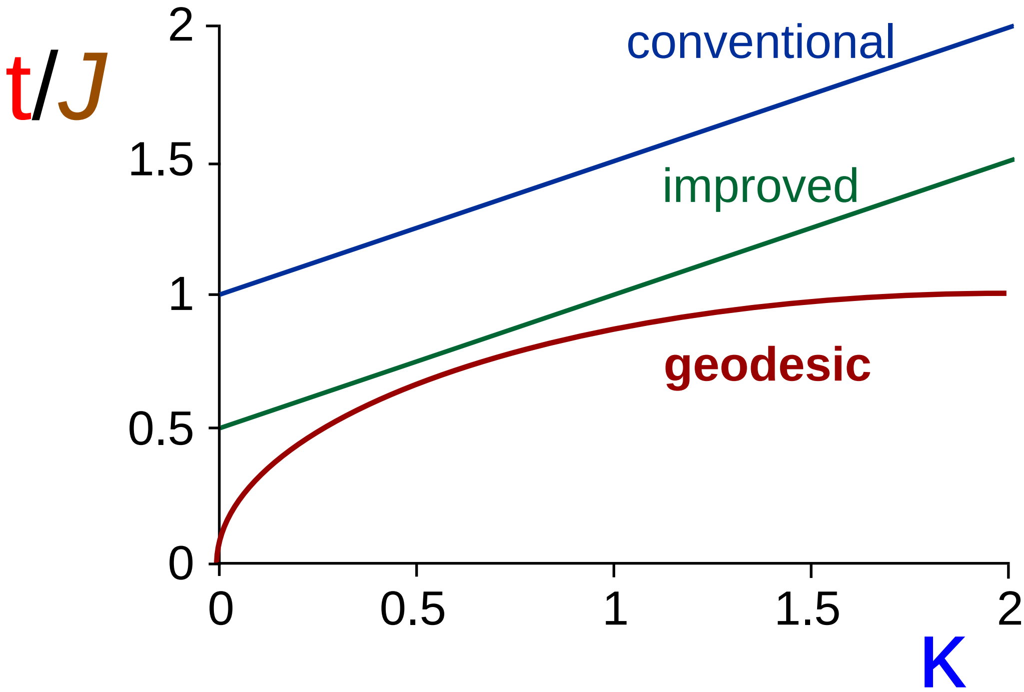
Given Hamiltonian:

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

Desired unitary transformation:

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

Duration **t** of pulse sequence:

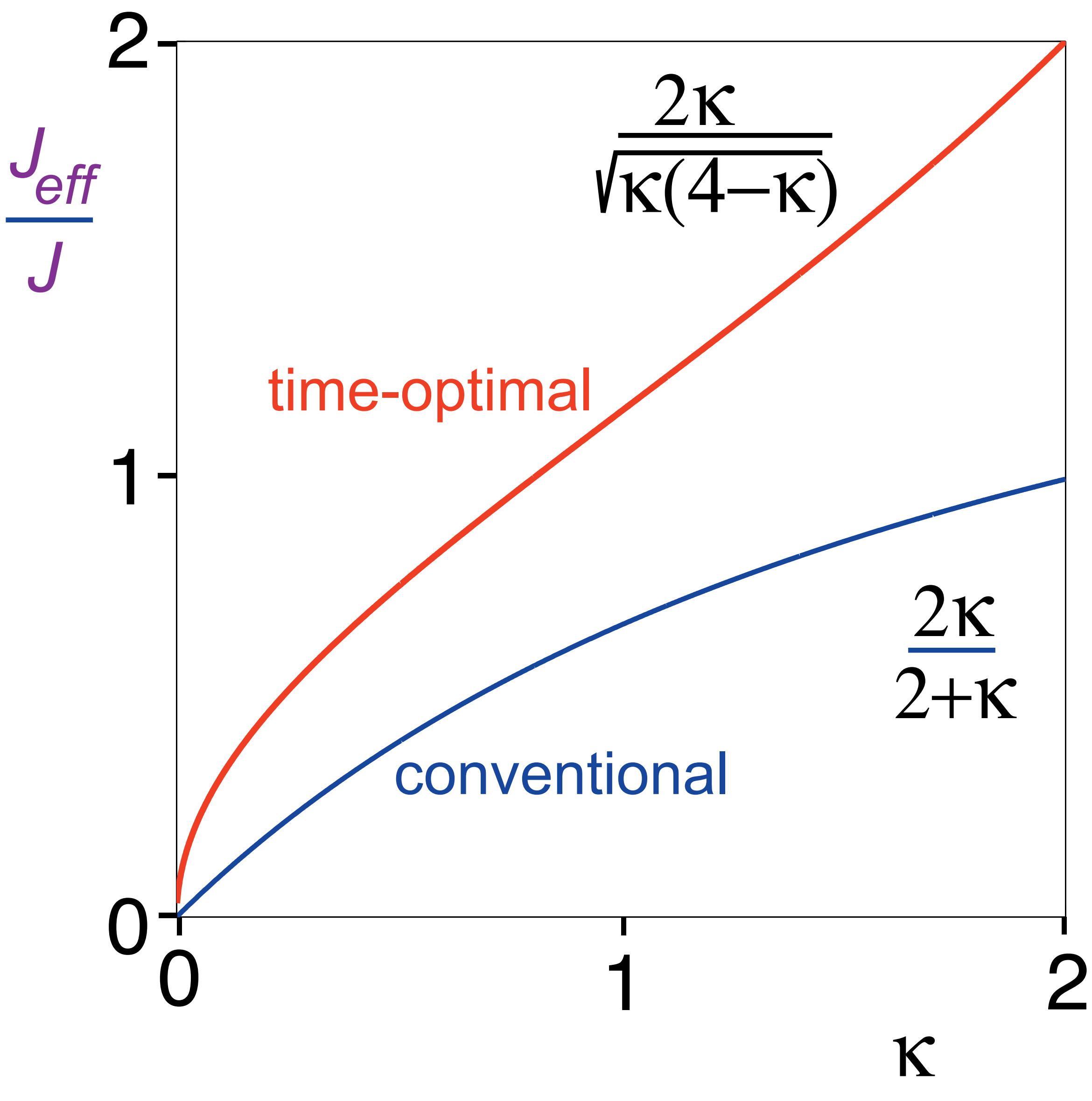


N. Khaneja, S. J. Glaser, R. Brockett,
Phys. Rev. A 65, 032301 (2002)

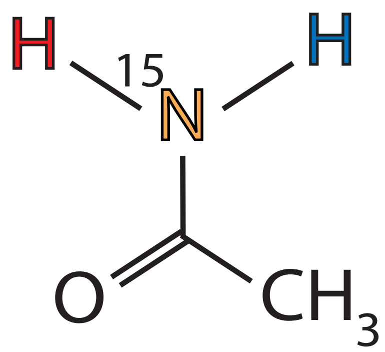
$$U = \exp\{-i\,\kappa\, 2\pi\, I_{1z} I_{2z} I_{3z}\}$$

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

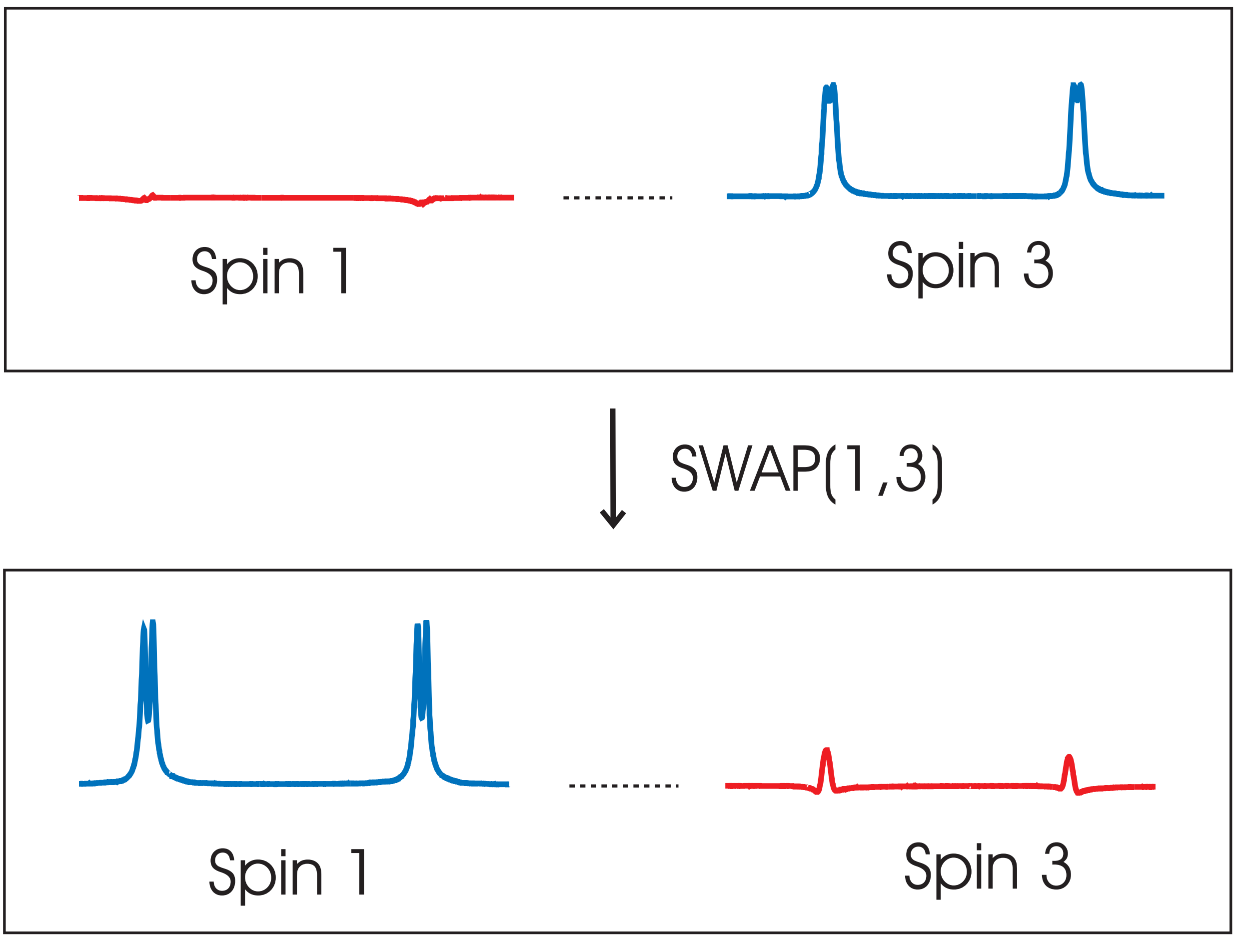
$$H_{eff} = 2\pi J_{eff}\,(I_{1z} I_{2z} I_{3z})$$



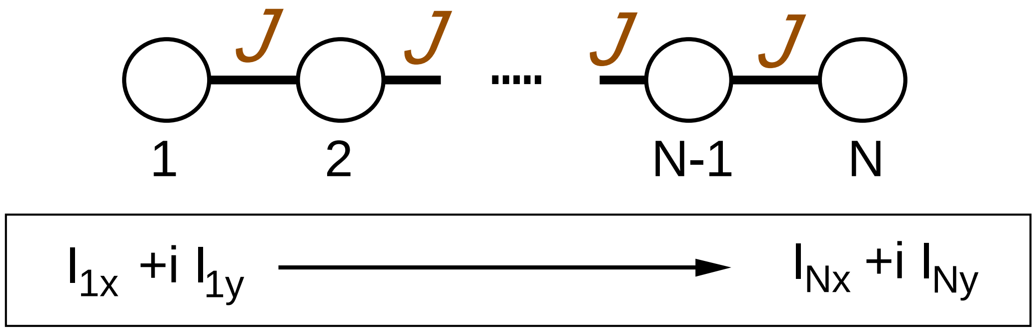
Indirect SWAP Operation

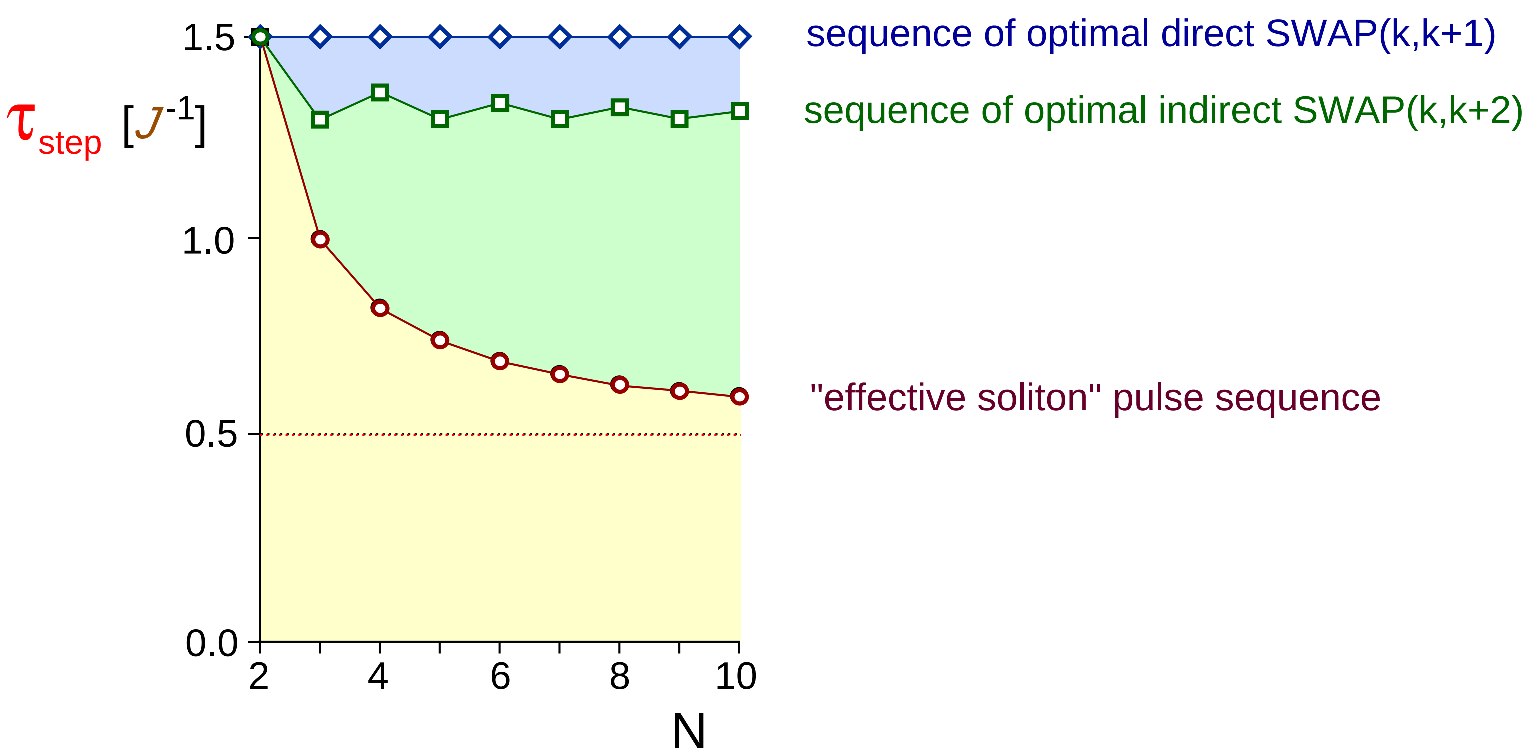


[^{15}N]-Acetamide

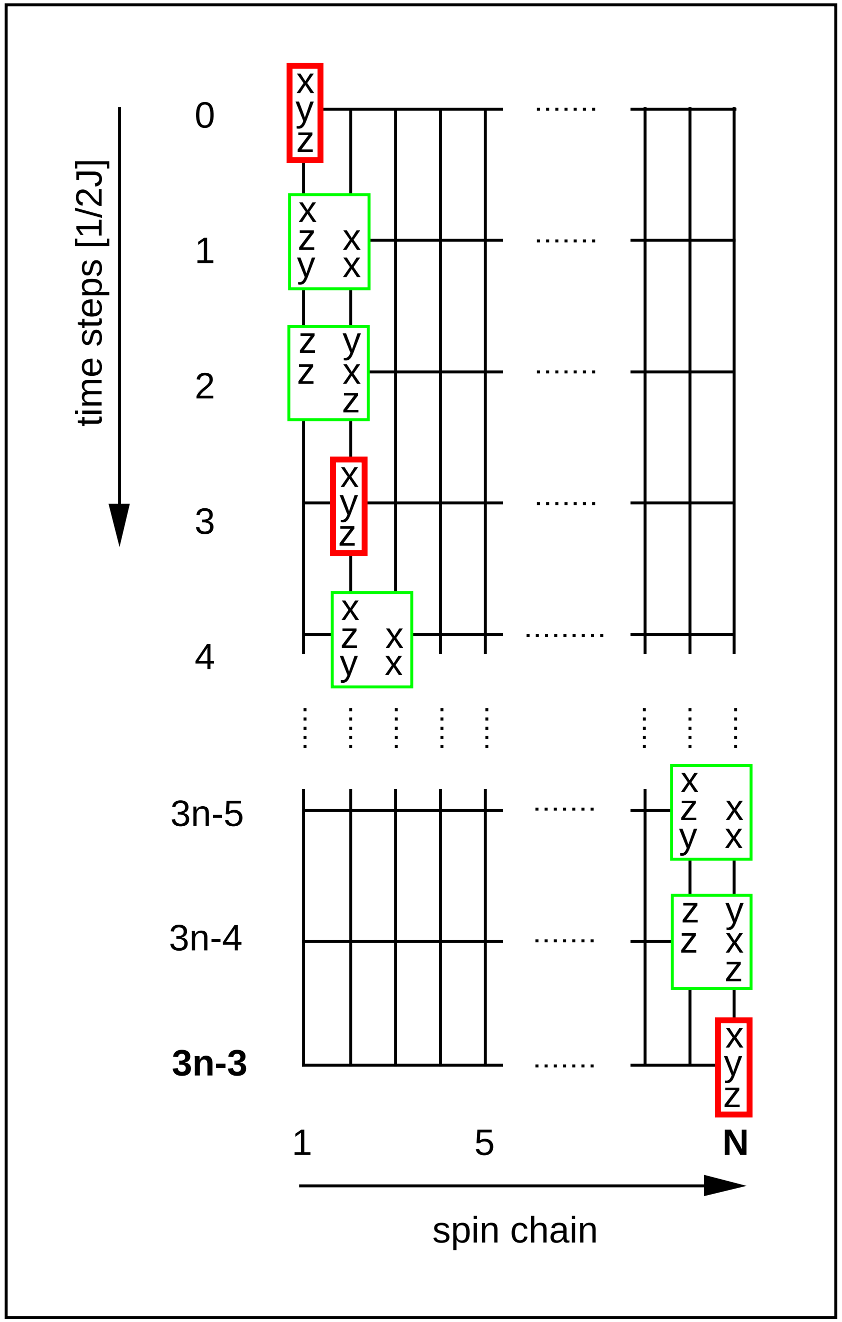


Coherence transfer in an N-spin chain

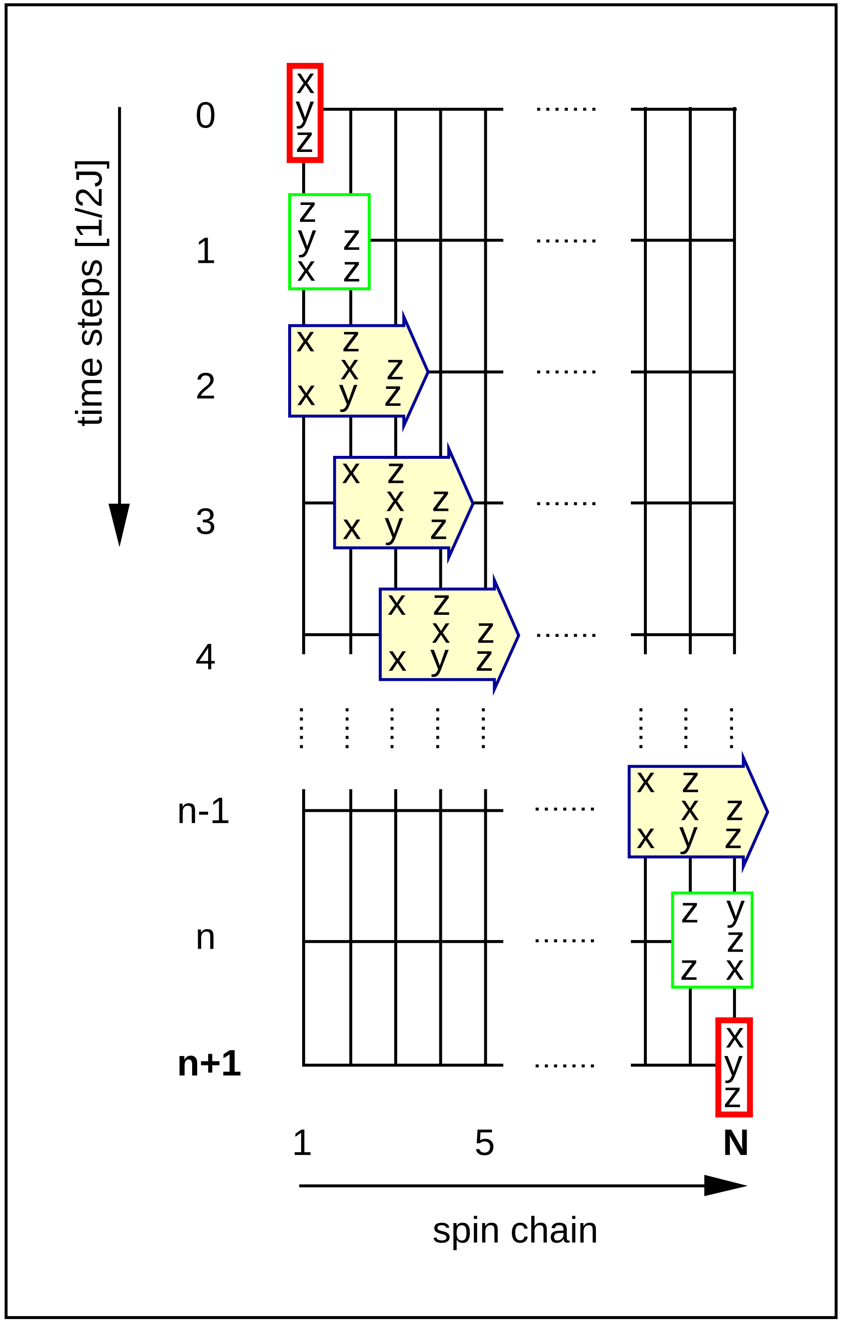


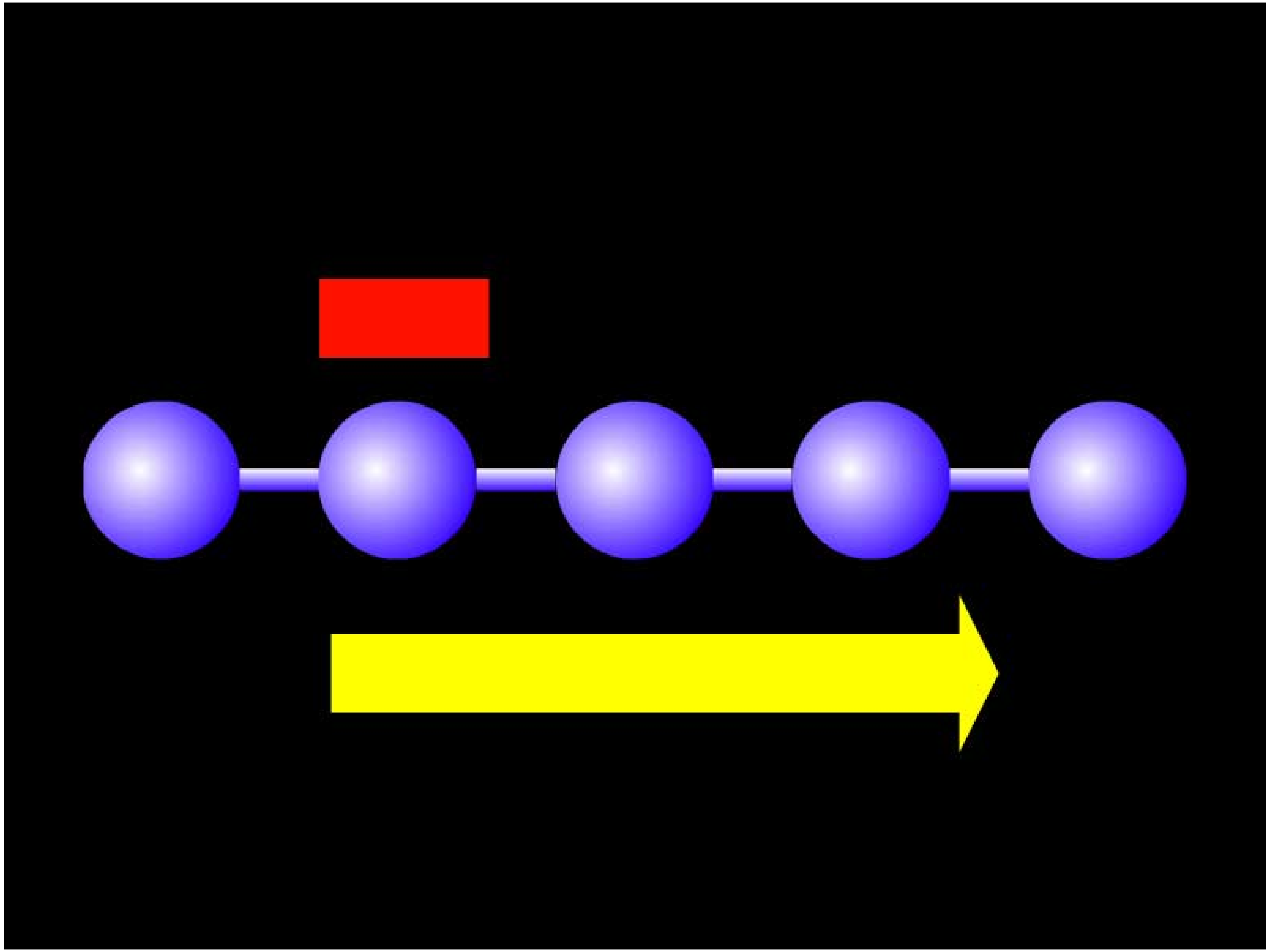


Sequence of direct SWAPs



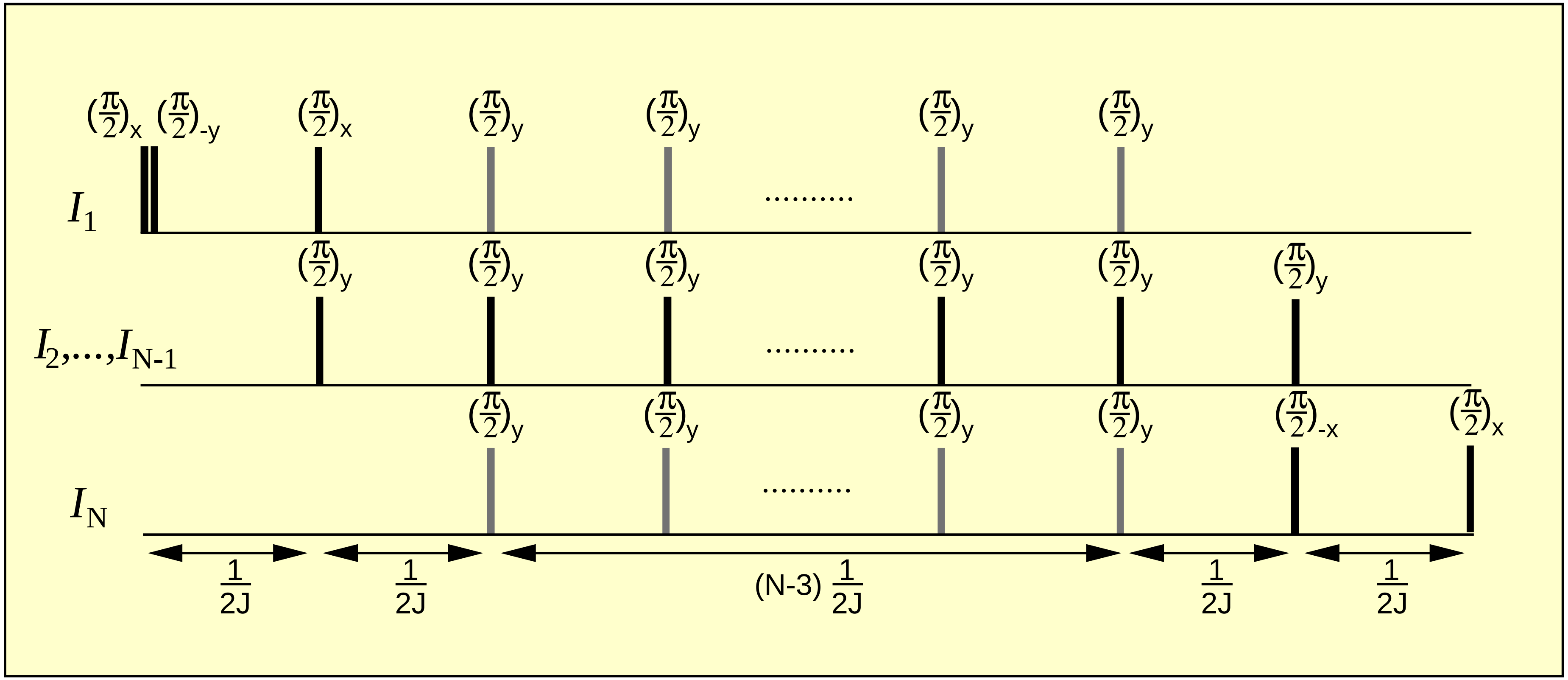
"effective soliton" sequence



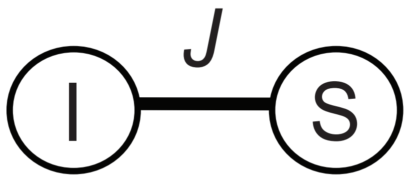


"effective soliton" sequence

$I_{1x} + i\, I_{1y} \longrightarrow I_{Nx} + i\, I_{Ny}$



Total duration: $(N+1)\,\frac{1}{2J}$



Dipol-Dipol Relaxation in the Spin-Diffusion Limit

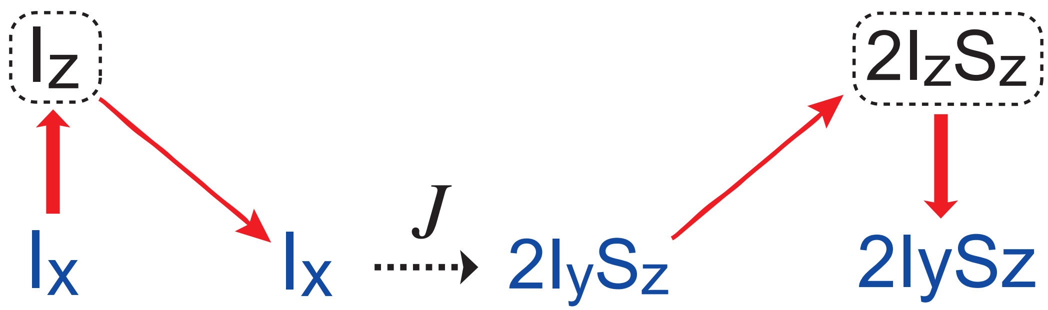
$$\dot{\rho} = \pi J\,[-i\,2I_z S_z, \rho] + \pi k\,[2I_z S_z, [2I_z S_z, \rho]]$$

$$I_x \xrightarrow{?} 2I_yS_z$$

Conventional transfer (INEPT)

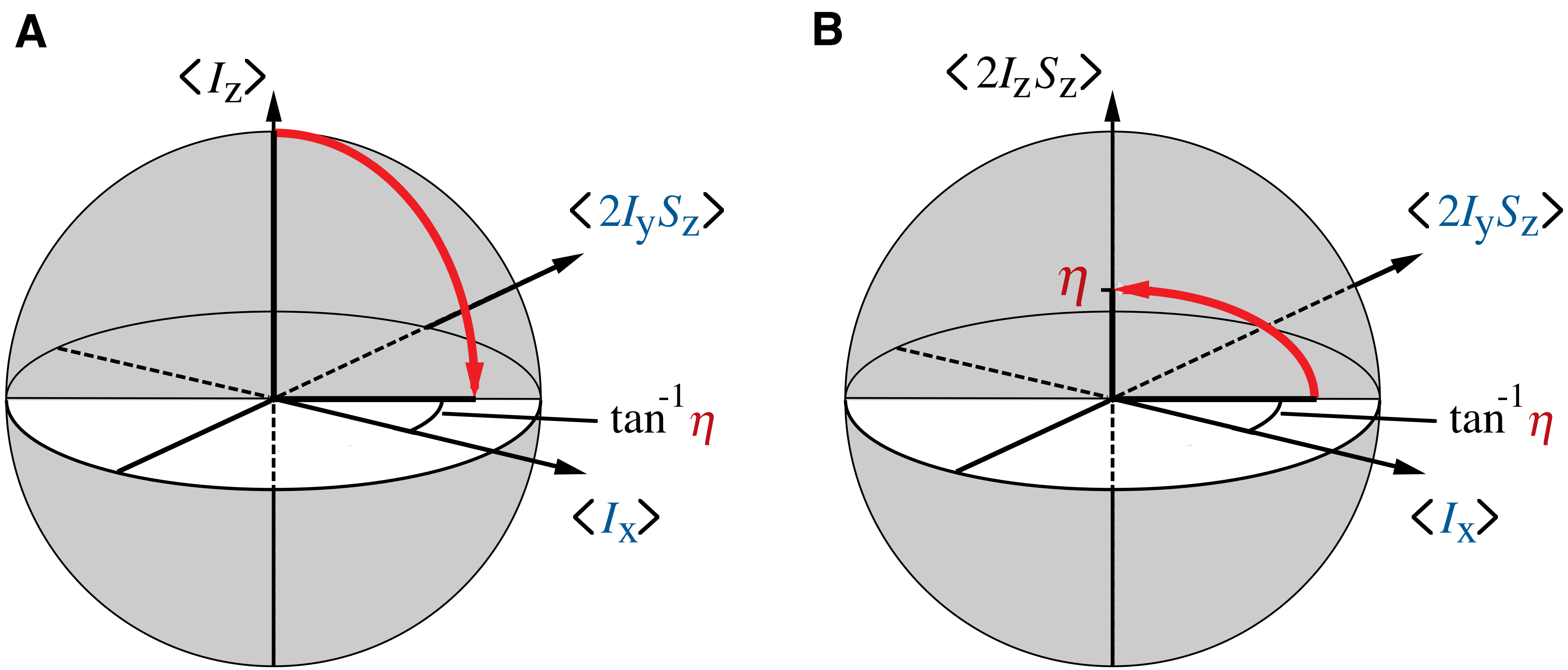
$$I_x \xrightarrow{J} 2I_yS_z$$

Relaxation-optimized transfer (ROPE)



quant-ph/0208050

ROPE Trajectory



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

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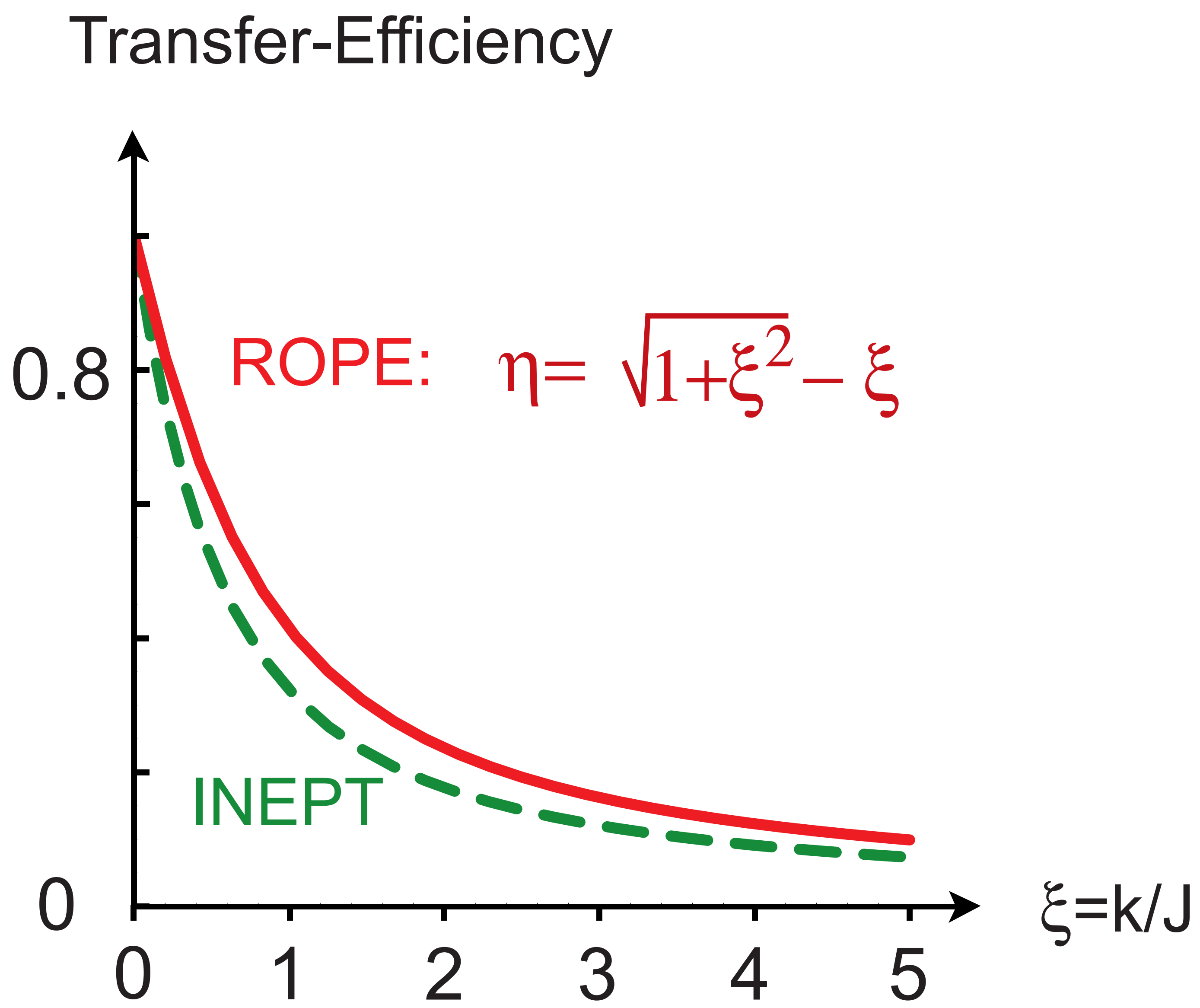

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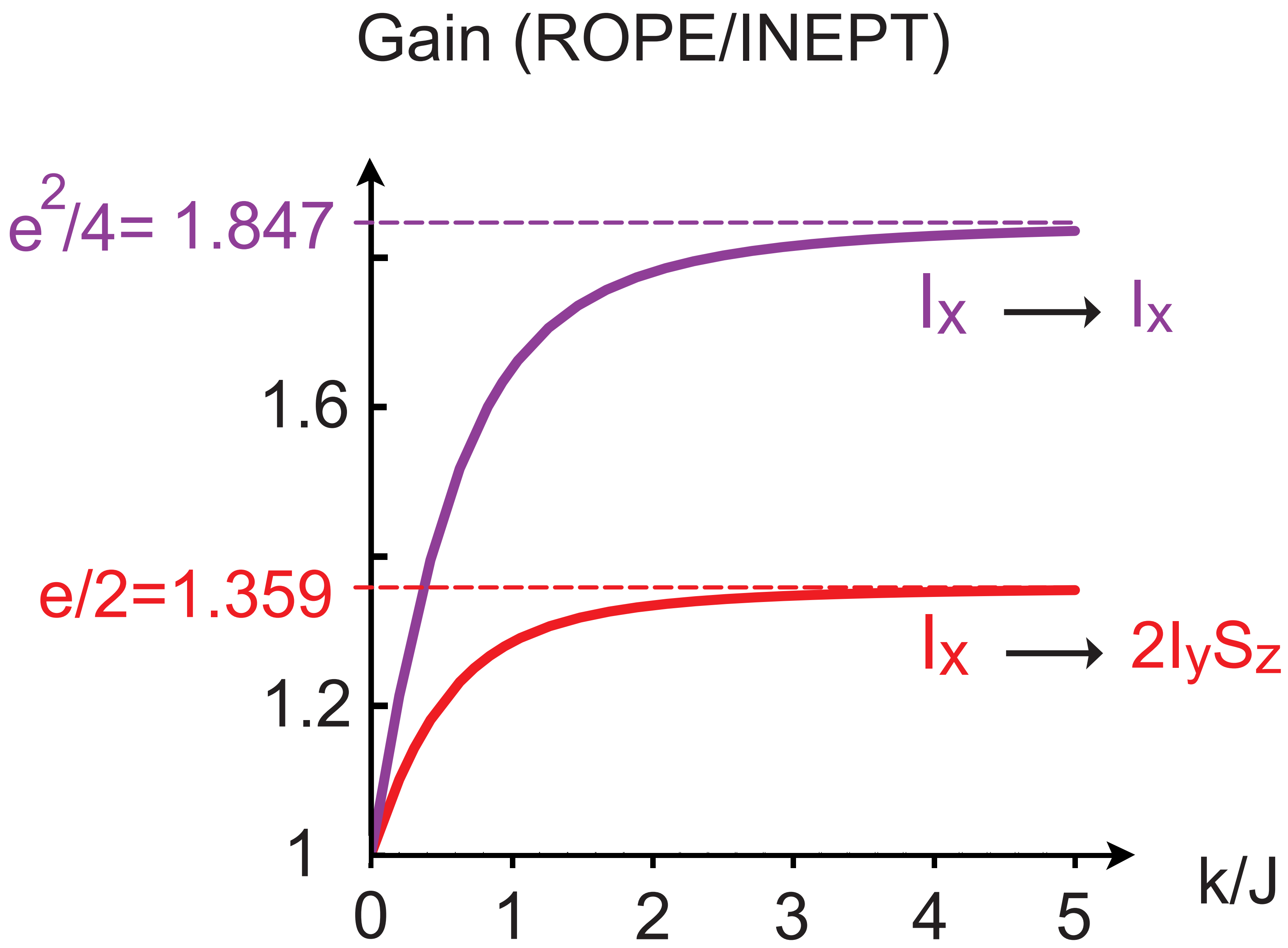

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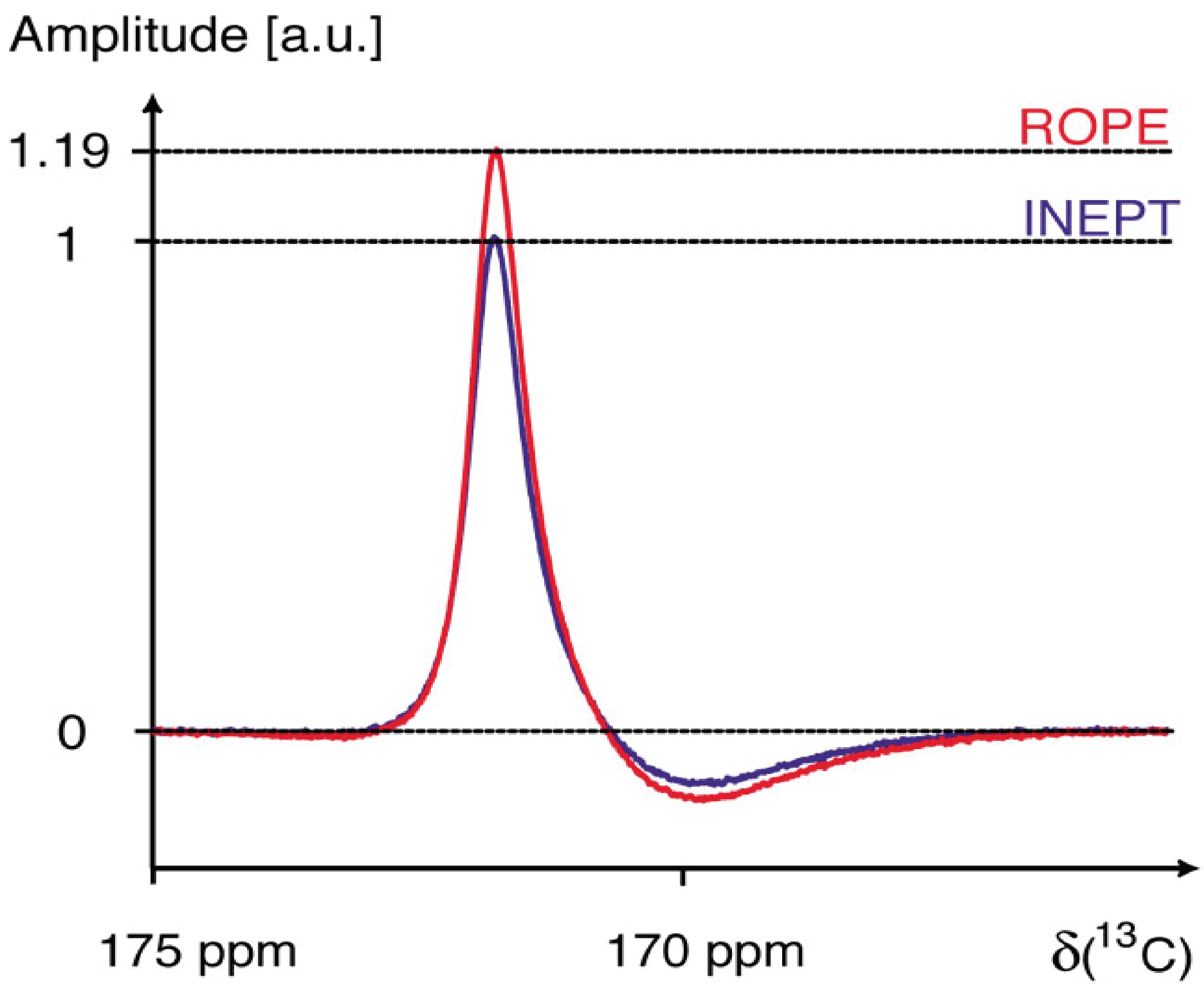

^{13}C-Formiate in 92% D_6-Glycerol and 8% D_2O (T=250 K)

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