Title: Quantum Theory (PHYS 605) - Lecture 15

Date: Oct 01, 2010 09:00 AM

URL: http://pirsa.org/10100001

Abstract:

NMR for quantum computing

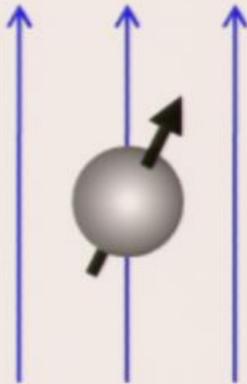Quantum Theory

PSI -- 1 Oct 2010

NMR for quantum computing

Quantum Theory
PSI -- 1 Oct 2010
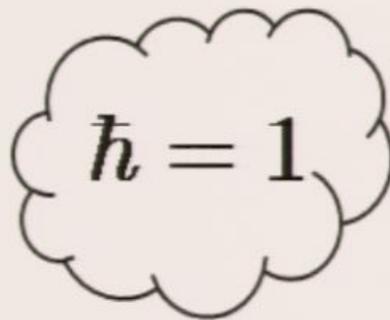
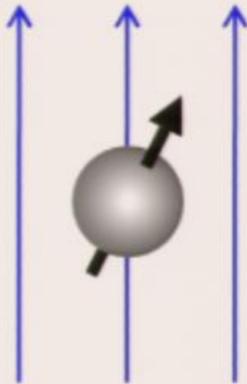$$\hbar = 1$$

Nuclear spin in a magnetic field

proton in a
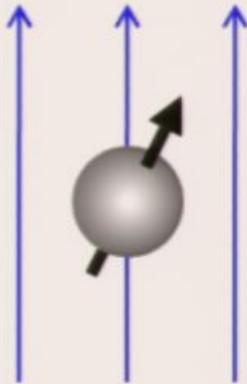10.00 T field

Nuclear spin in a magnetic field

Nuclear magnetic moment couples to external field:

$$H_0 = -\vec{\mu} \cdot \vec{B}_0 = -\frac{\Omega}{2} Z$$

proton in a
10.00 T field

Nuclear spin in a magnetic field

proton in a
10.00 T field

$\Omega/2\pi = 425.7$ MHz

Nuclear magnetic moment couples to external field:

$$H_0 = -\vec{\mu} \cdot \vec{B}_0 = -\frac{\Omega}{2} Z$$

Time evolution from external field only:

$$U_0(t) = \exp(-iH_0 t) = \exp\left(i\frac{\Omega t}{2} Z\right)$$

$$= \cos(\Omega t/2)\, \mathbf{1} + i \sin(\Omega t/2)\, Z$$

Nuclear spin in a magnetic field

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proton in a
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$\Omega/2\pi = 425.7$ MHz

Actual Hamiltonian includes extra stuff

$$i\frac{d}{dt}|\psi(t)\rangle = (H_0 + H)|\psi(t)\rangle$$
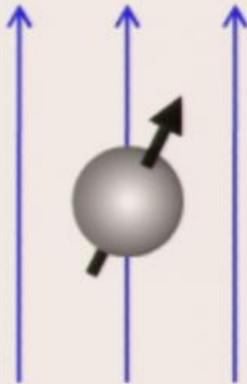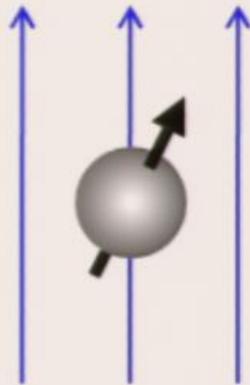
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proton in a
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$$i\frac{d}{dt} |\psi(t)\rangle = (H_0 + H) |\psi(t)\rangle$$

external
field

other
effects

Rotating frame picture

Rotating frame picture

Adopt: "Heisenberg" picture for H_0
"Schrödinger" picture for H

$$\left|\hat{\psi}(t)\right\rangle = U_0(t)^\dagger \left|\psi(t)\right\rangle$$

$$\hat{H}(t) = U_0(t)^\dagger H\, U_0(t)$$

Rotating frame picture

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$$\boxed{\; i\frac{d}{dt} \left| \hat{\psi}(t) \right\rangle = \hat{H}(t) \left| \hat{\psi}(t) \right\rangle \;}$$

Rotating frame picture

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This is related to the "interaction picture".

Our "reference frame" precesses at Ω like an unperturbed nuclear spin.

Rotating frame picture

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This is related to the "interaction picture".

Our "reference frame" precesses at Ω like an unperturbed nuclear spin.

Possible terms: $\quad H = \varepsilon_0 \mathbf{1} + \varepsilon_x X + \varepsilon_y Y + \varepsilon_z Z$

What do these look like in the rotating frame picture?

Rotating frame picture

Rotating frame picture

$$H = \varepsilon_0 \mathbf{1} + \varepsilon_x X + \varepsilon_y Y + \varepsilon_z Z$$

$$\hat{H}(t) = U_0(t)^\dagger H\, U_0(t) \qquad U_0(t) = \cos\left(\Omega t/2\right) \mathbf{1} + i \sin\left(\Omega t/2\right) Z$$

Rotating frame picture

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$$+\, i \sin\left(\Omega t/2\right) Z$$

How does rotating frame U_0 affect Pauli operators?

$$U_0^\dagger \mathbf{1} U_0 = \mathbf{1}$$
$$U_0^\dagger Z U_0 = Z$$
$$U_0^\dagger X U_0 = \cos \Omega t\, X + \sin \Omega t\, Y$$
$$U_0^\dagger Y U_0 = \cos \Omega t\, Y - \sin \Omega t\, X$$

Rotating frame picture

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Rotating frame Hamiltonian

$$\hat{H}(t) = \varepsilon_0 \mathbf{1} + (\varepsilon_x \cos\Omega t - \varepsilon_y \sin\Omega t)X$$
$$+ (\varepsilon_x \sin\Omega t + \varepsilon_y \cos\Omega t)Y + \varepsilon_z Z$$

Rotating frame picture

$$H = \varepsilon_0 \mathbf{1} + \varepsilon_x X + \varepsilon_y Y + \varepsilon_z Z$$

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Rotating frame Hamiltonian

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overall
E-shift
(ignore)

Rotating frame picture

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Rotating frame Hamiltonian

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overall E-shift (ignore)

rapidly oscillating (avg. to zero!)

Rotating frame picture

$$H = \varepsilon_0 1 + \varepsilon_x X + \varepsilon_y Y + \varepsilon_z Z$$

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Rotating frame Hamiltonian

*rapidly
oscillating
(avg. to zero!)*

$$\hat{H}(t) = \boxed{\varepsilon_0 1} + \boxed{(\varepsilon_x \cos \Omega t - \varepsilon_y \sin \Omega t) X}$$
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E-shift
(ignore)*

Radio pulses

Radio pulses

Radio pulse produces a time-dependent perturbation

$$\mathsf{H} = A(t)\ (\cos(\Omega't - \phi)\mathsf{X} - \sin(\Omega't - \phi)\mathsf{Y})$$

$A(t) = \text{"envelope" or "shape" of pulse}$

Radio pulses

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$$H = A(t)\,(\cos(\Omega' t - \phi)X - \sin(\Omega' t - \phi)Y)$$

$A(t) = $ "envelope" or "shape" of pulse

In rotating frame

$$\hat{H} = A(t)\left(\cos\left((\Omega - \Omega')t + \phi\right)X + \sin\left((\Omega - \Omega')t + \phi\right)Y\right)$$

This will quickly average to zero unless $\Omega' = \Omega$.
("*Resonance*" is the R in "NMR"!)

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Resonant pulse yields

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Resonant pulse yields

$$\hat{H} = A(t)(\cos\phi\,X + \sin\phi\,Y)$$

We can control
- How $A(t)$ turns on, off
- Phase shift ϕ

Radio pulses

$$\hat{\mathsf{H}} = A(t)(\cos\phi\,\mathsf{X} + \sin\phi\,\mathsf{Y})$$

Radio pulses

$$\hat{\mathsf{H}} = A(t)(\cos\phi\,\mathsf{X} + \sin\phi\,\mathsf{Y})$$

Total strength of resonant pulse $\quad \displaystyle\int_{-\infty}^{\infty} A(t)\,dt = \frac{\beta}{2}$

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$A(t)$

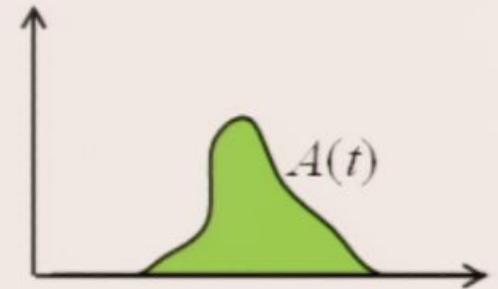By choosing phases $\phi = 0$ or $\phi = \pi/2$, we can produce

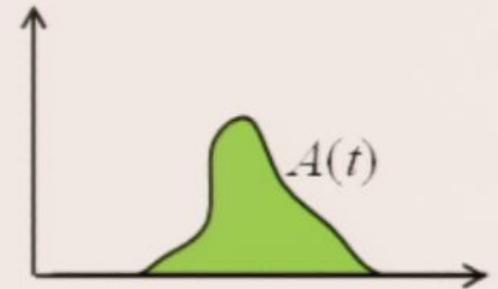$$\hat{R}_x(\beta) = e^{-i(\beta/2)X} = \cos(\beta/2)\mathbf{1} - i\sin(\beta/2)X$$
$$\hat{R}_y(\beta) = e^{-i(\beta/2)Y} = \cos(\beta/2)\mathbf{1} - i\sin(\beta/2)Y.$$

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From a sequence of such pulses, we can create any 1-qubit gate!

Radio pulses

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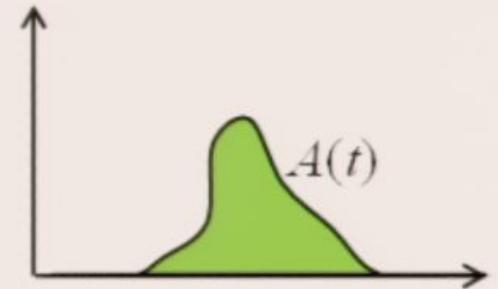By choosing phases $\phi = 0$ or $\phi = \pi/2$, we can produce

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Radio pulses

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Total strength of resonant pulse $\displaystyle\int_{-\infty}^{\infty} A(t)\,dt = \frac{\beta}{2}$

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$$
\begin{aligned}
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From a sequence of such pulses, we can create any 1-qubit gate!

$\hat{R}_x(\pi) = -i\mathsf{X}$

$\hat{R}_y(\pi) = -i\mathsf{Y}$

Radio pulses

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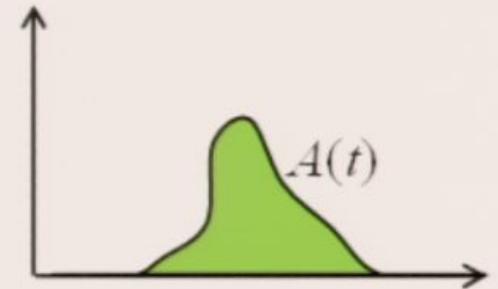From a sequence of such pulses, we can create any 1-qubit gate!

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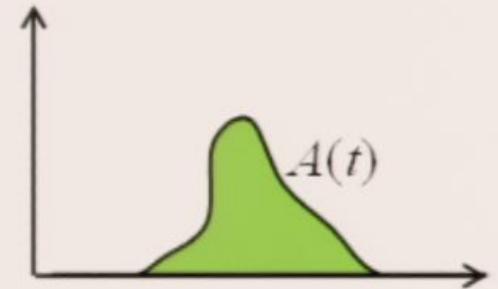From a sequence of such pulses, we can create any 1-qubit gate!

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From a sequence of such pulses, we can create any 1-qubit gate!

$$
\begin{aligned}
\hat{R}_x(\pi) &= -iX & \hat{R}_y(\pi)\hat{R}_x(\pi) &= -iZ \\
\hat{R}_y(\pi) &= -iY & \hat{R}_x(\pi)\hat{R}_y(\pi/2) &= -iH
\end{aligned}
$$

for Atoms

$$R_x(\beta) = \begin{pmatrix} \cos \beta/2 \\ & \cos \beta/2 \end{pmatrix}$$

$$R_x(\beta) = \begin{pmatrix} \cos \beta/2 & -i\sin \beta/2 \\ -i\sin \beta/2 & \cos \beta/2 \end{pmatrix}$$

$$R_y(\beta) = \begin{pmatrix} \cos \beta/2 & \\ & \cos \beta/2 \end{pmatrix}$$

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$$R_x(\pi) R_y\left(\pi/2\right) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}\Bigg($$

$$R_x(\beta) = \begin{pmatrix} \cos \beta/2 & -i\sin\beta/2 \\ -i\sin\beta/2 & \cos\beta/2 \end{pmatrix}$$

$$R_y(\beta) = \begin{pmatrix} \cos\beta/2 & -\sin\beta/2 \\ \sin\beta/2 & \cos \end{pmatrix}$$

$$R_x(\pi)R_y(\tfrac{\pi}{2}) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{ }}\begin{pmatrix} -i \\ \end{pmatrix}$$

WHAT PART
THE QUANTU
THEORY DON'T
UNDERSTAND

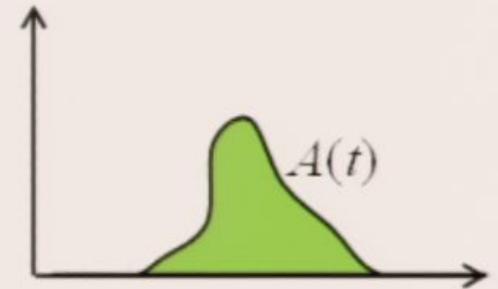$$R_x(\beta) = \begin{pmatrix} \cos \beta/2 & -i\sin \beta/2 \\ -i\sin \beta/2 & \cos \beta/2 \end{pmatrix}$$

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$$= -iH$$

Radio pulses

$$\hat{H} = A(t)(\cos\phi\, X + \sin\phi\, Y)$$

Total strength of resonant pulse $\quad \displaystyle\int_{-\infty}^{\infty} A(t)\, dt = \frac{\beta}{2}$

$A(t)$

By choosing phases $\phi = 0$ or $\phi = \pi/2$, we can produce

$$\hat{R}_x(\beta) \;=\; e^{-i(\beta/2)X} \;=\; \cos(\beta/2)\mathbf{1} - i\sin(\beta/2)X$$
$$\hat{R}_y(\beta) \;=\; e^{-i(\beta/2)Y} \;=\; \cos(\beta/2)\mathbf{1} - i\sin(\beta/2)Y.$$

From a sequence of such pulses, we can create any 1-qubit gate!

$$\hat{R}_x(\pi) = -iX \qquad\qquad \hat{R}_y(\pi)\hat{R}_x(\pi) = -iZ$$
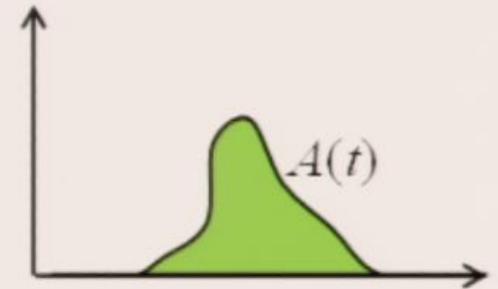
Note: Overall phases

$$\hat{R}_y(\pi) = -iY \qquad\qquad \hat{R}_x(\pi)\hat{R}_y(\pi/2) = -iH$$

are unimportant.

Radio pulses

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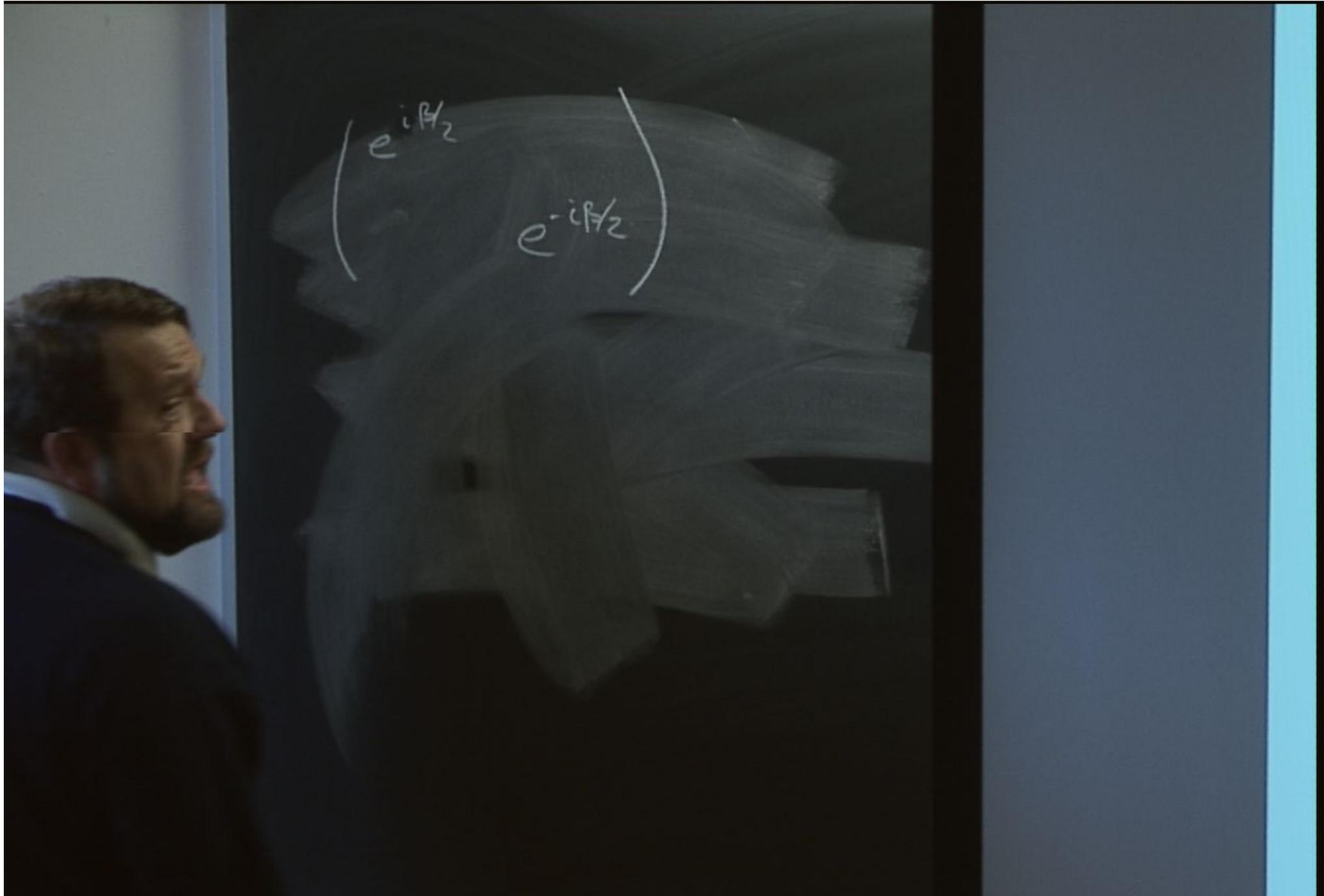From a sequence of such pulses, we can create any 1-qubit gate!

$$\hat{R}_x(\pi) = -iX \qquad \hat{R}_y(\pi)\hat{R}_x(\pi) = -iZ \qquad \text{Note: Overall phases}$$
$$\hat{R}_y(\pi) = -iY \qquad \hat{R}_x(\pi)\hat{R}_y(\pi/2) = -iH \qquad \text{are unimportant}$$

$$\begin{pmatrix} e^{i\beta/2} \\ e^{-i\beta/2} \end{pmatrix}$$

$$e^{-i\beta/2} \left(e^{i\beta/2} \right)$$

$$e^{-i\beta/2}$$

$$= \left(\begin{array}{c} 1 \\ \\ e^{-i\beta} \end{array} \right)$$

$$e^{-i\beta/2}\begin{pmatrix} e^{i\beta/2} & \\ & e^{-i\beta/2} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \\ & e^{-i\beta} \end{pmatrix}$$

Two spins!

Two spins!

Two spins!

Rotating frame for both spins:

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Terms in $H^{(12)}$

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overall E-shift (ignore) $\mathbf{1}^{(1)} \otimes \mathbf{1}^{(2)}$	$\mathbf{1}^{(1)} \otimes X^{(2)}$	$\mathbf{1}^{(1)} \otimes Y^{(2)}$	$\mathbf{1}^{(1)} \otimes Z^{(2)}$
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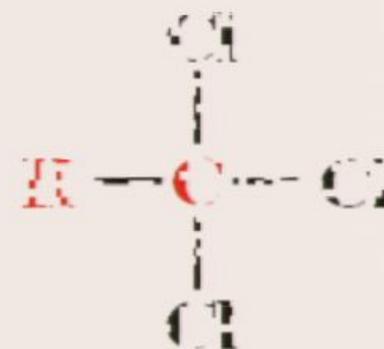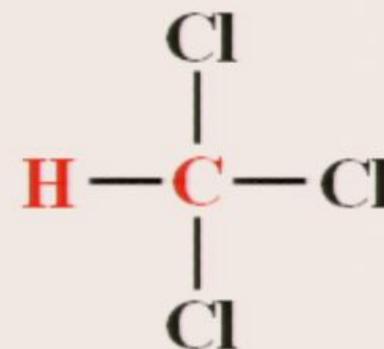
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Chemical shifts
for spins 1 and 2

J-coupling
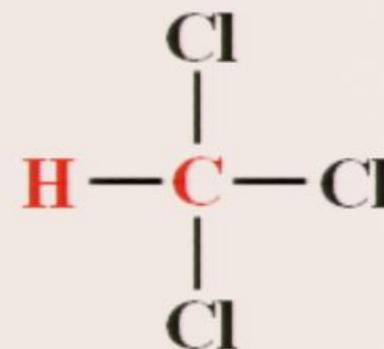mediated by
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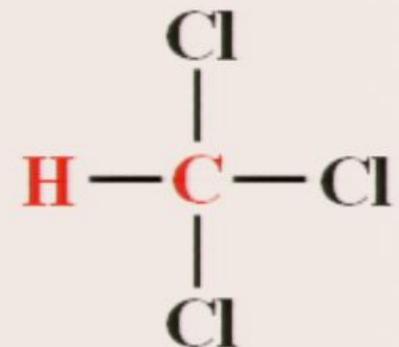
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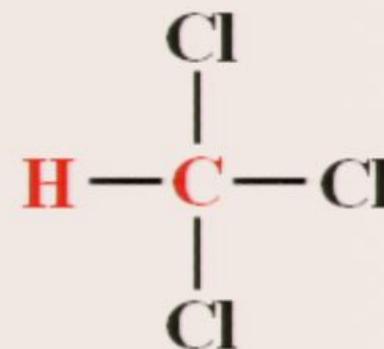$$\hat{H}^{(12)} = \varepsilon_1 Z^{(1)} + \varepsilon_2 Z^{(2)} + \varepsilon_{12} Z^{(1)} \otimes Z^{(2)}$$

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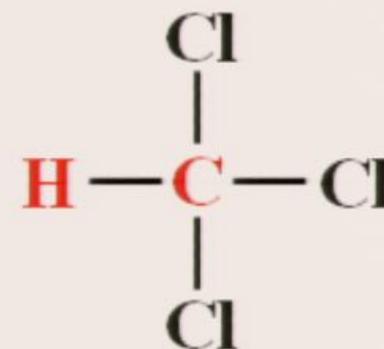
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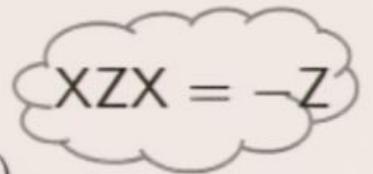
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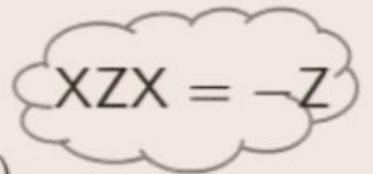
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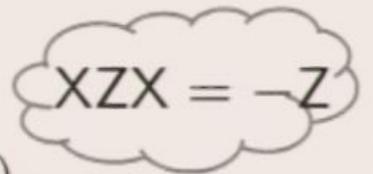
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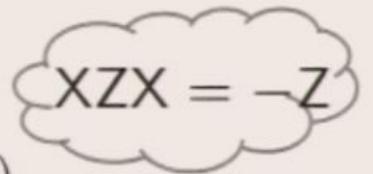
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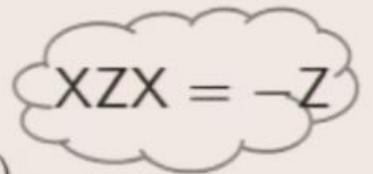
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Controlled-Z gate!

NMR quantum computing

1-qubit and 2-qubit gates provide a universal set for quantum computation!

Note: We must be able to address spins *individually* with resonant pulses.

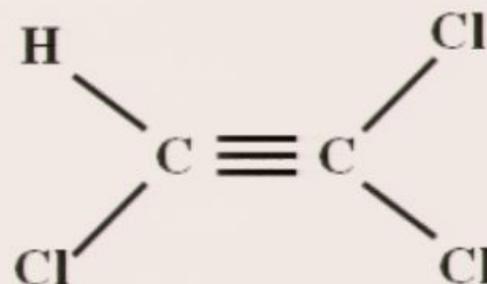Chemical shifts must separate similar nuclei in frequency.

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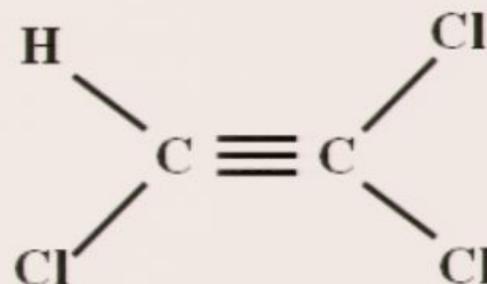
Resonant pulses must be very narrow in frequency -- this limits the speed of 1-qubit gates.

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Use "pseudopure" states, do computation on ~10^{18} molecules.

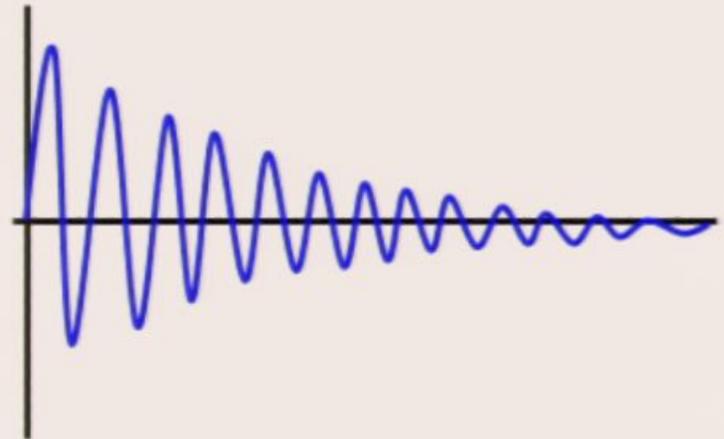$$\omega = \left(\frac{1-\eta}{d}\right) \mathbf{1} + \eta |\psi\rangle\langle\psi| \qquad \eta = \text{"purity"}$$

Measurement

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Free-induction decay (FID): Freely
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Only transverse (X and Y) components of
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From amplitude and phase information in
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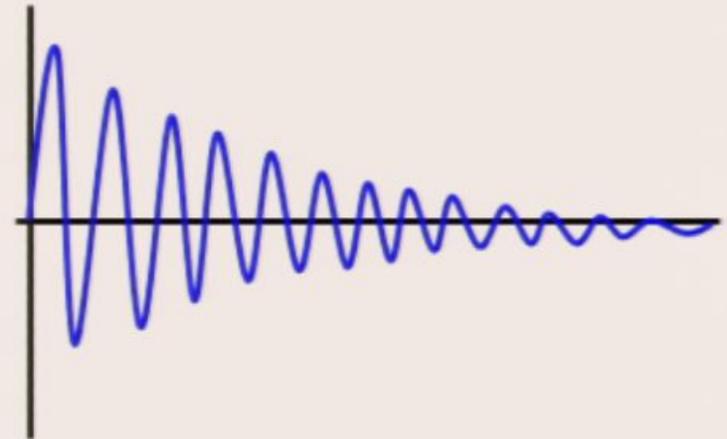 averages for $\langle X \rangle$ and $\langle Y \rangle$.

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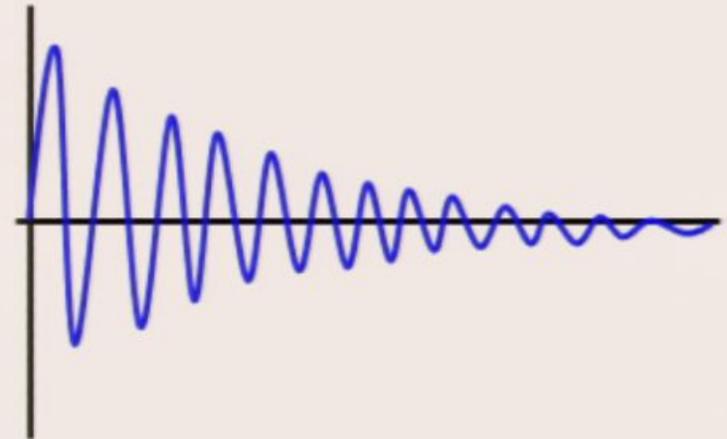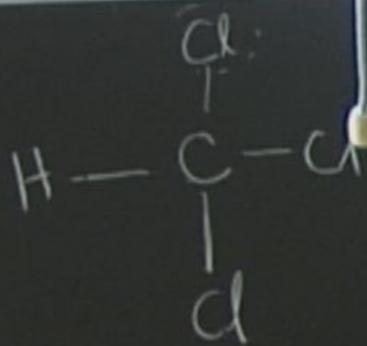
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Lindblad operators (simplified):

Longitudinal $\quad \lambda^{1/2}\,|0\rangle\langle 1| \qquad\qquad$ Transverse $\quad \mu^{1/2}\mathsf{Z}$

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Relaxation times

Nuclear spins: Open systems with both "longitudinal" and "transverse" relaxation processes.

$$\dot{\rho} = \frac{1}{i\hbar}[H, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\}\right)$$

Lindblad operators (simplified):

Longitudinal $\quad \lambda^{1/2}|0\rangle\langle 1|$ $\quad\quad$ Transverse $\quad \mu^{1/2}Z$
$\quad\quad\quad\quad\quad\quad\quad \lambda^{1/2}|1\rangle\langle 0|$

- Populations decay toward equilibrium with time constant T_1.
- Coherences decay toward zero with time constant T_2 (faster).
- For ^{13}C in chloroform, $T_2 \approx 0.3$ s -- enough time for many quantum gates!

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