Ressonância Magnética Nuclear: Ecos, Imagens e Computação Quântica

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- Fundamentos de RMN
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  - Ecos
  - Espectroscopia
- Imagens por RMN (MRI)
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  - Métodos de contraste
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RMN

Ecos, Imagens e Computação Quântica

1940 1980 2000

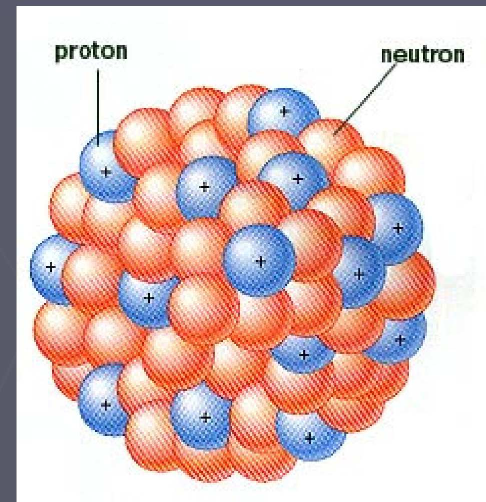
Alguns marcos históricos da RMN

- Rabi (1937): ressonância em feixes de moléculas de H_2.
  - Prêmio Nobel de Física - 1944.
- Bloch (1946): absorção de RF em água.
  - Prêmio Nobel de Física - 1952.
- Purcell (1946): absorção de RF em parafina.
  - Prêmio Nobel de Física - 1952.
- Hahn (1949): ecos de spin.
- Packard (1951): deslocamento químico em etanol.
- Andrew, Lowe (1959): RMN no estado sólido.
- Ernst (1964): RMN com transformada de Fourier.
  - Prêmio Nobel de Química - 1991.
- Wüthrich (1968): RMN aplicada ao estudo de macromoléculas biológicas.
  - Prêmio Nobel de Química - 2002.
- Lauterbur, Mansfeld (1973): imagem por RMN (MRI).
  - Prêmio Nobel de Medicina - 2003.

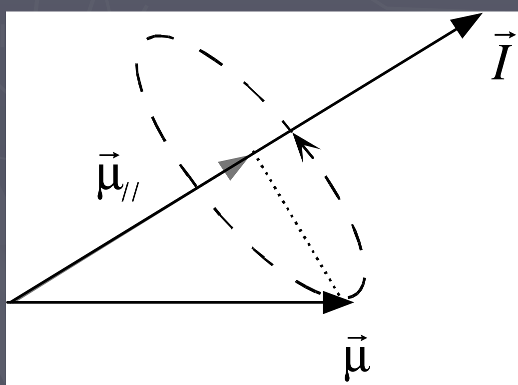
Spin nuclear e momento de dipolo magnético nuclear

$$\vec{\mathbf{I}} = \sum_{k=1}^{A}\left(\vec{\boldsymbol{l}}_k + \vec{\boldsymbol{s}}_k\right)$$

O *spin nuclear*:
- Número quântico *I*.
- Inteiro ou semi-inteiro.



$$\vec{\mu} = (\mu_{\mathrm{N}} / \hbar)\left[\sum_{k=1}^{Z}\vec{\boldsymbol{l}}_k + \sum_{k=1}^{Z} g_{sp}\vec{\boldsymbol{s}}_k + \sum_{k=Z+1}^{A} g_{sn}\vec{\boldsymbol{s}}_k\right]$$



$$\vec{\mu}_{efetivo} = \frac{\langle \vec{\mu} \cdot \vec{\mathbf{I}} \rangle}{I(I+1)\hbar^2}\vec{\mathbf{I}} = \gamma\vec{\mathbf{I}}$$

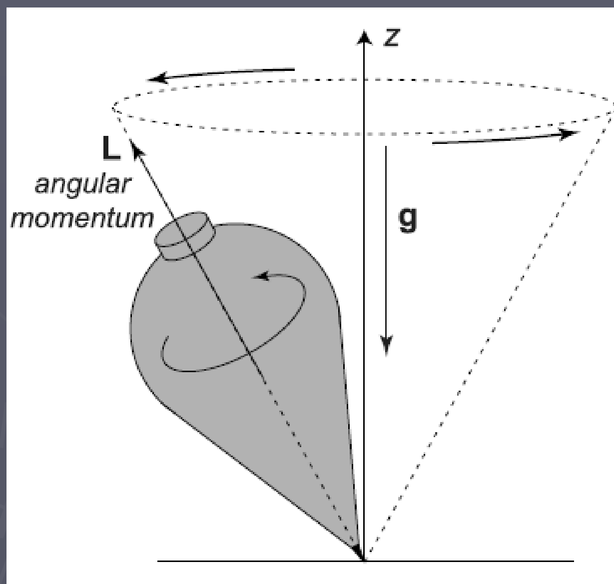
Fator giromagnético

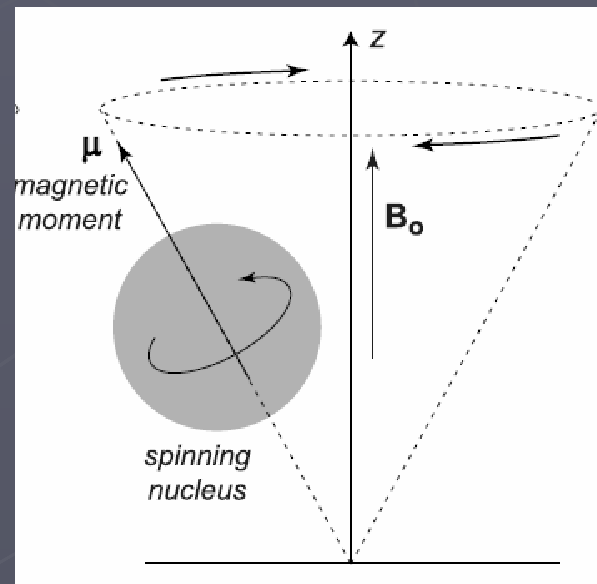
Alguns núcleos de interesse para RMN

Nuclídeo	*Abundância Natural* (%)	*I*	μ (múltiplos de μ_N)	*Q* (barns)
^{1}H	99,99	1/2	2,7928	0
^{13}C	1,11	1/2	0,7024	0
^{14}N	99,63	1	0,4036	0,01
^{15}N	0,37	1/2	0,2831	0
^{19}F	100	1/2	2,6287	0
^{27}Al	100	5/2	3,6414	0,150
^{29}Si	4,70	1/2	0,5553	0
^{31}P	100	1/2	1,1317	0
^{55}Mn	100	5/2	3,4680	0,400
^{59}Co	100	7/2	4,6490	0,400
^{155}Gd	14,73	3/2	0,2700	1,300
^{157}Gd	15,68	3/2	0,3600	1,500

Fundamentos de RMN

Núcleo atômico na presença de um campo magnético estático:





$$\vec{\tau} = \vec{r} \times m\vec{g}$$

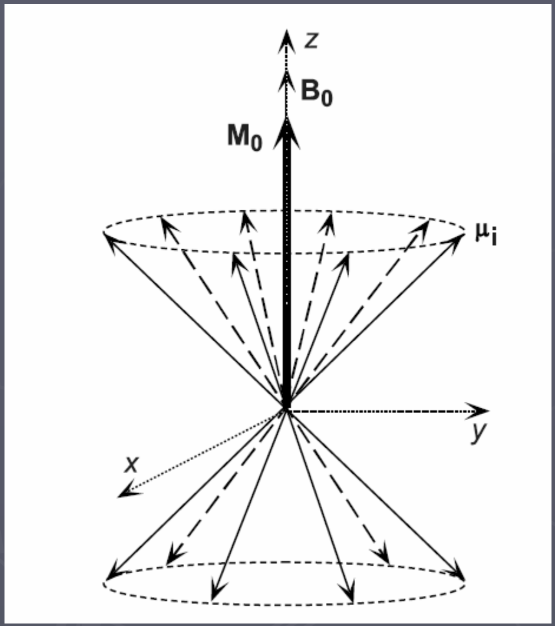
$$\omega = \frac{mgr}{L}$$

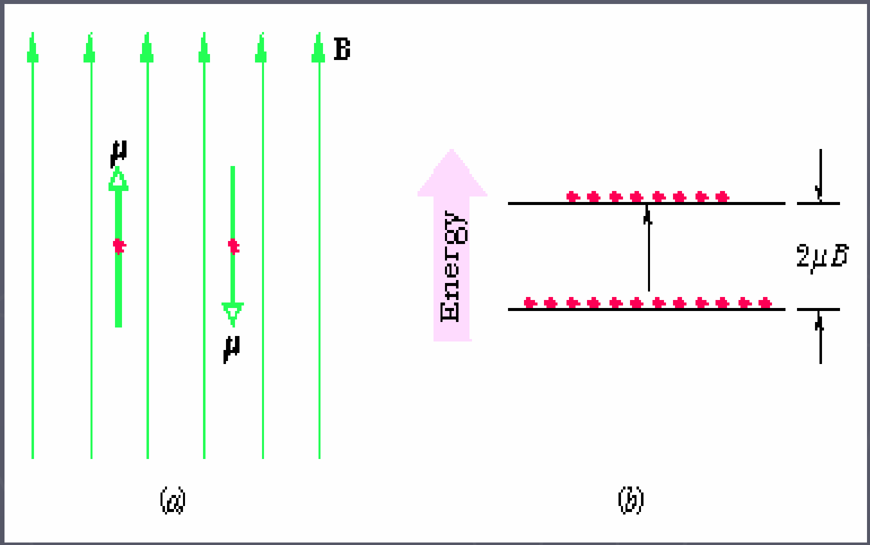
$$\vec{\mu} = \gamma \vec{I}$$

$$\vec{\tau} = \vec{\mu} \times \vec{B}_0$$

$$\omega_L = \gamma B_0$$

Paramagnetismo nuclear



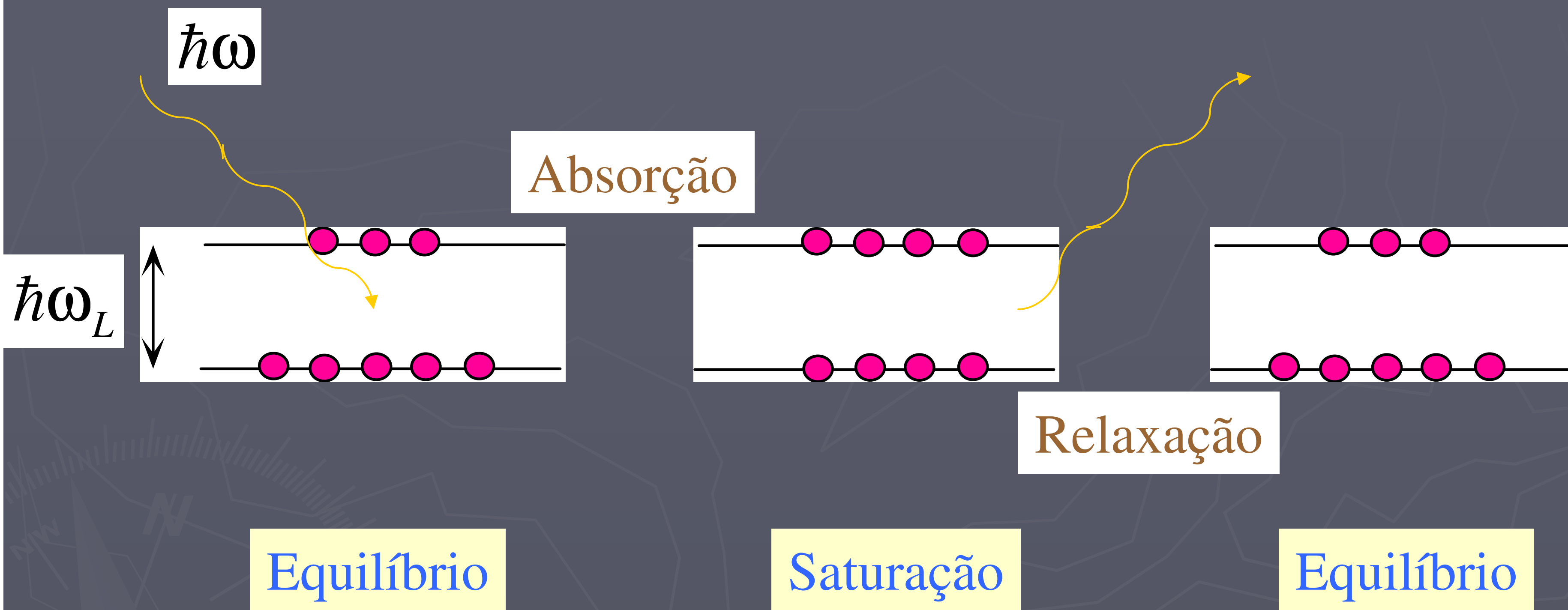


$$M_0 = \frac{N\mu^2 B_0}{3kT}$$

$$E = -\vec{\mu}\cdot\vec{B}_0 = -\gamma m\hbar B_0 = -m\hbar\omega_L$$

$$\frac{n_-}{n_+} = e^{(-\hbar\omega_L / kT)}$$

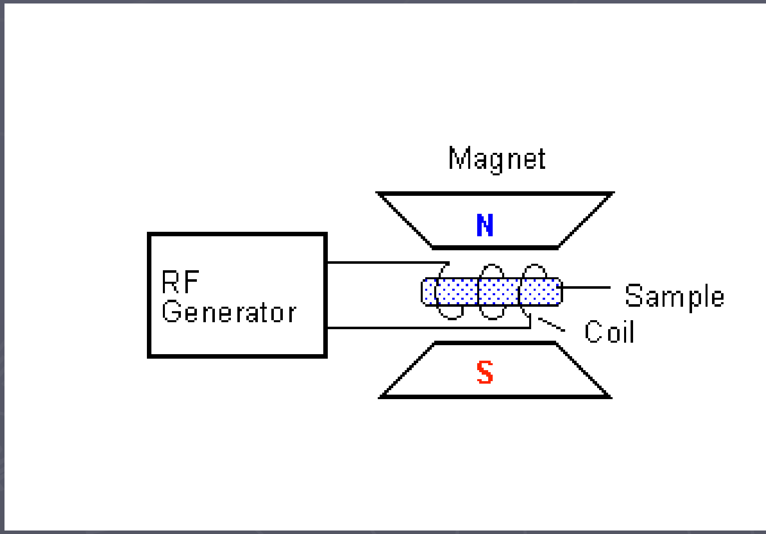
Transições de spin nuclear



Probabilidade de transição: $P_{m \to n} = P_{n \to m} \propto \gamma^2 B_1^2 \left| \langle m | \mathbf{I}_x | n \rangle \right|^2 \delta(\omega - \omega_L)$

Excitação do sistema de spins

$$B_0 \sim 1\text{T} \;\Rightarrow\; \begin{cases} f_L \sim 43 \text{ MHz} \;\; (^1\text{H}) \\ f_L \sim 28 \text{ GHz} \;\; (\text{elétron}) \end{cases}$$



Campo de RF: $B_1 \sim 10\text{G} = 10^{-3}\text{T}$

Campo da Terra: $B_T \sim 10^{-5}\text{T}$

$$\vec{B}_0 = B_0 \hat{z}$$

$$\vec{B}_1 = (2B_1 \cos \omega t)\hat{x}$$

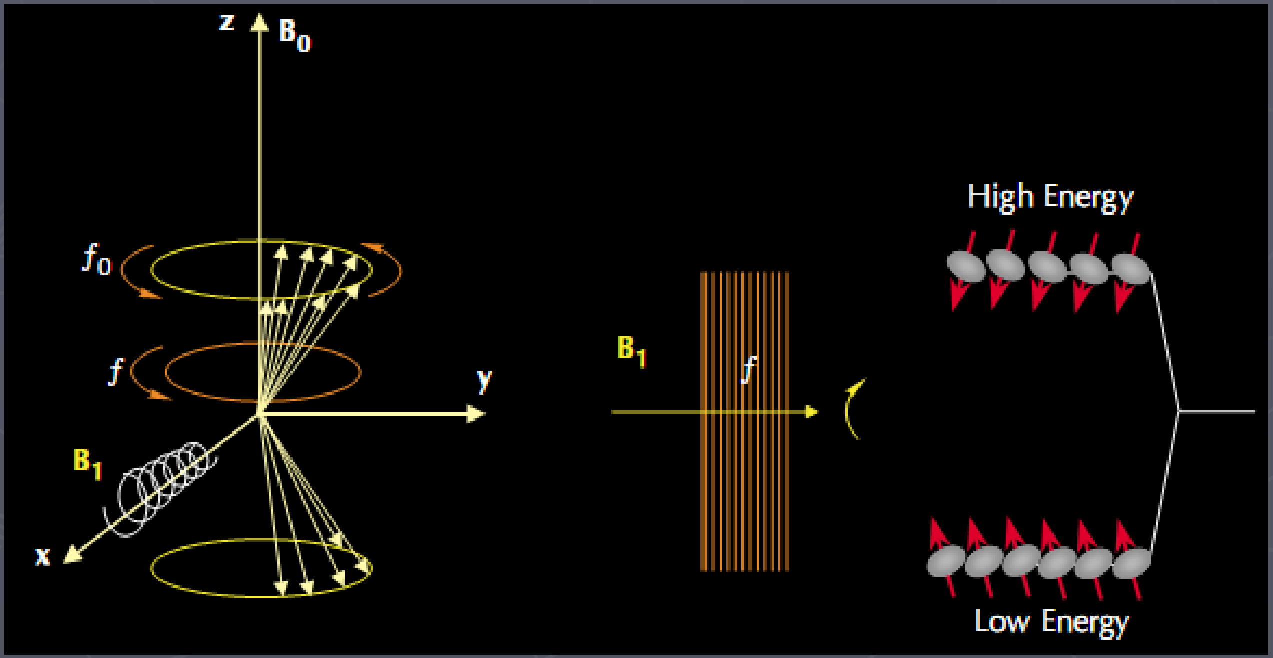
Condição de ressonância

$$\vec{B}_1 = (2B_1 \cos \omega t)\hat{x}$$

$$\cancel{\vec{B}_1^{\,+} = B_1\left[(\cos \omega t)\ \hat{x} + (\mathrm{sen}\ \omega t)\ \hat{y}\right]}$$

$$\boxed{\vec{B}_1^{\,-} = B_1\left[(\cos \omega t)\ \hat{x} - (\mathrm{sen}\ \omega t)\ \hat{y}\right]}$$

$$\omega \cong \omega_L$$



Efeitos do campo de RF sobre a magnetização

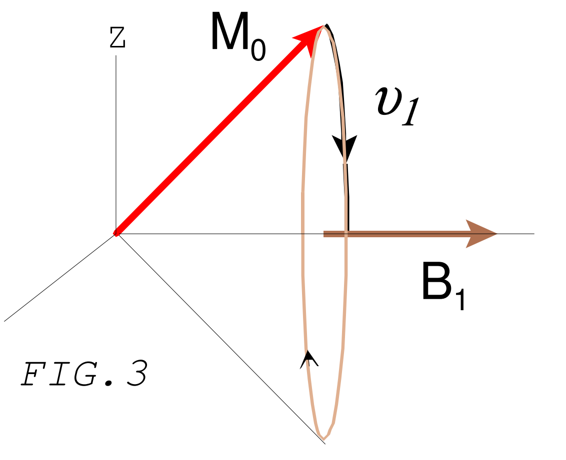


FIG. 3

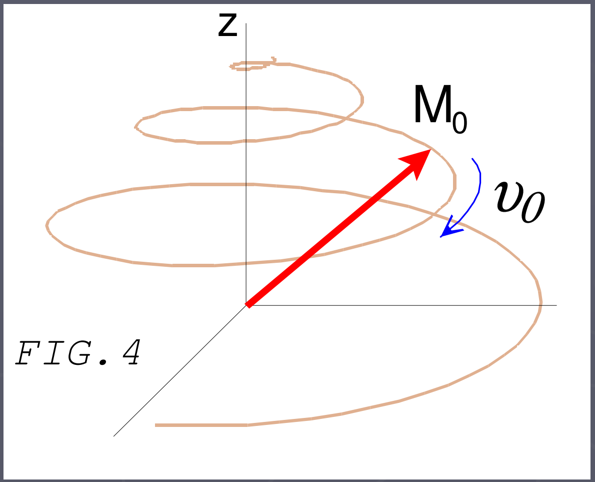


FIG. 4

Sistema girante de coordenadas:

$$\vec{\omega} = -\omega\,\hat{z}$$

$$\vec{B}_{ef} = \gamma^{-1}(\omega_L - \omega)\hat{z} + B_1\hat{x}$$

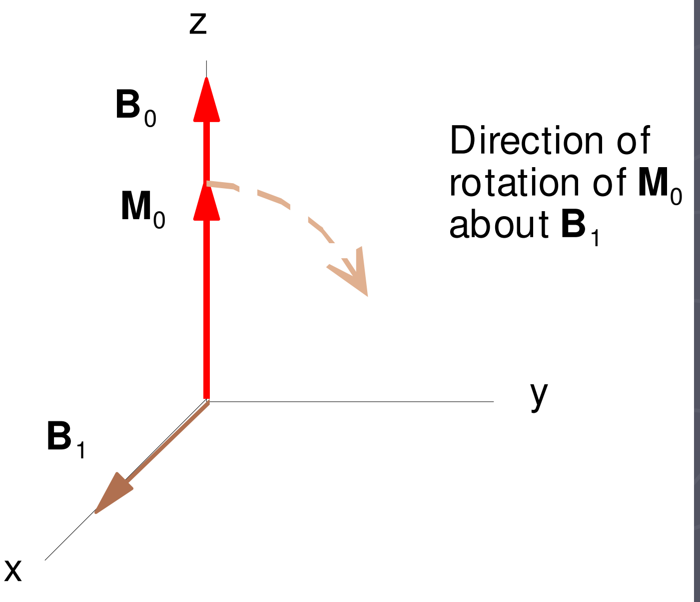
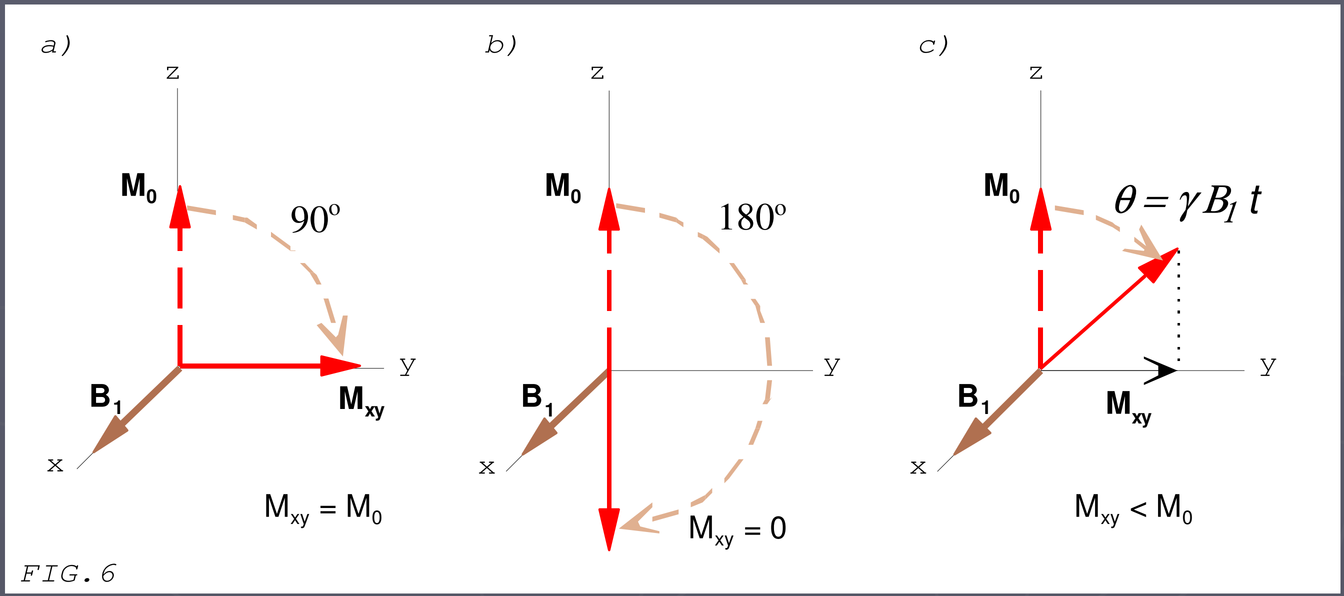


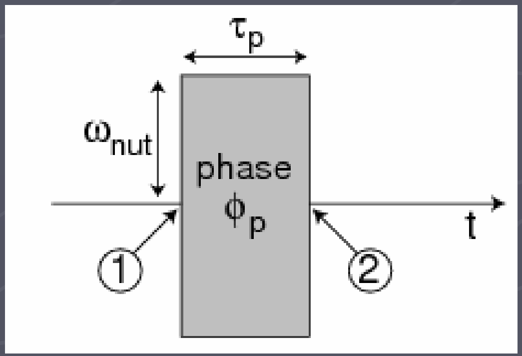
FIG. 5

Pulsos de RF

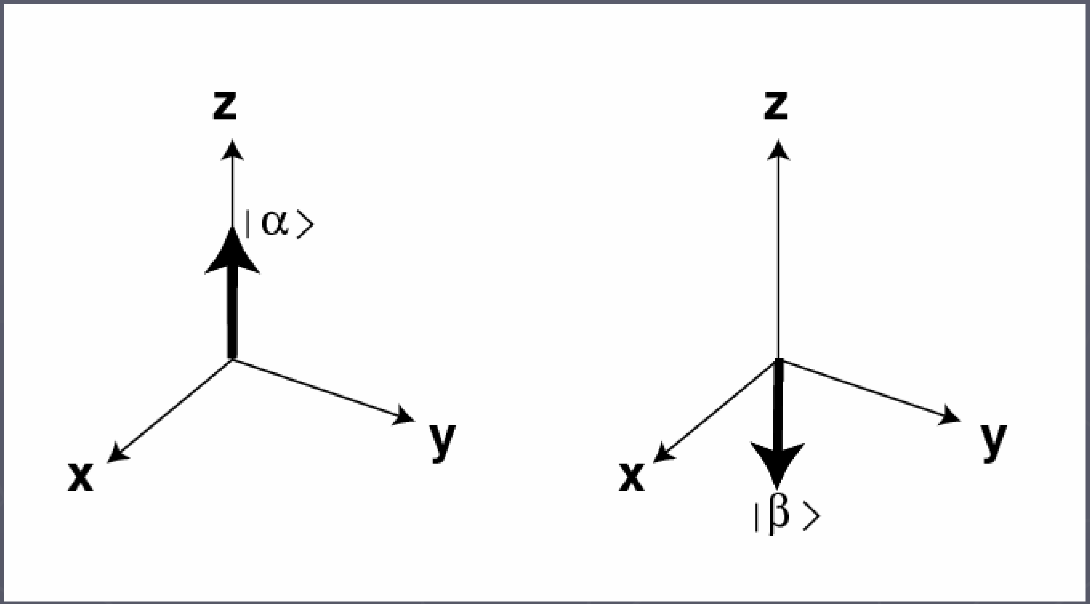


Pulso $\pi/2$ Pulso π Pulso θ

Controle
- Duração (~ µs)
- Amplitude (~ 10^2 kHz)
- Fase

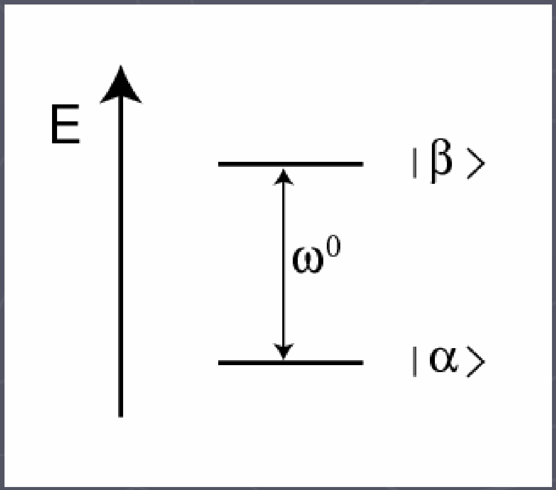


Spin ½ em um campo magnético



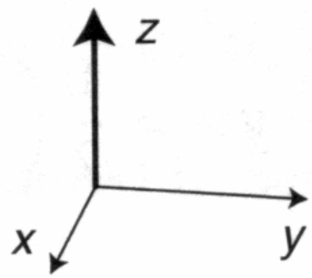
$I_z|\alpha\rangle = +\frac{1}{2}|\alpha\rangle$

$I_z|\beta\rangle = -\frac{1}{2}|\beta\rangle$

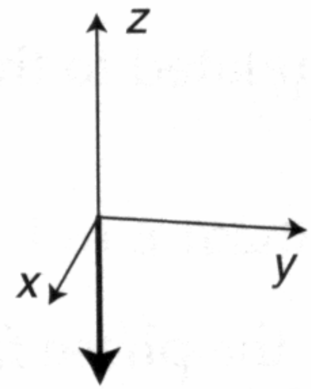


Alguns vetores de estado

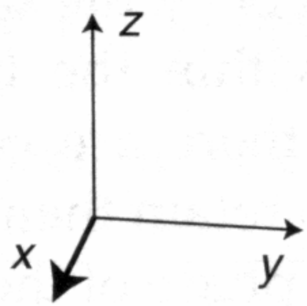
$$|\alpha> = \begin{pmatrix}1\\0\end{pmatrix} =$$



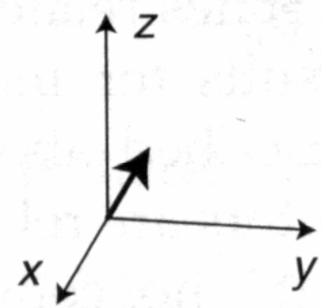
$$|\beta> = \begin{pmatrix}0\\1\end{pmatrix} =$$



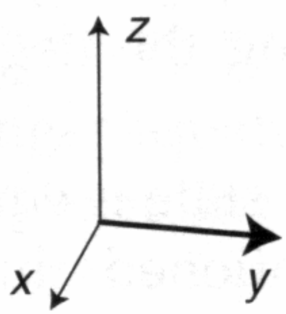
$$|+x> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} =$$



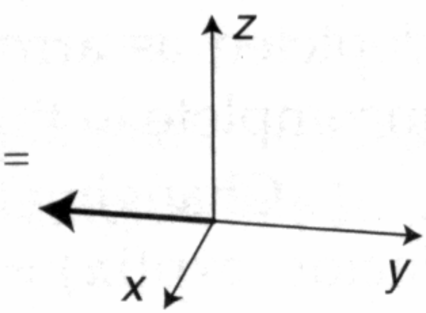
$$|-x> = \frac{1}{\sqrt{2}}\begin{pmatrix}-i\\+i\end{pmatrix} =$$



$$|+y> = \frac{1}{2}\begin{pmatrix}1-i\\1+i\end{pmatrix} =$$

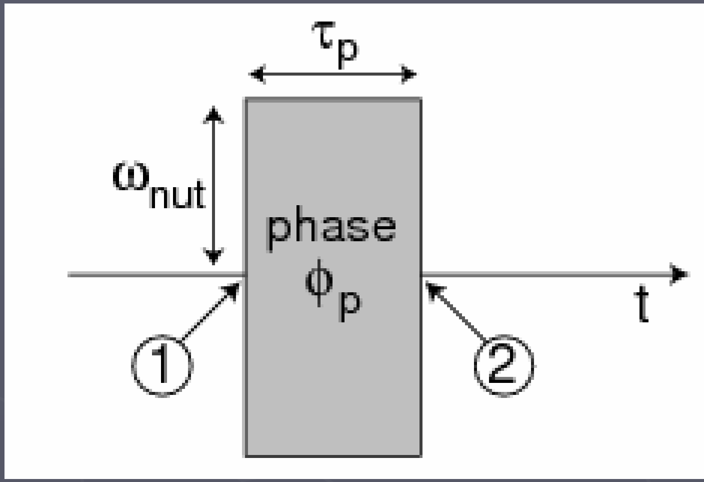


$$|-y> = \frac{1}{2}\begin{pmatrix}1+i\\1-i\end{pmatrix} =$$



Pulsos de RF: matrizes de rotação

Solução da equação de Shrödinger no sistema girante de coordenadas:



$$\theta = \gamma B_1 t_P$$

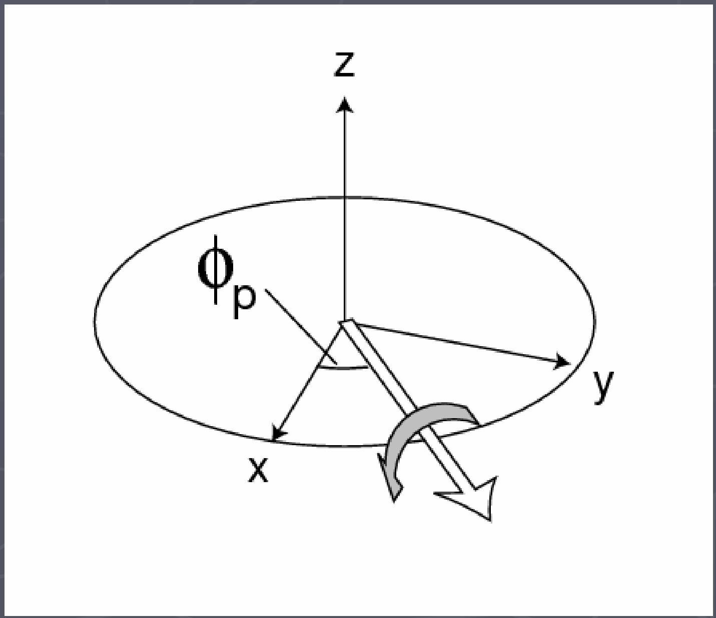
(ângulo de nutação)

$$\omega_{nut} = \gamma B_1$$

(freqüência de nutação)

$$|\psi\rangle_2 = R_{\phi_P}(\theta)|\psi\rangle_1$$

$$R_{\phi_P}(\theta) = \begin{pmatrix} \cos\frac{1}{2}\theta & -i\mathrm{sen}\frac{1}{2}\theta \mathrm{e}^{-i\phi_P} \\ -i\mathrm{sen}\frac{1}{2}\theta \mathrm{e}^{-i\phi_P} & \cos\frac{1}{2}\theta \end{pmatrix}$$



Pulsos de RF: matrizes de rotação

$$R_x(\theta) = \begin{pmatrix} \cos\frac{1}{2}\theta & -i\text{sen}\,\frac{1}{2}\theta \\ -i\text{sen}\,\frac{1}{2}\theta & \cos\frac{1}{2}\theta \end{pmatrix}$$

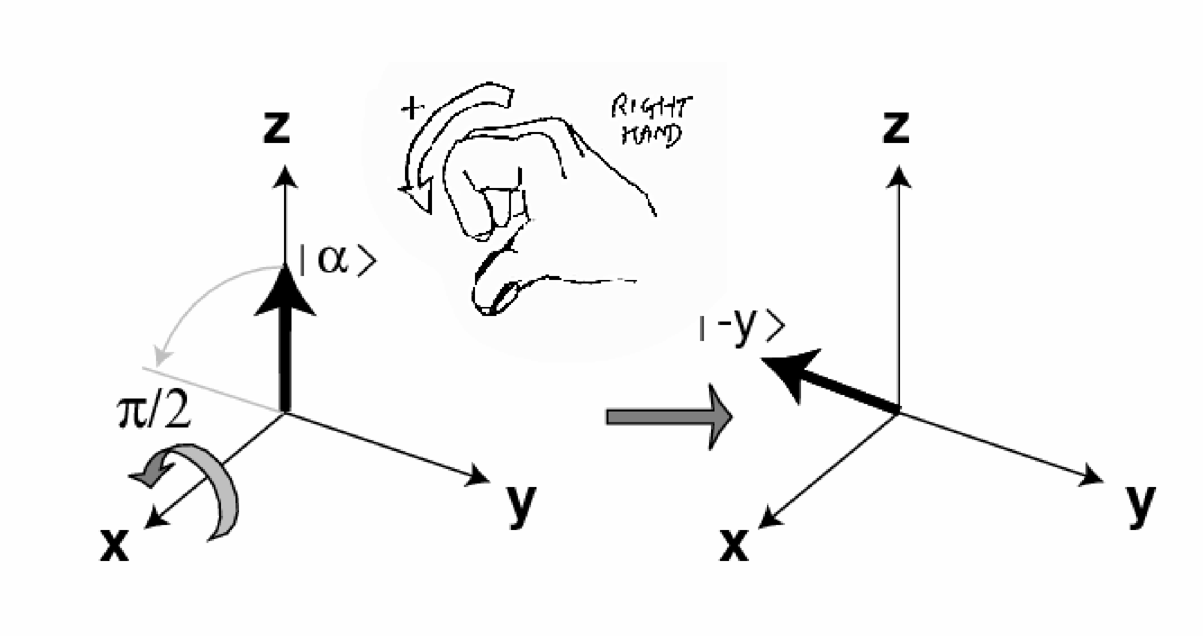
$$\theta = \gamma B_1 t_P$$

(ângulo de nutação)

$$R_x(\pi/2)|\alpha\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = e^{-i\pi/4}|-y\rangle$$

***Exemplo* 1**:

Pulso $\pi/2$ na direção *x* atuando sobre estado inicial com spin na direção *z*:



Pulsos de RF: matrizes de rotação

$$R_x(\theta) = \begin{pmatrix} \cos\frac{1}{2}\theta & -i\mathrm{sen}\frac{1}{2}\theta \\ -i\mathrm{sen}\frac{1}{2}\theta & \cos\frac{1}{2}\theta \end{pmatrix}$$

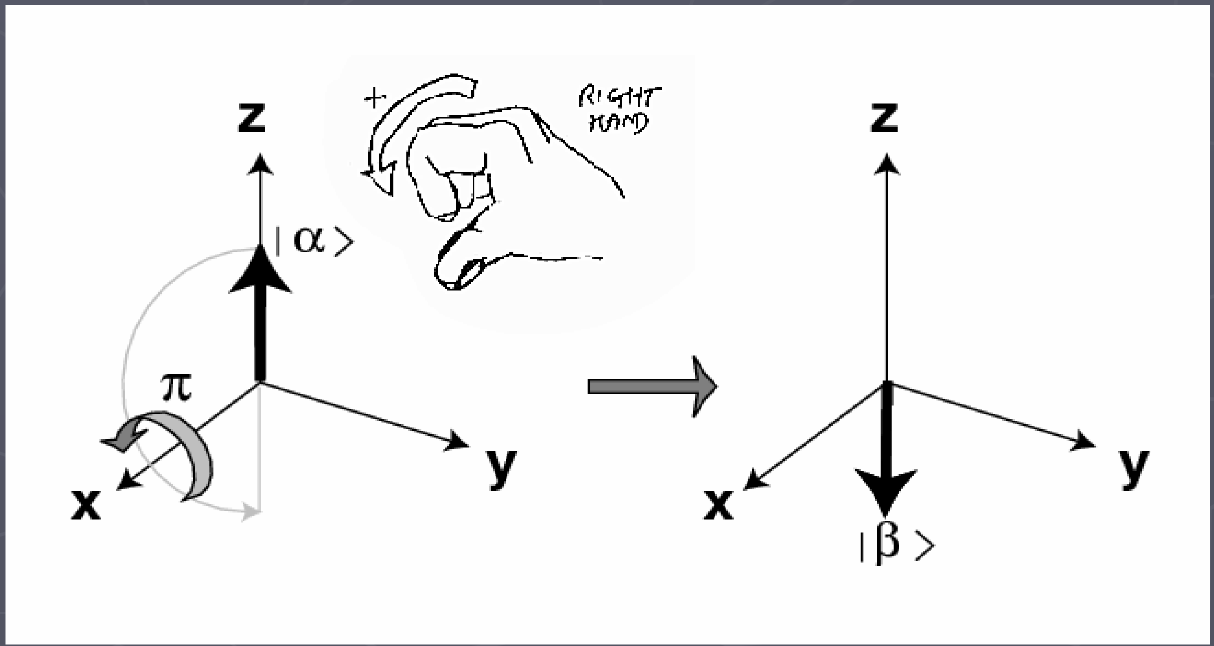
$$\theta = \gamma B_1 t_P$$

(ângulo de nutação)

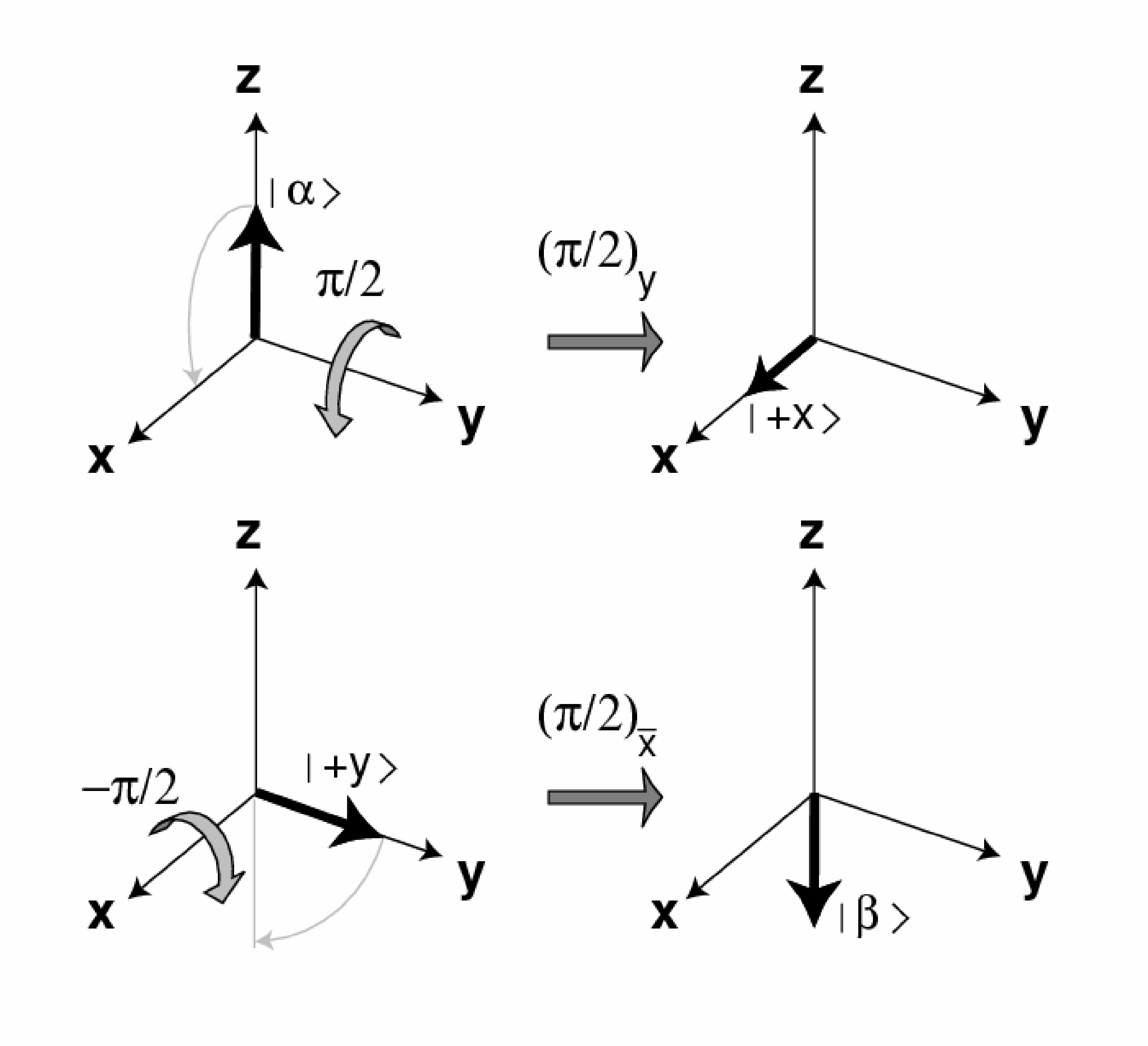
$$R_x(\pi)\left|\alpha\right\rangle = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -i\left|\beta\right\rangle$$

***Exemplo* 2**:

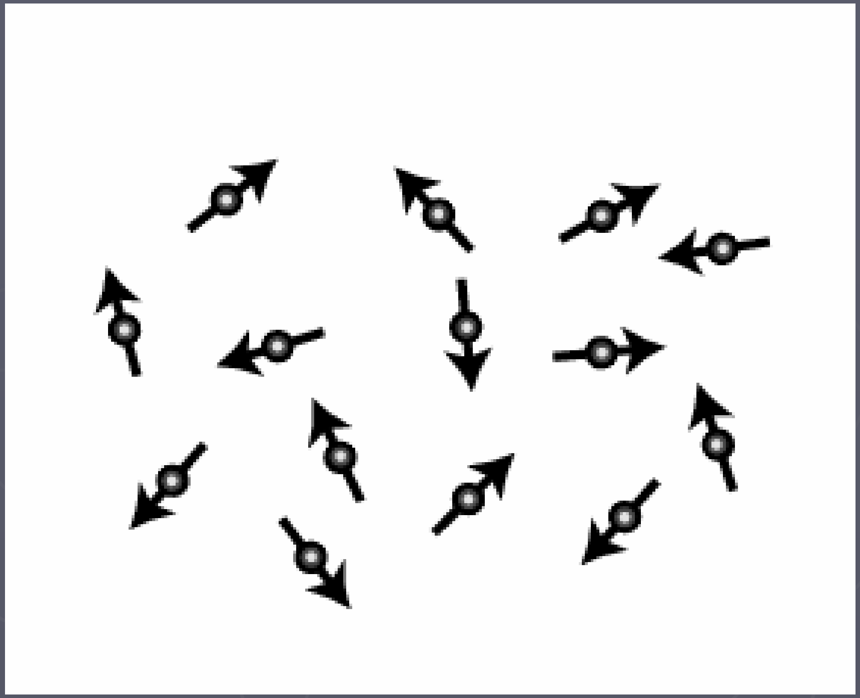
Pulso π na direção *x* atuando sobre estado inicial com spin na direção *z*:



Outros exemplos



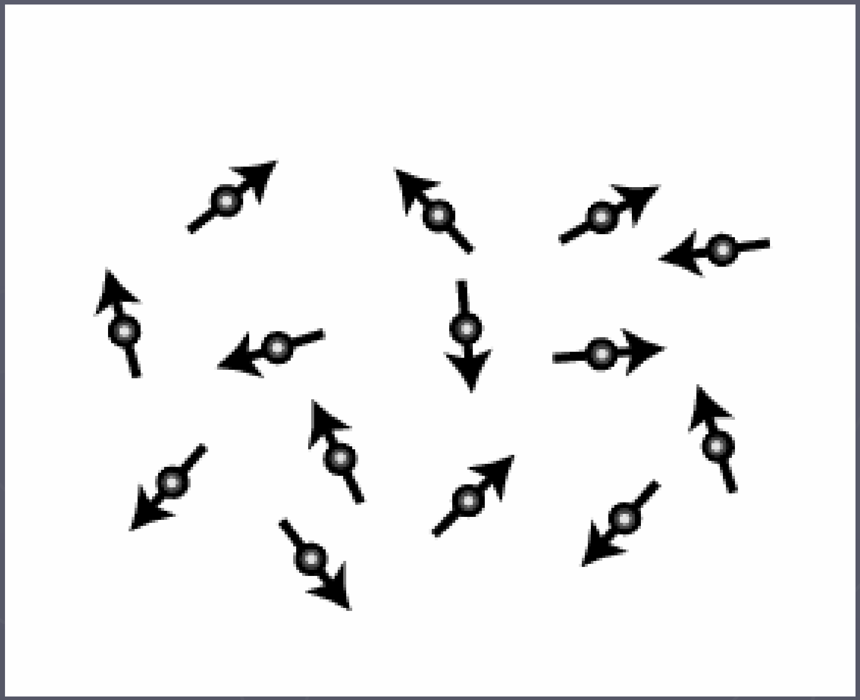
“Ensemble” de spins ½



Estado de um spin: $$|\psi\rangle = \begin{pmatrix} c_\alpha \\ c_\beta \end{pmatrix}$$

Matriz densidade para um spin: $$|\psi\rangle\langle\psi| = \begin{pmatrix} c_\alpha c_\alpha^* & c_\alpha c_\beta^* \\ c_\beta c_\alpha^* & c_\beta c_\beta^* \end{pmatrix}$$

"Ensemble" de spins ½



Matriz densidade para o ensemble: $\rho = \begin{pmatrix} \rho_{\alpha\alpha} & \rho_{\alpha\beta} \\ \rho_{\beta\alpha} & \rho_{\beta\beta} \end{pmatrix} = \begin{pmatrix} \overline{c_\alpha c_\alpha^*} & \overline{c_\alpha c_\beta^*} \\ \overline{c_\beta c_\alpha^*} & \overline{c_\beta c_\beta^*} \end{pmatrix}$

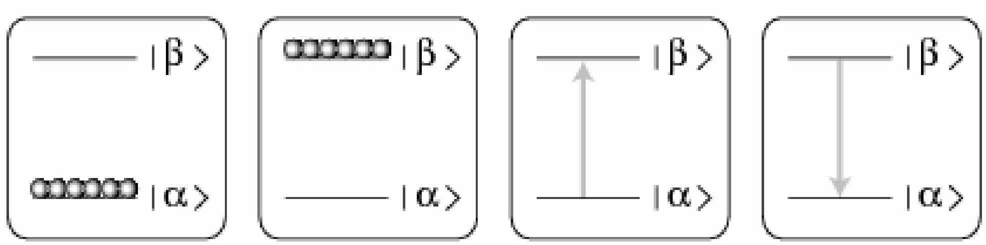
Cálculos de valores médios para o ensemble: $\langle A \rangle = \mathrm{Tr}\{\rho A\}$

Populações e coerências

$$\rho = \begin{pmatrix} \rho_{\alpha\alpha} & \rho_{\alpha\beta} \\ \rho_{\beta\alpha} & \rho_{\beta\beta} \end{pmatrix} = \begin{pmatrix} \rho_{\boxed{\alpha}} & \rho_{\boxed{+}} \\ \rho_{\boxed{-}} & \rho_{\boxed{\beta}} \end{pmatrix}$$

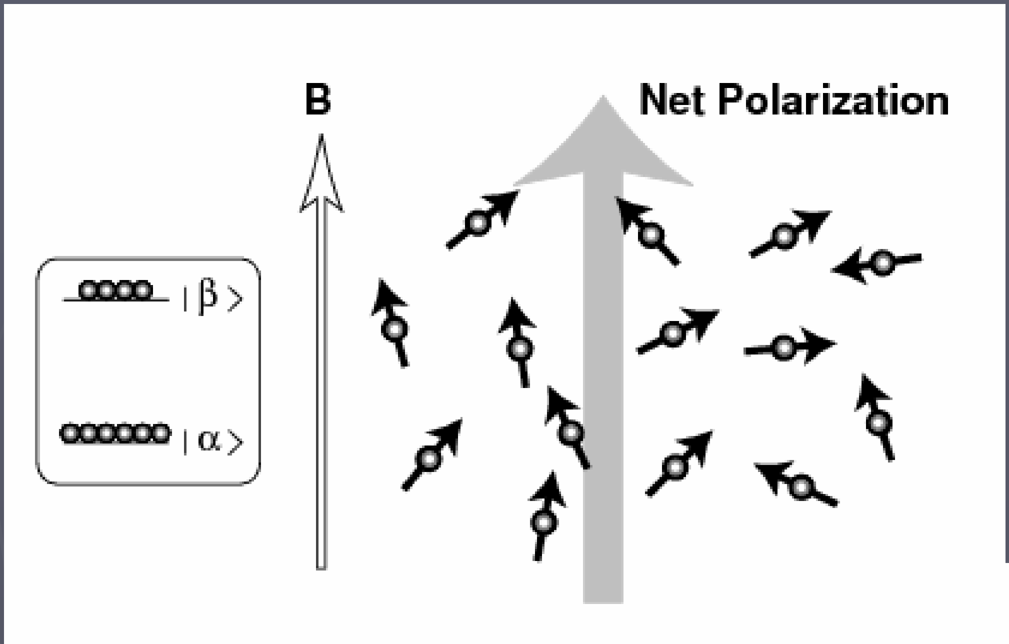
Populações: $\rho_{\boxed{\alpha}}$ $\rho_{\boxed{\beta}}$ $\rho_{\boxed{\alpha}} + \rho_{\boxed{\beta}} = 1$

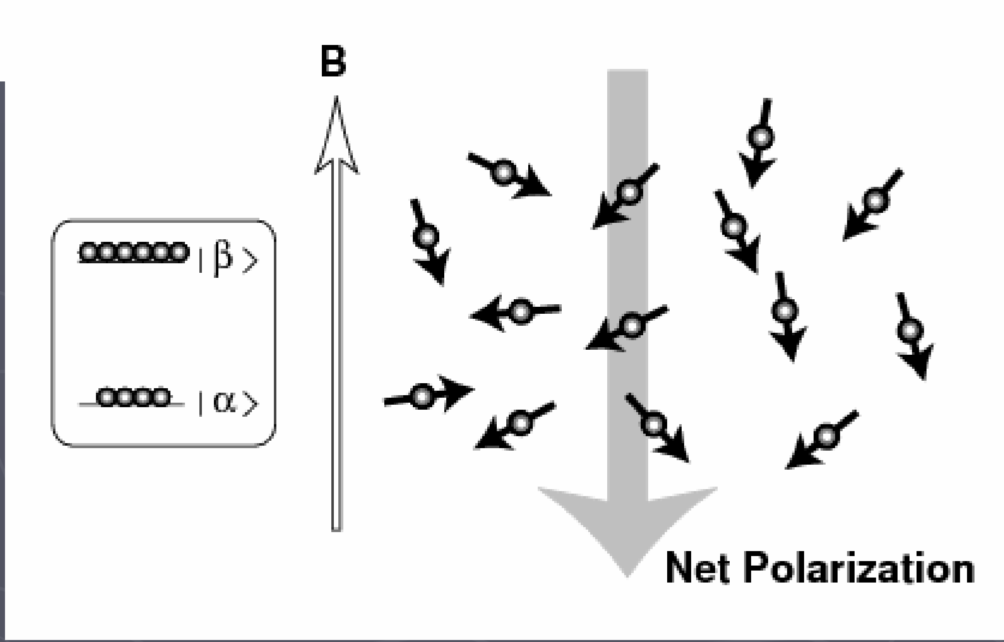
Coerências: $\rho_{\boxed{+}}$ $\rho_{\boxed{-}}$ $\rho_{\boxed{+}} = \rho_{\boxed{-}}^{*}$



$\rho_{\boxed{\alpha}}$ $\rho_{\boxed{\beta}}$ $\rho_{\boxed{-}}$ $\rho_{\boxed{+}}$

Interpretação física das populações

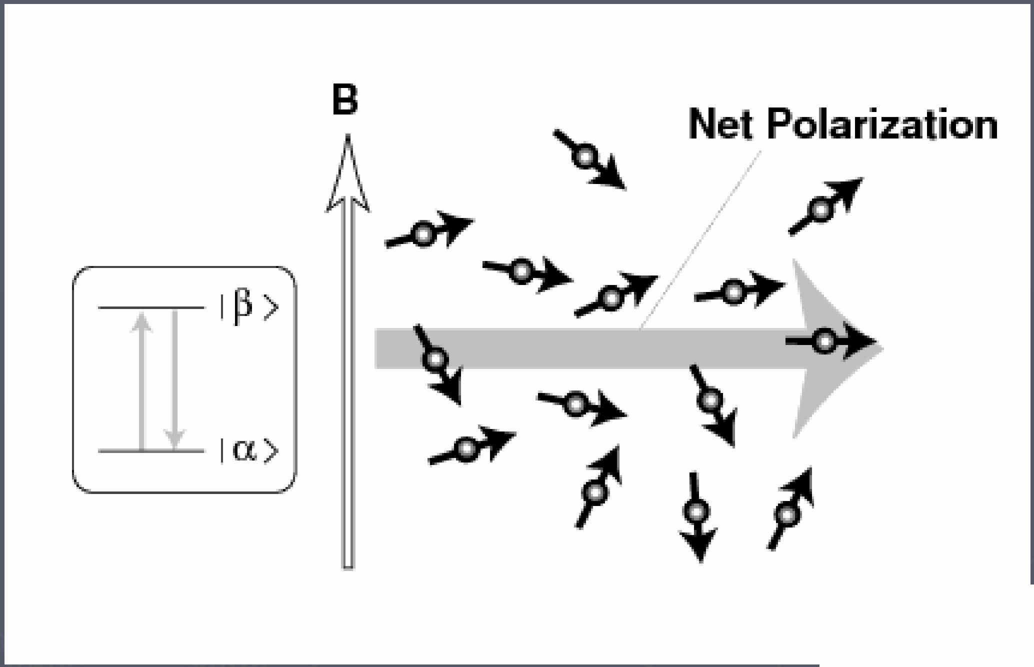




$$|\alpha\rangle\langle\alpha| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

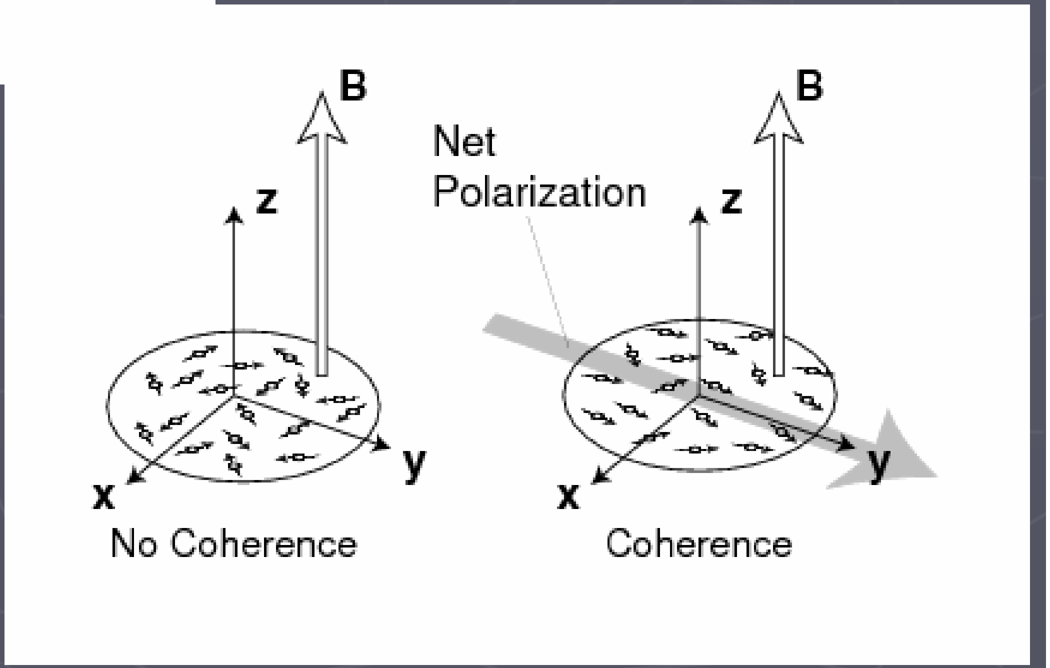
$$|\beta\rangle\langle\beta| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Interpretação física das coerências



$$|x\rangle\langle x| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$|y\rangle\langle y| = \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$$



Equilíbrio térmico

$$\rho_{eq} = \frac{e^{-H/kT}}{Z}$$

$$\rho_{eq} \cong \frac{1}{Z} - \underbrace{\frac{1}{Z}\frac{H}{kT}}_{\text{Desvio}}$$

$$U\rho_{eq}U^{\dagger} \cong \frac{1}{Z} - \frac{1}{Z}\frac{1}{kT}UHU^{\dagger}$$

$$\rho_{eq} = \begin{pmatrix} \frac{1}{2}+\frac{1}{4}\varepsilon & 0 \\ 0 & \frac{1}{2}-\frac{1}{4}\varepsilon \end{pmatrix} = \tfrac{1}{2}\mathbf{1} + \tfrac{1}{4}\mathbf{I}_z$$

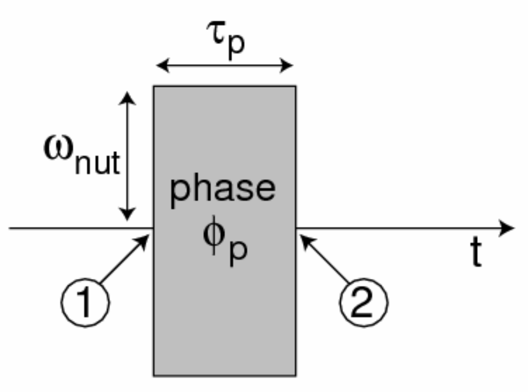
$$\varepsilon = \frac{\hbar\gamma B_0}{kT} \approx 10^{-4}$$

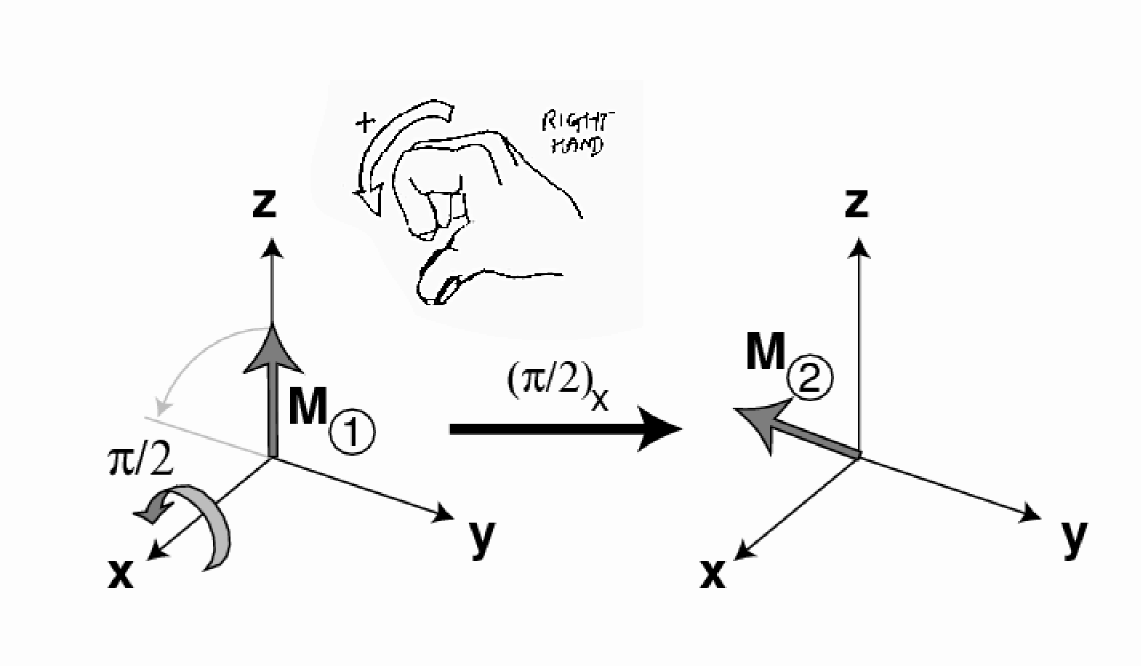
Magnetização:

$$\rho_{\boxed{\alpha}} = \tfrac{1}{2} + \tfrac{1}{4}\varepsilon\, M_z \qquad \rho_{\boxed{\beta}} = \tfrac{1}{2} - \tfrac{1}{4}\varepsilon\, M_z$$

$$\rho_{\boxed{+}} = \tfrac{1}{4}\varepsilon(M_x - iM_y) \qquad \rho_{\boxed{-}} = \tfrac{1}{4}\varepsilon(M_x + iM_y)$$

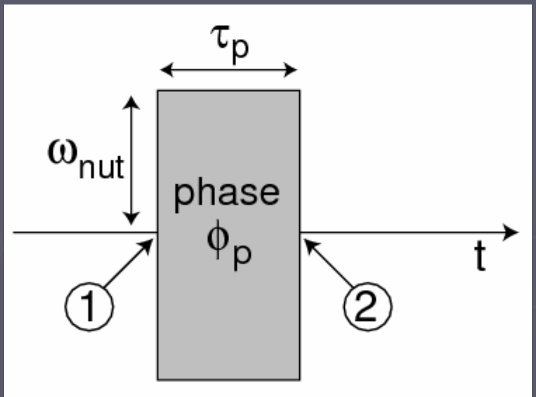
Atuação de pulsos de RF

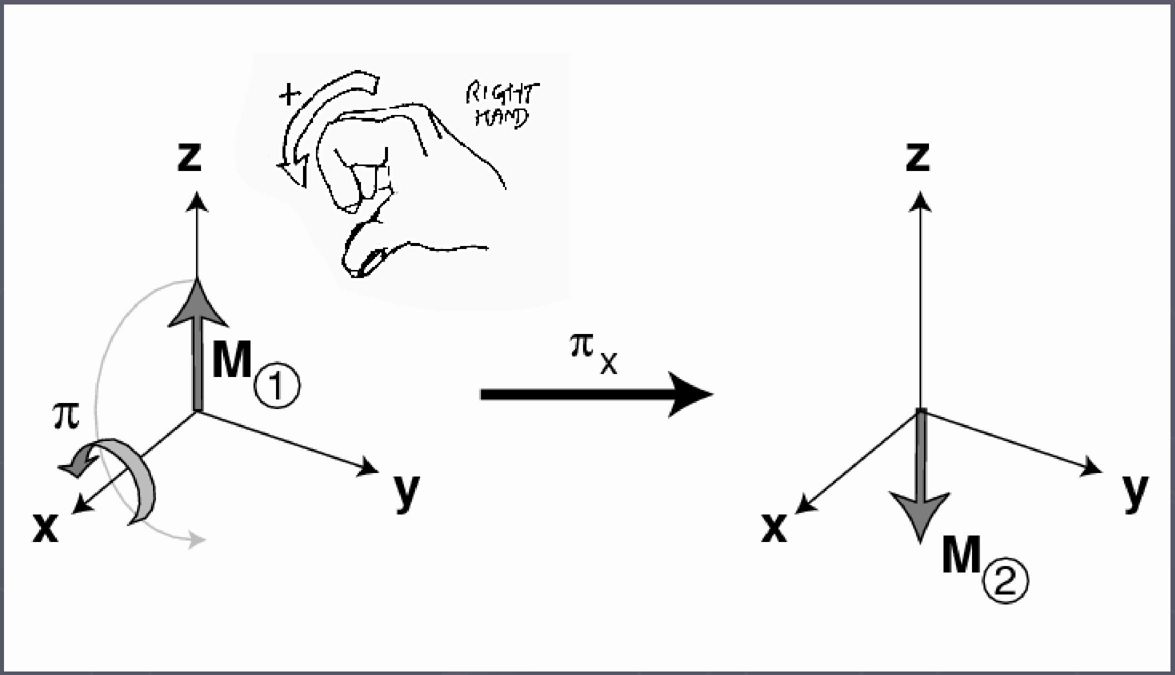




$$\rho_1 = \begin{pmatrix} \frac{1}{2}+\frac{1}{4}\varepsilon & 0 \\ 0 & \frac{1}{2}-\frac{1}{4}\varepsilon \end{pmatrix} \xrightarrow{(\pi/2)_x} \rho_2 = \begin{pmatrix} \frac{1}{2} & -\frac{1}{4i}\varepsilon \\ \frac{1}{4i}\varepsilon & \frac{1}{2} \end{pmatrix}$$

Atuação de pulsos de RF



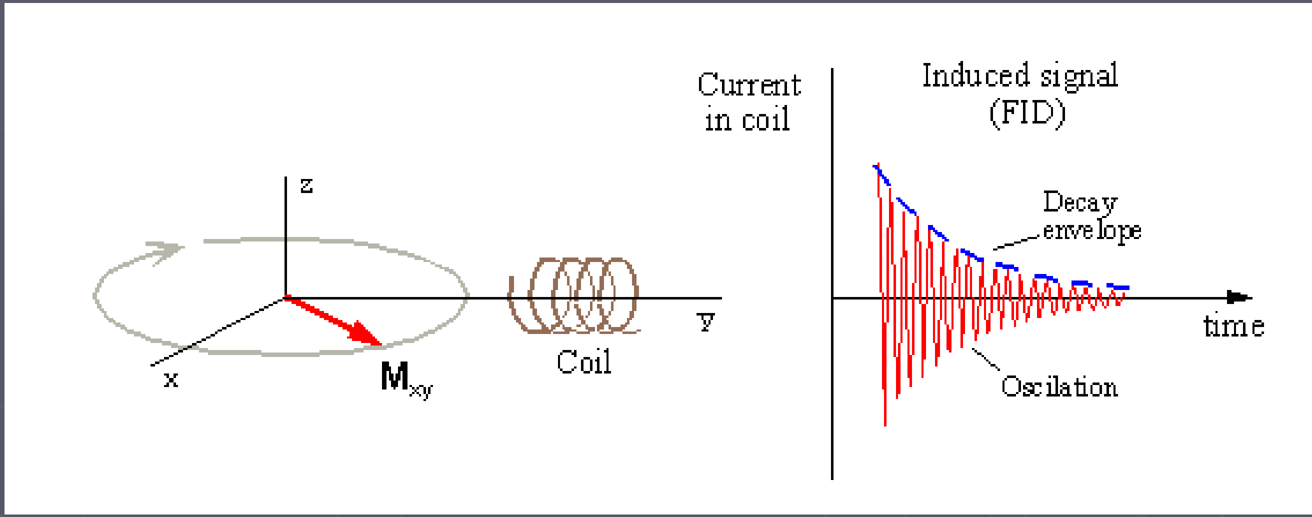


$$\rho_1 = \begin{pmatrix} \frac{1}{2}+\frac{1}{4}\varepsilon & 0 \\ 0 & \frac{1}{2}-\frac{1}{4}\varepsilon \end{pmatrix} \xrightarrow{(\pi)_x} \rho_2 = \begin{pmatrix} \frac{1}{2}-\frac{1}{4}\varepsilon & 0 \\ 0 & \frac{1}{2}+\frac{1}{4}\varepsilon \end{pmatrix}$$

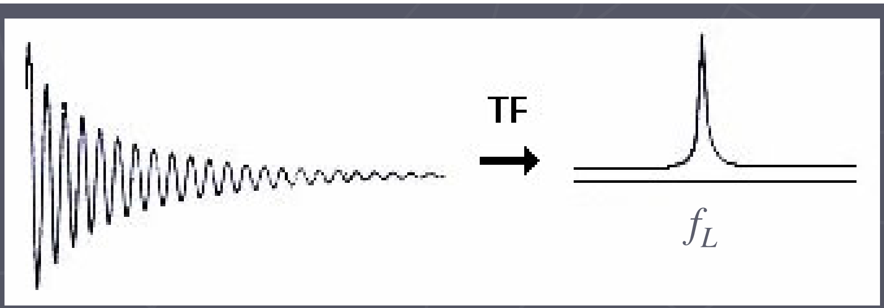
Detecção do sinal de RMN

FID = decaimeno livre de indução

ω_L



Transformada de Fourier (FT)

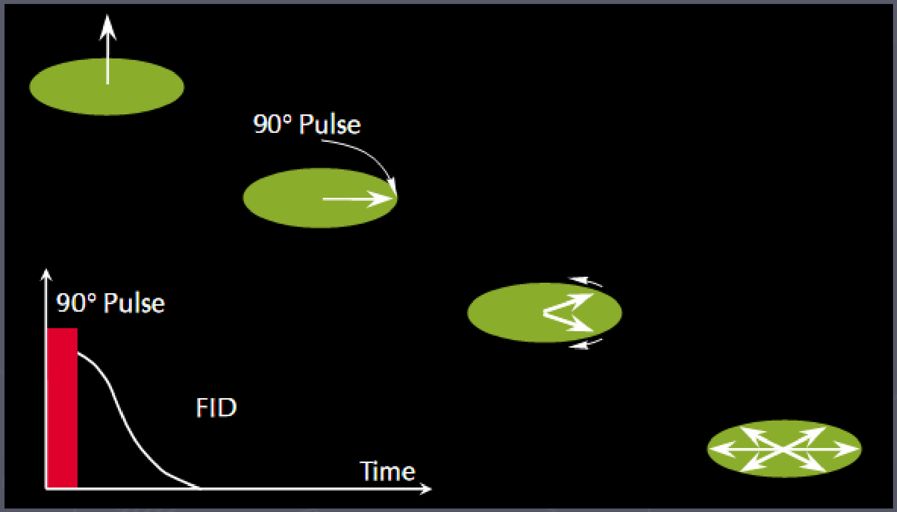


FID

Espectro

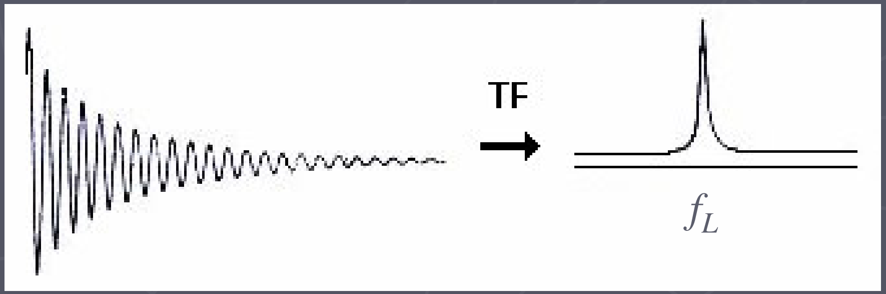
Um experimento simples de RMN (1D)

Experimento de **pulso simples** ou **decaimento de Bloch**:



Sinal detectado com frequência:
$\Delta f = f_L - f_{RF}$ (áudio)

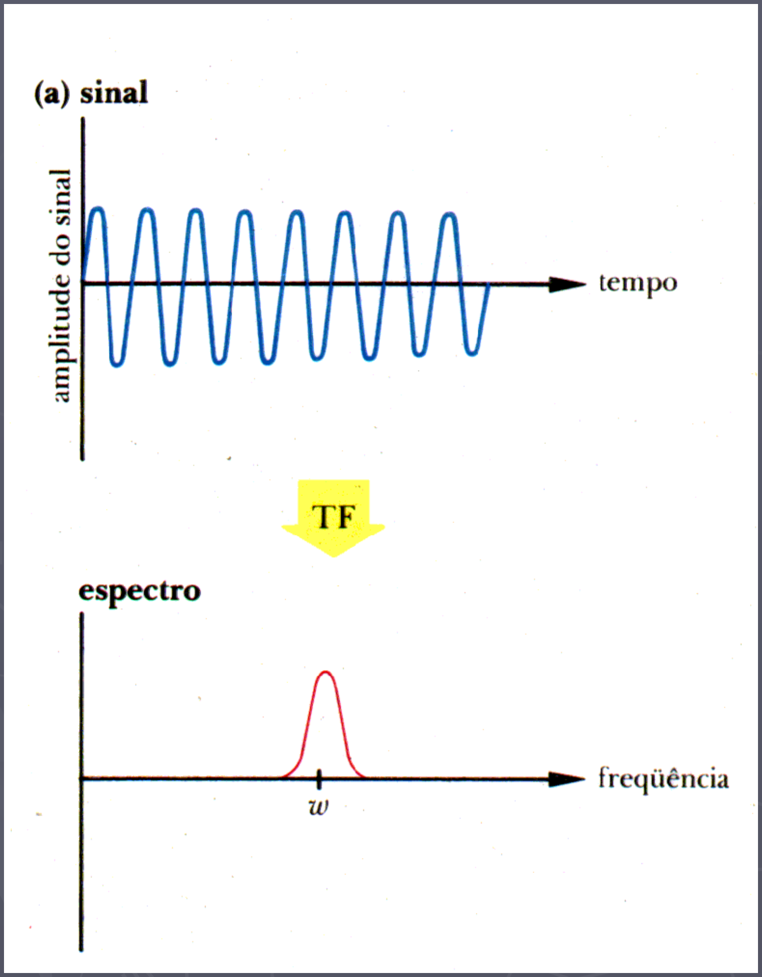
Sinal em ressonância: $\Delta f = 0$

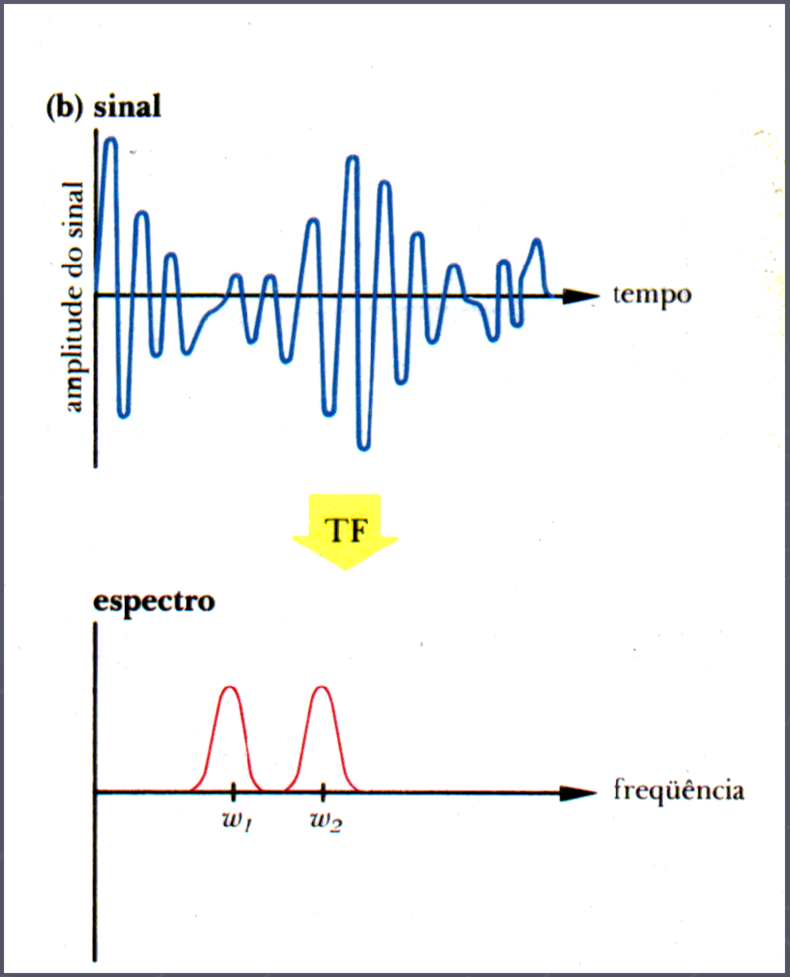


FID

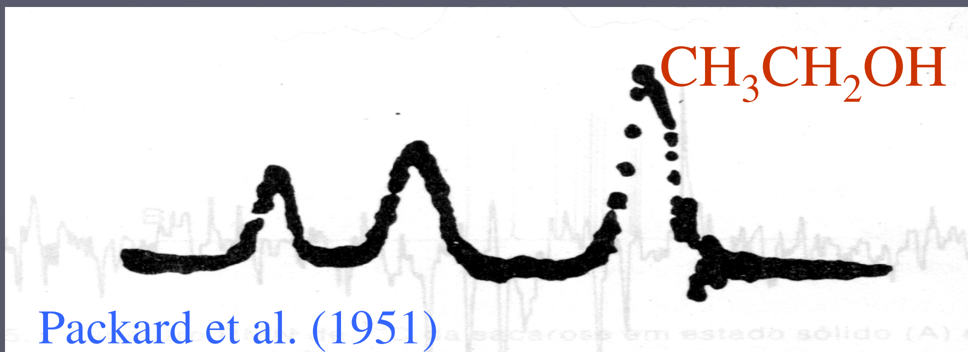
Espectro

Método da transformada de Fourier

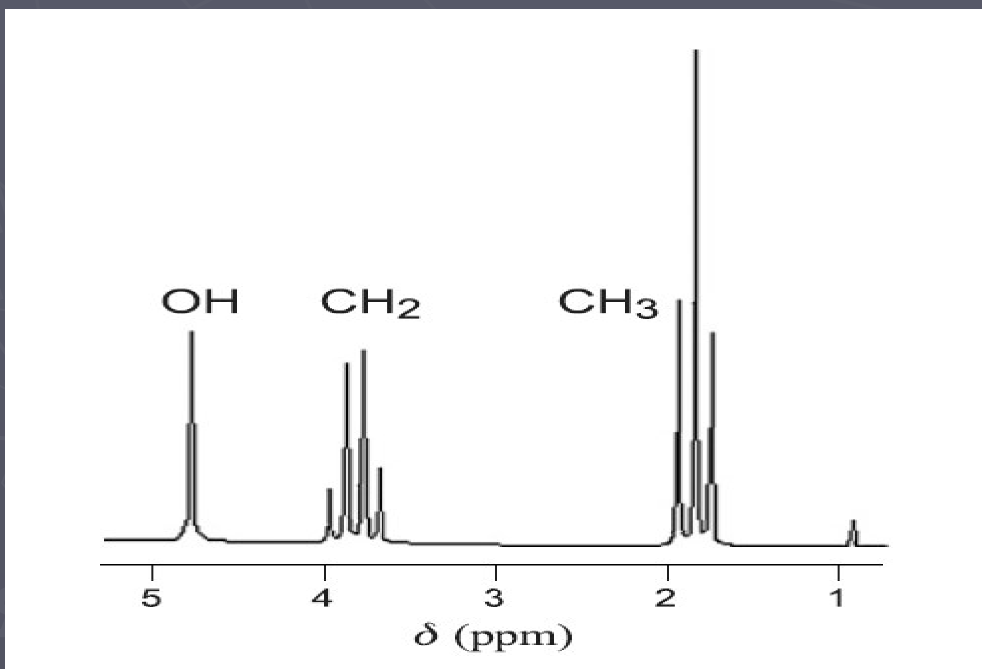




Espectros de RMN de ^{1}H - etanol



Packard et al. (1951)



Deslocamento químico:

$$\vec{B}_{loc} = (1-\tilde{\sigma})\vec{B}_0$$

$$f_{obs} = \frac{\gamma B_{loc}}{2\pi} = f_L(1-\sigma_{iso})$$

$$\delta = \frac{f_{obs} - f_{ref}}{f_{ref}}$$

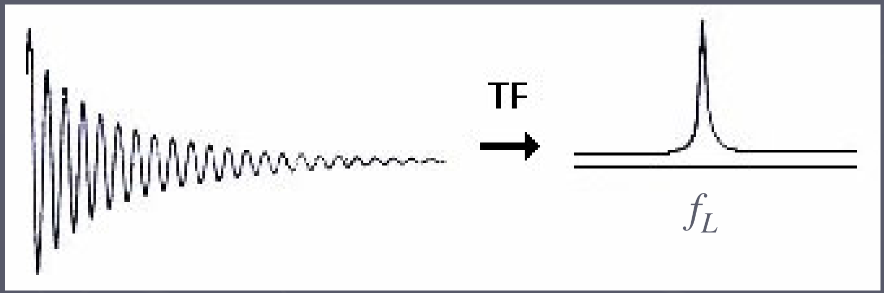
Valores típicos (^{1}H):

f_{ref} ~ 400MHz (TMS)

$f_{obs} - \nu_{ref}$ ~ 400-4000 Hz

$\delta \sim 10^{-6}$: partes por milhão (ppm)

Interações de spin nuclear



$$f_L = \gamma B_0 / 2\pi$$

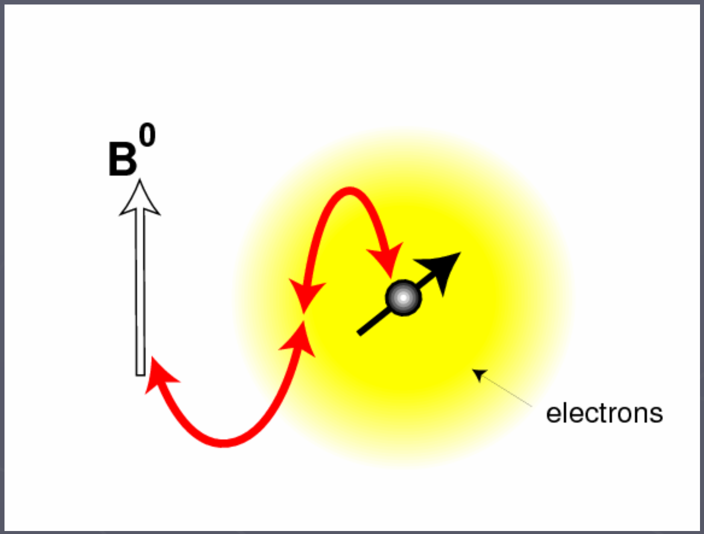
- Núcleo atômico isolado: medida de f_L fornece B_0 ou γ.
- Núcleo atômico na matéria: espectros de RMN (contendo vários valores ou distribuições de f_L) fornecem informações sobre a estrutura da matéria.

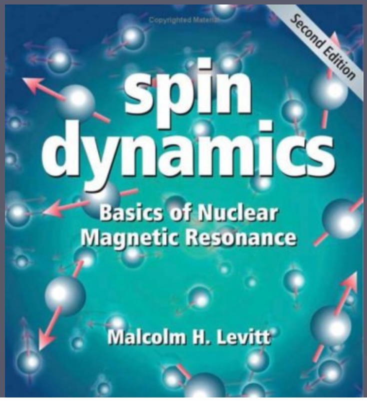
Interações de spin nuclear

Materiais isolantes e diamagnéticos:

- Deslocamento químico: Termo isotrópico + parte anisotrópica
- Interação dipolar direta: Homonuclear ou heteronuclear.
- Acoplamento escalar *(J)*: Termo isotrópico.
- Interação quadrupolar: $I > 1/2$.

Deslocamento químico ("chemical shift")





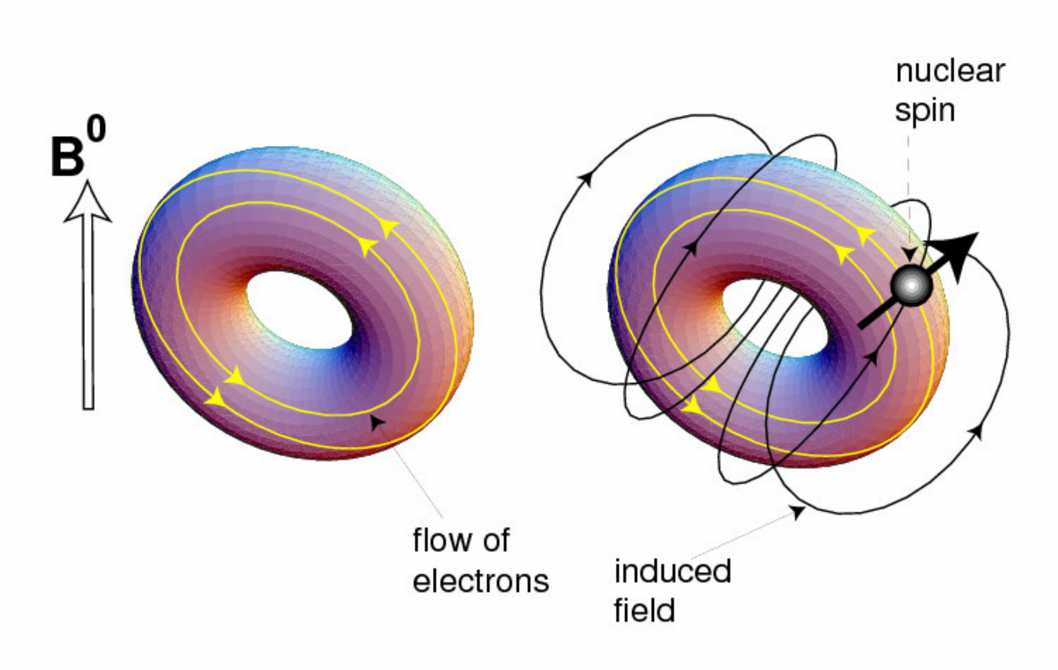
Em líquidos:

$$\omega = \gamma B_{loc} = \gamma(1-\sigma_{iso})B_0$$

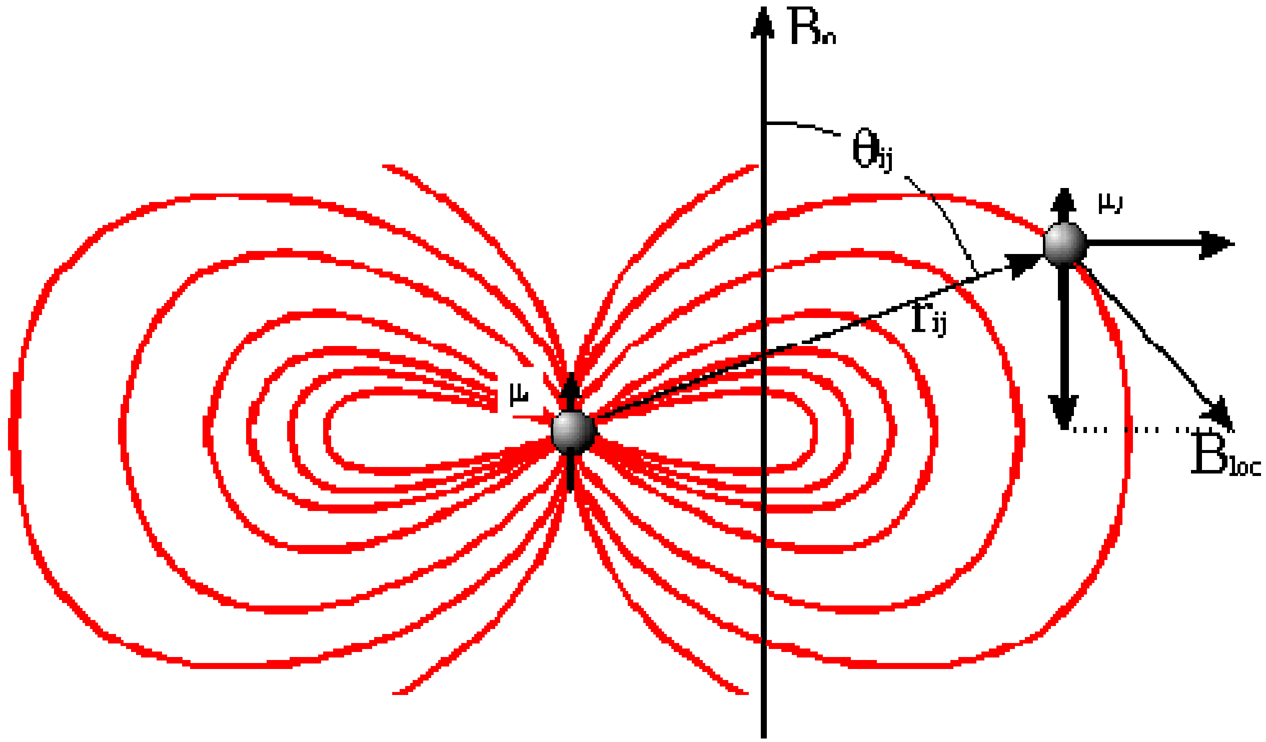
$$\delta = (f_{obs} - f_{ref}) / f_{ref}$$

ppm

TMS



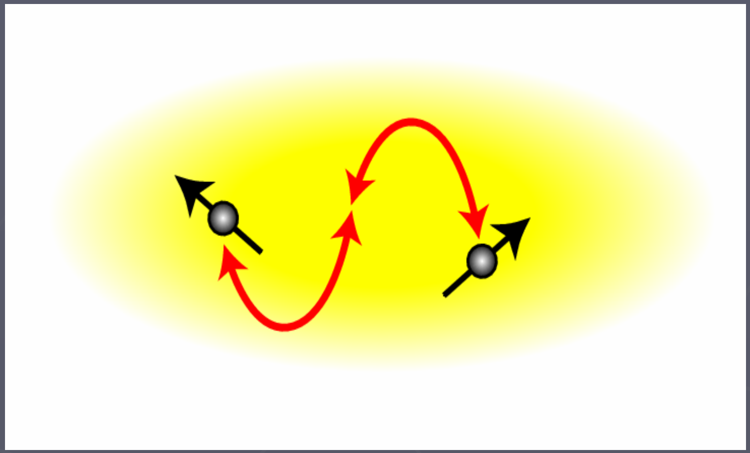
Interação dipolar internuclear

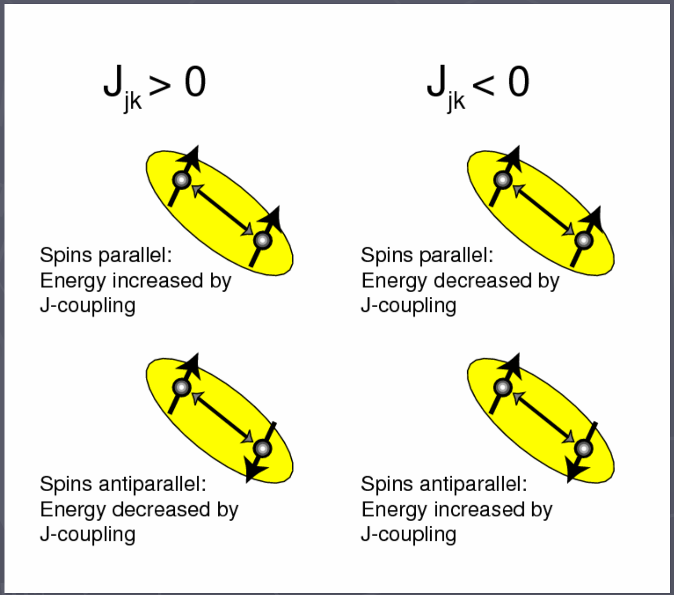


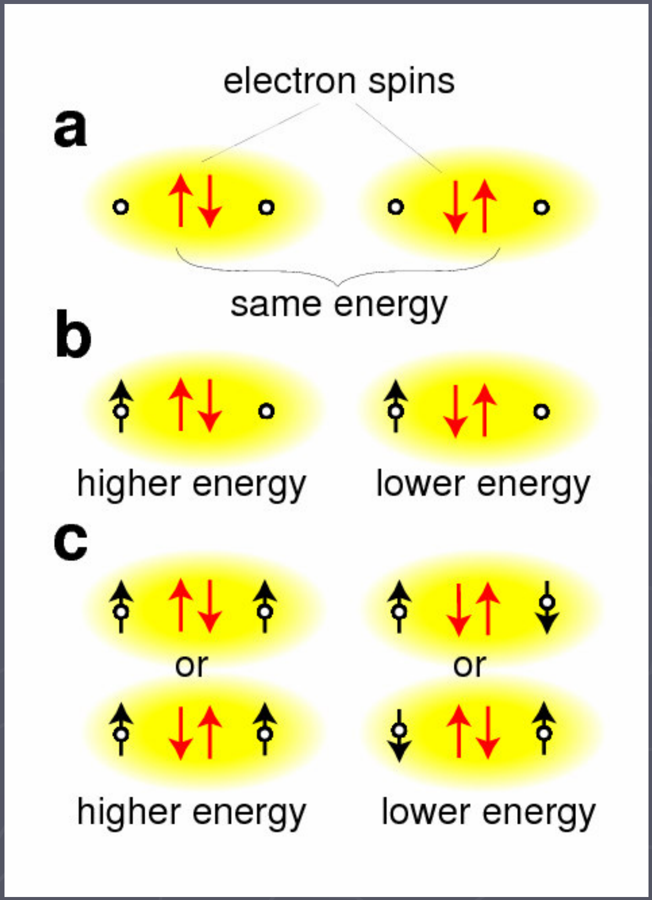
$$B_z^{(loc)} = \frac{\mu}{r_{ij}^3}(3\cos^2\theta - 1)$$

Interação através do espaço

Acoplamento escalar ou indireto (*J*)

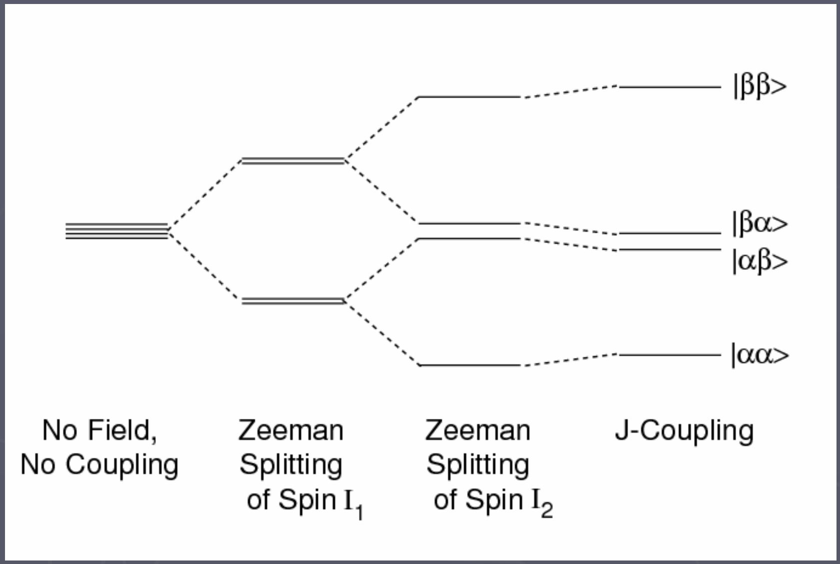


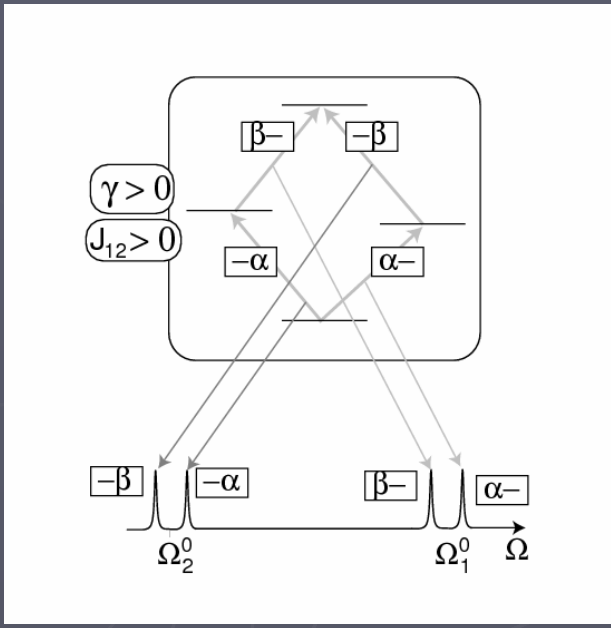




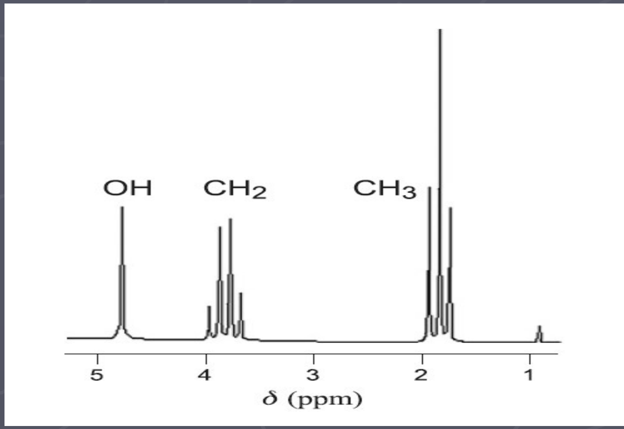
Interação através de ligações químicas

Acoplamento escalar ou indireto (*J*)





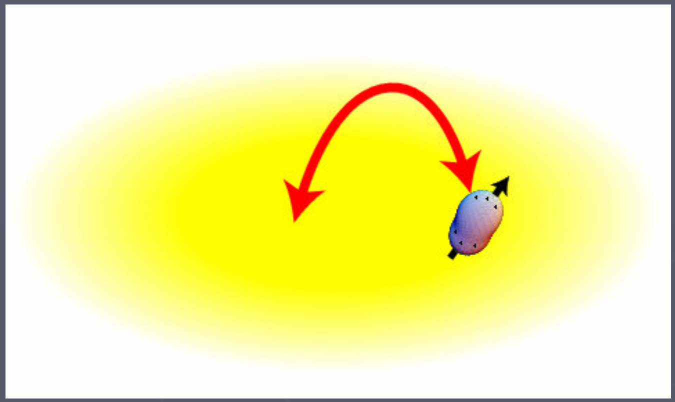
$$H \cong \omega_1 I_{1z} + \omega_2 I_{2z} + 2\pi J I_{1z} I_{2z}$$

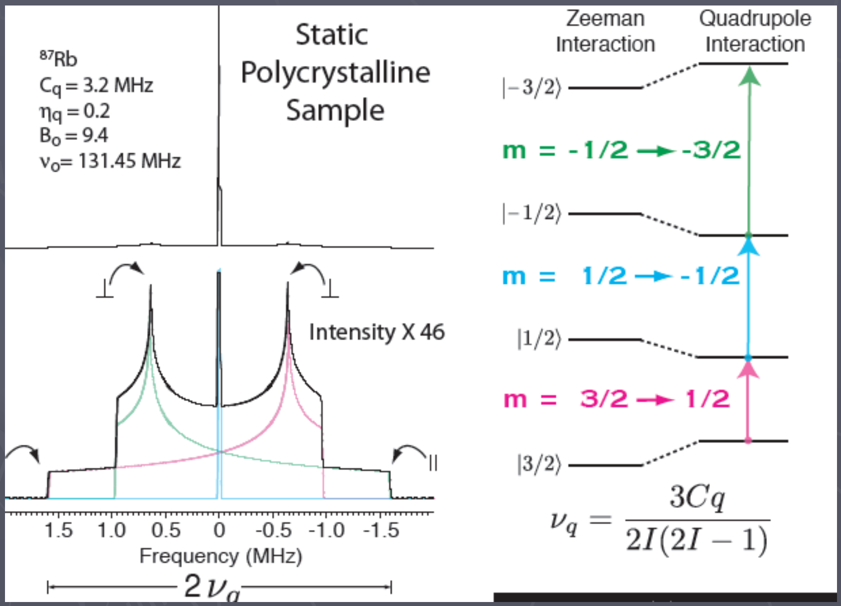


- Termo isotrópico.
- Importante principalmente em líquidos.

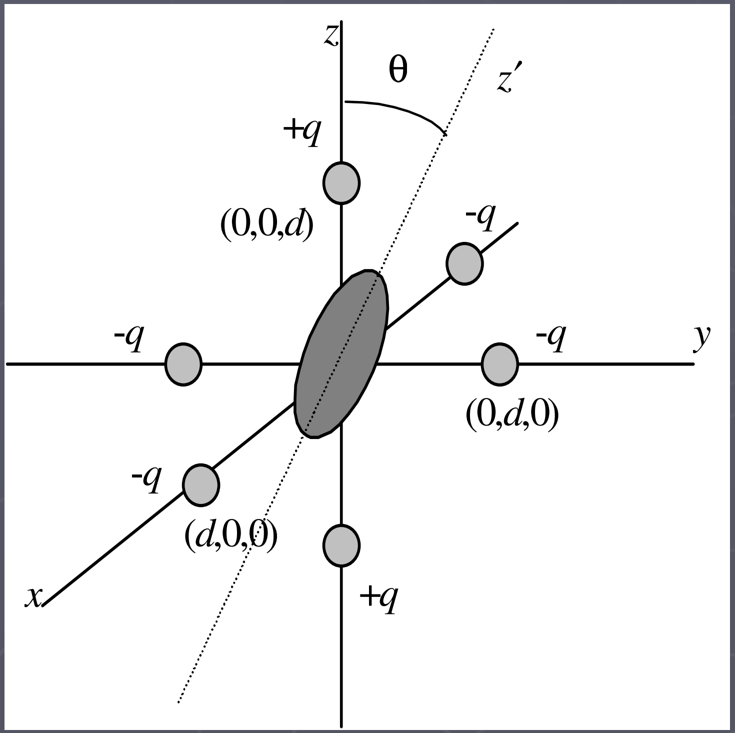
Interação quadrupolar elétrica

Núcleos quadrupolares (I > ½):
^{2}H, ^{23}Na, ^{25}Mg, ^{27}Al, ^{35}Cl, ^{55}Mn, ...



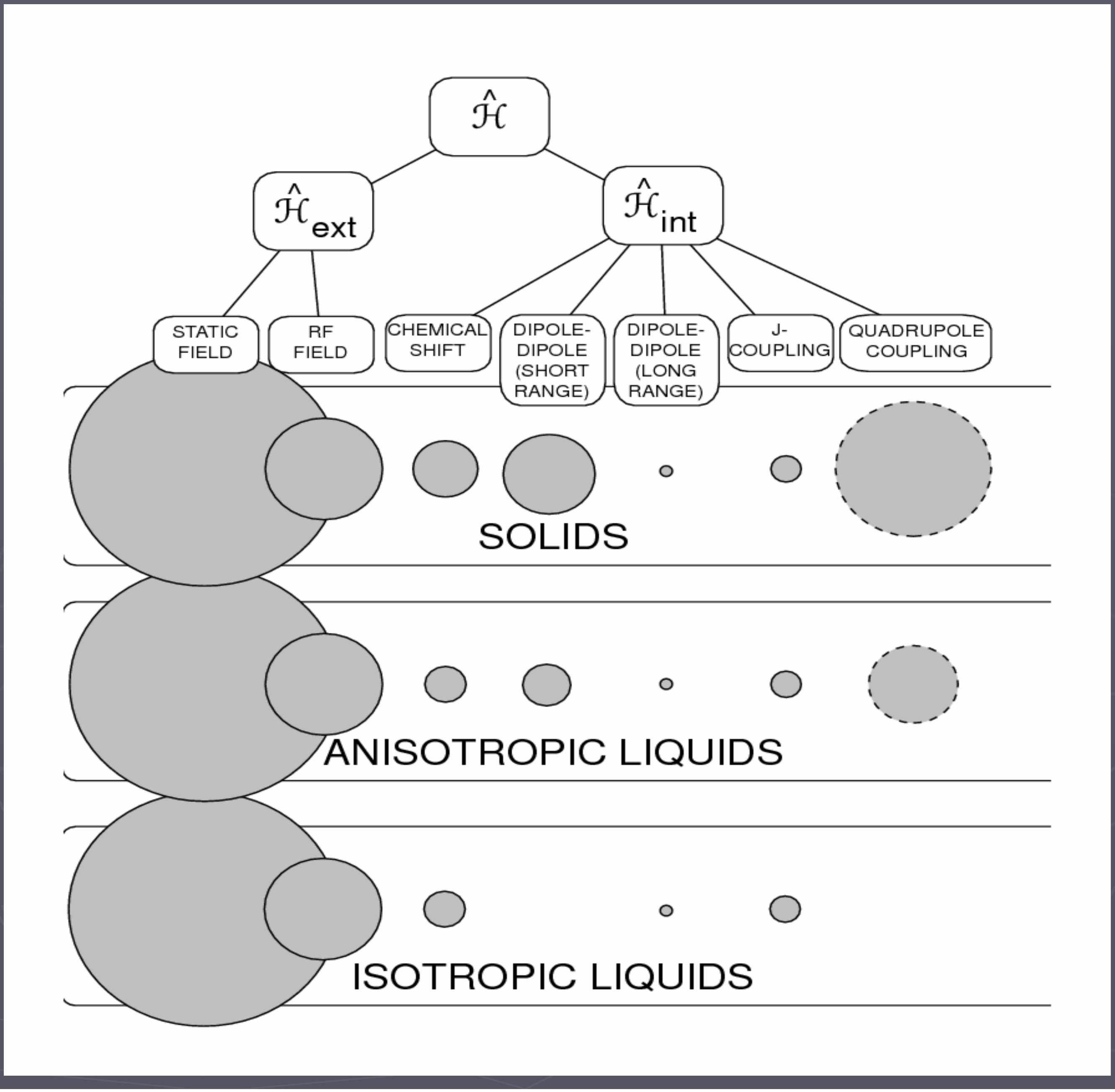


$$\nu_q = \frac{3Cq}{2I(2I-1)}$$

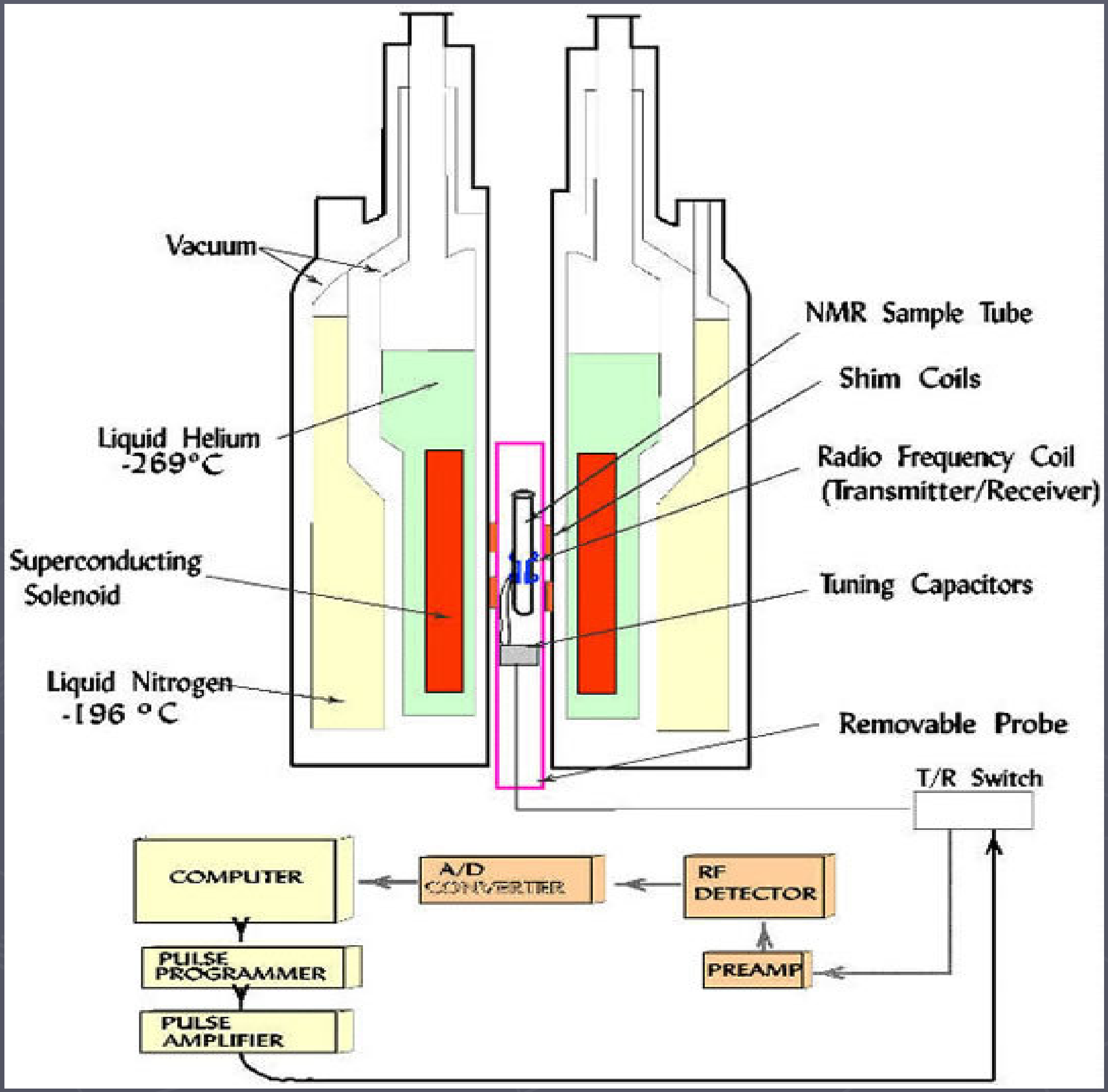


$$E_Q = (eqQ/d^3)(3\cos^2\theta - 1)$$

Interações de spin nuclear: resumo

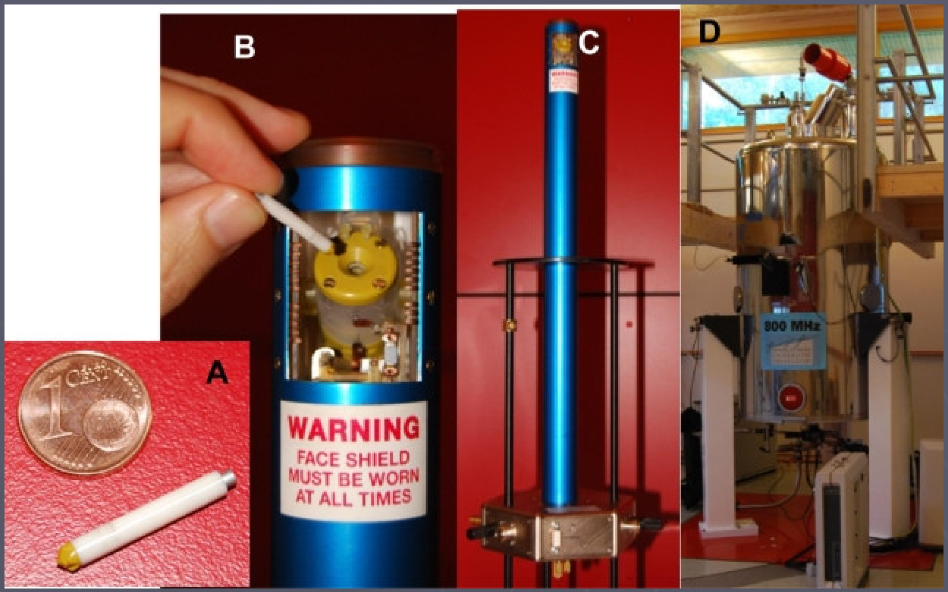


Espectrômetro de RMN

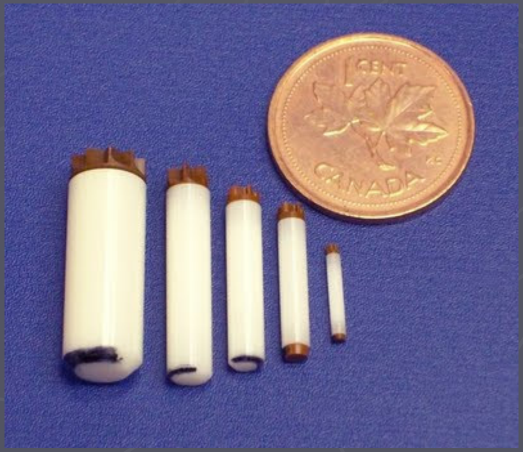


Espectrômetro de RMN

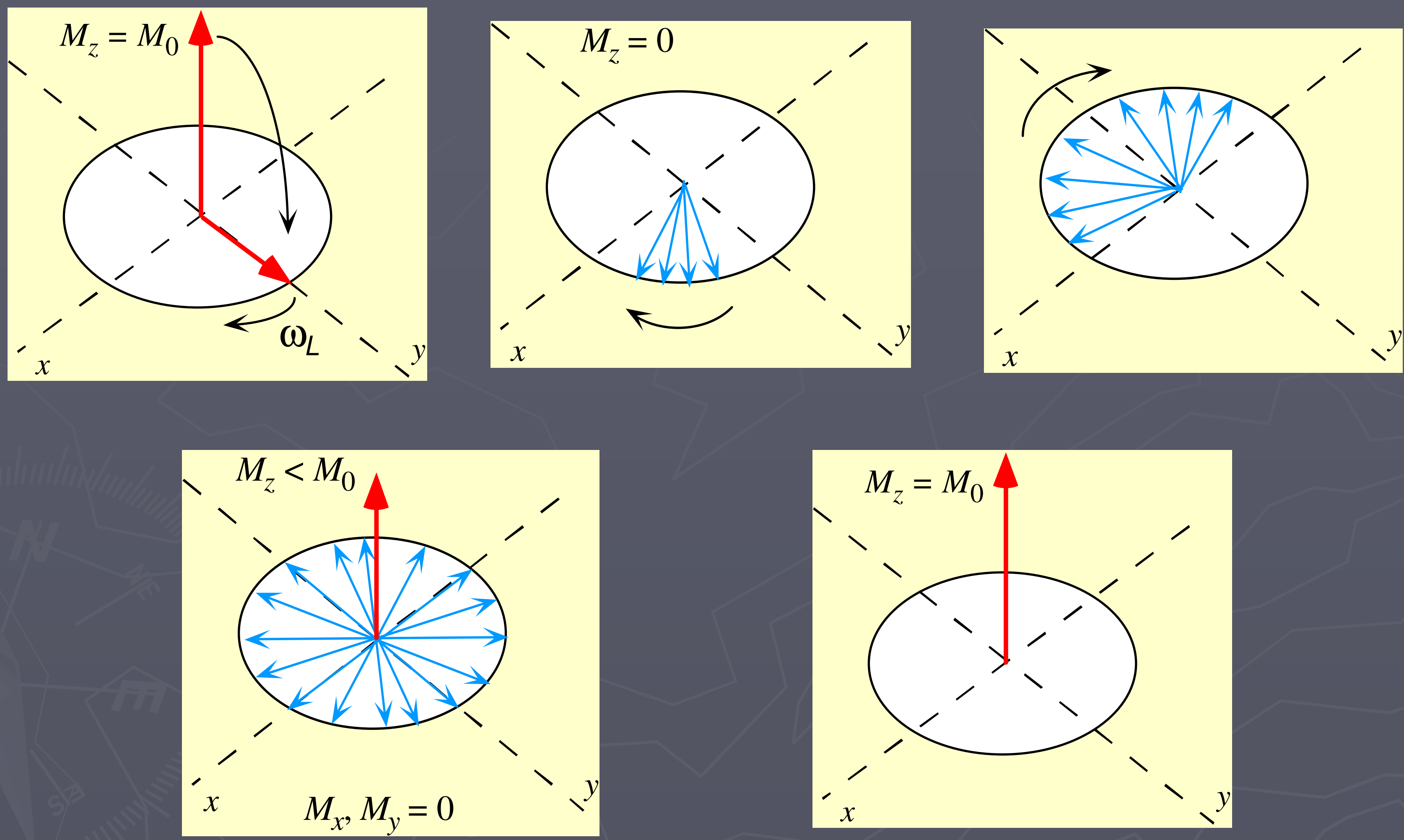
RMN no estado sólido: probes e rotores



- Rotores menores:
  - ✓ Frequências de MAS maiores.
    - 7mm: $f_{MAS} < 8$ kHz.
    - 2,5mm: $f_{MAS} < 35$ kHz.
  - ✓ Menor sensibilidade.



Relaxação do sistema de spins



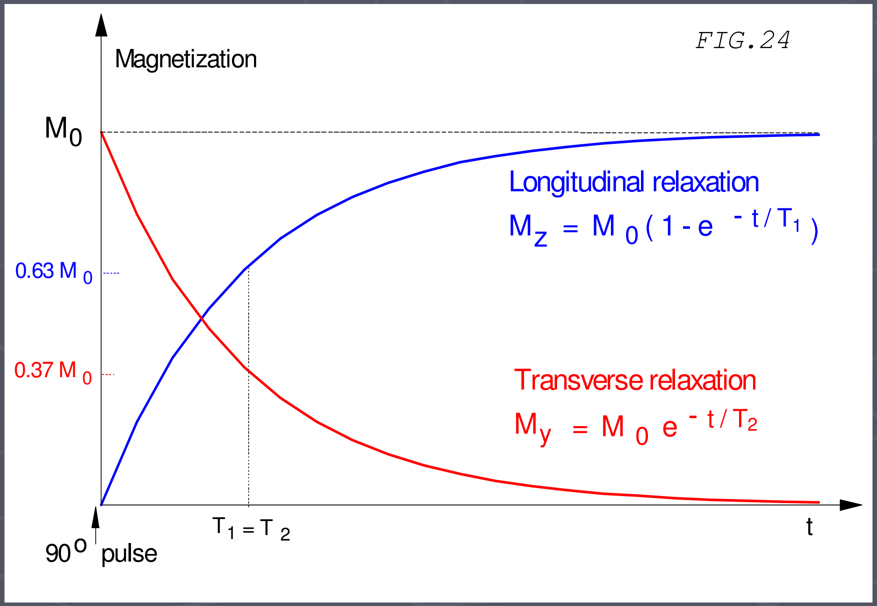
Relaxação do sistema de spins

- Relaxação longitudinal (T_1):
  - Trocas de energia entre spins e “rede”.
  - Existência de campos flutuantes com freqüências ~ ω_L.
  - Restauração do equilíbrio térmico.
- Relaxação transversal (T_2):
  - Perda de coerência entre os spins no plano transversal.
  - Distribuições de freqüências de precessão.
  - Interações entre os spins.

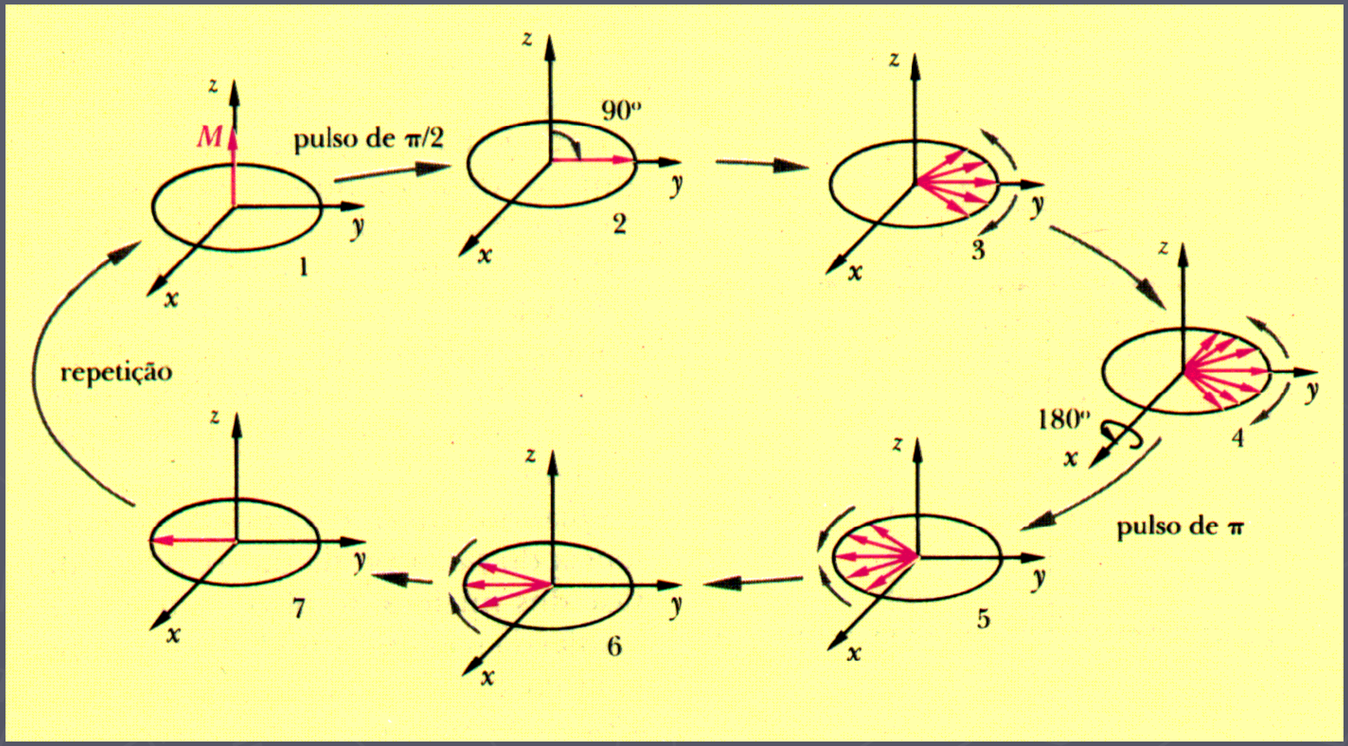
Líquidos: $T_1 \approx T_2$

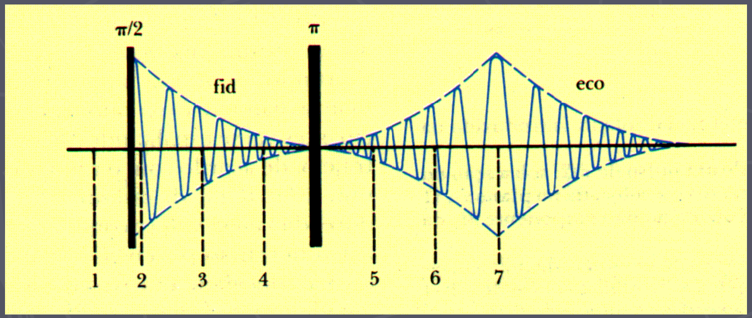
Sólidos: $T_1 >> T_2$

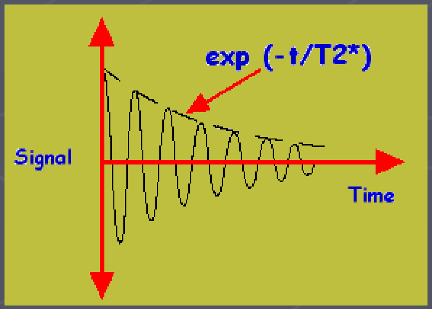
$T_1 \geq T_2$



Técnica dos ecos de spin ("spin-echoes")

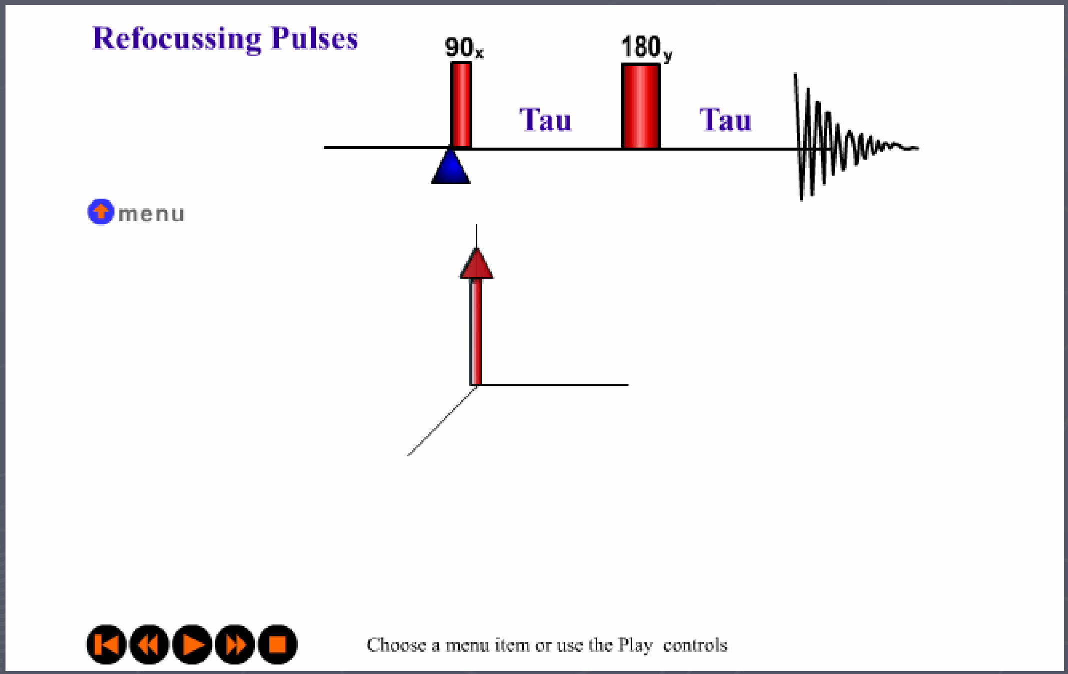






Hahn (1950)

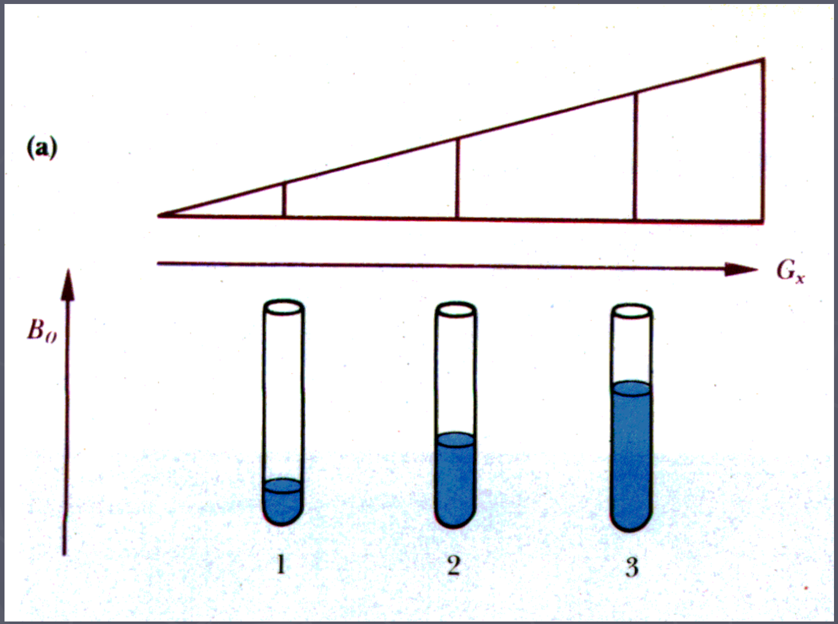
Formação dos ecos de spin

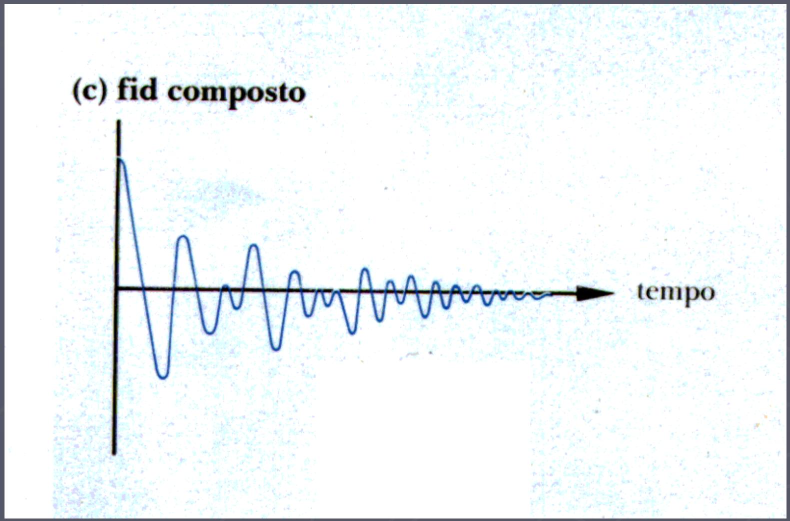


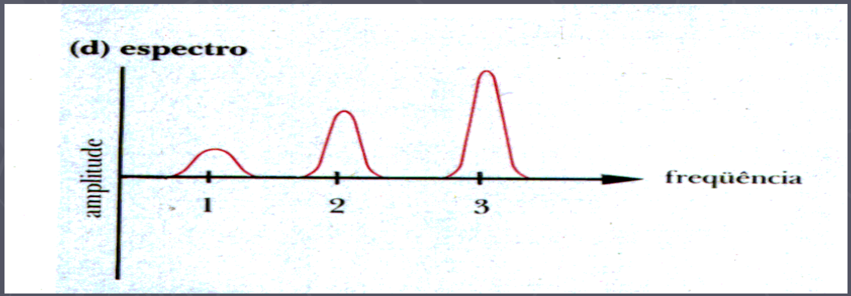
http://www.chem.queensu.ca/FACILITIES/NMR/nmr/webcourse/list.htm

Formação de imagens por RMN (MRI)

➢ Utilização de gradientes de campo magnético:

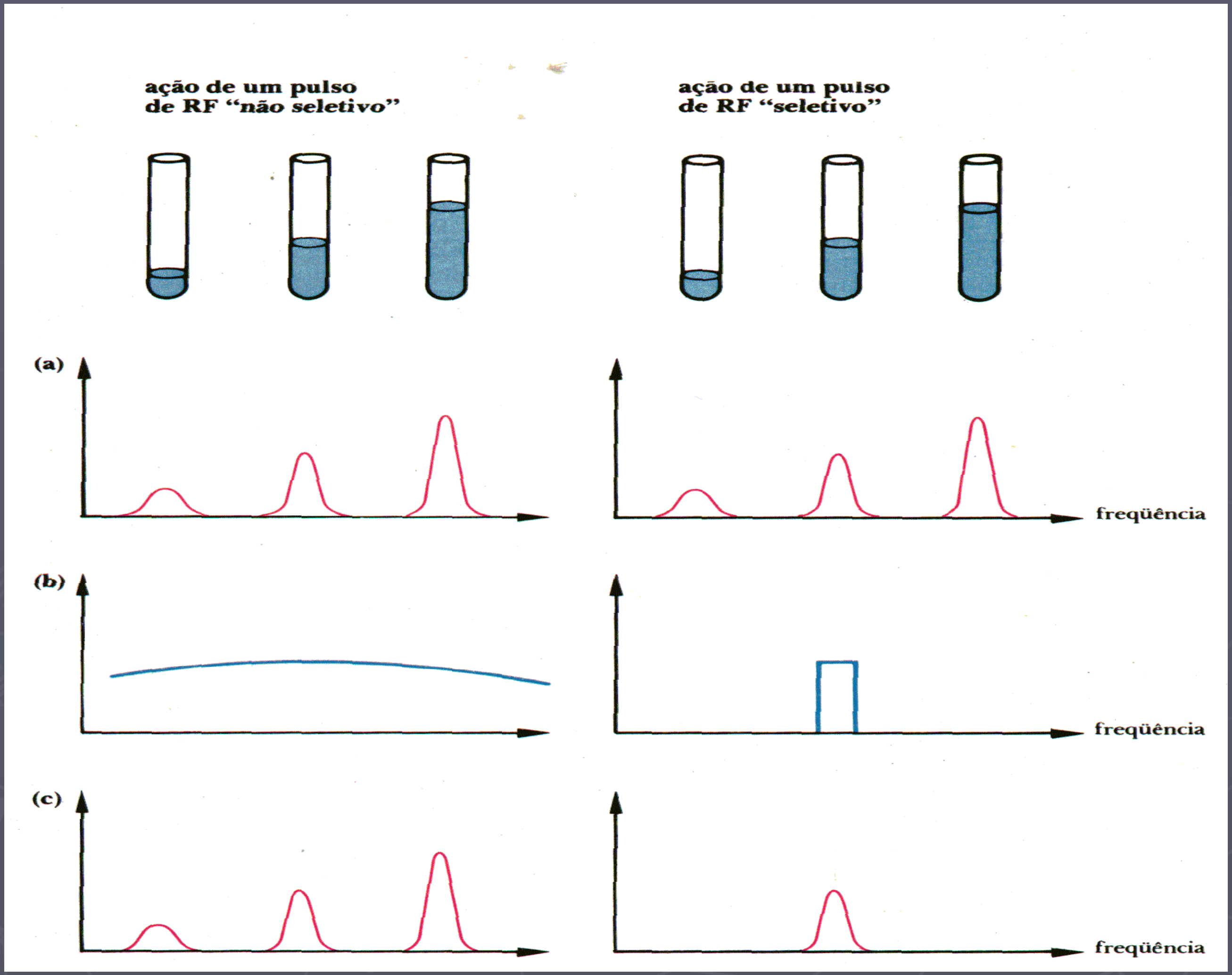




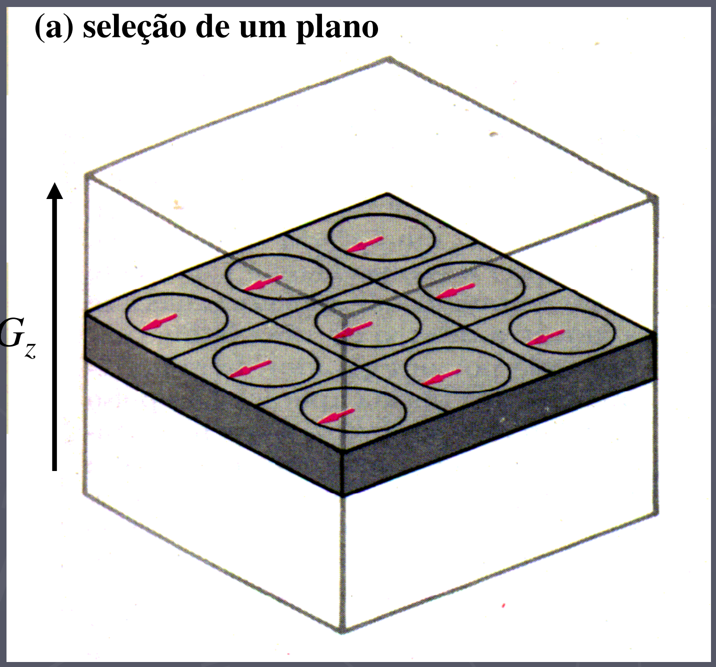


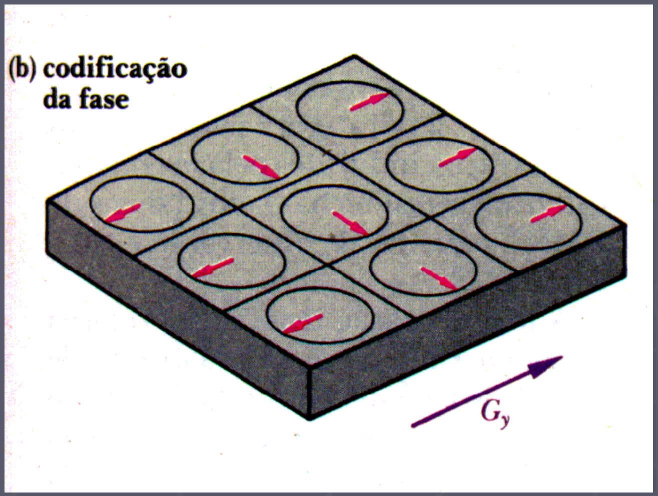
- Discriminação espacial de freqüências.
- Distribuição de densidade de prótons.

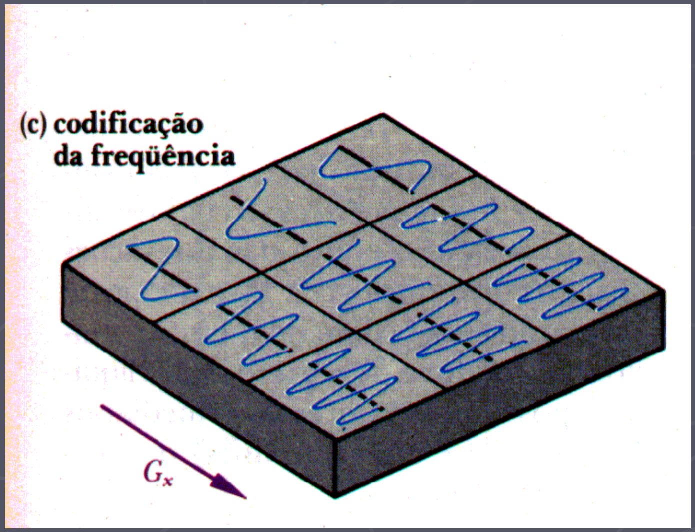
Excitação seletiva



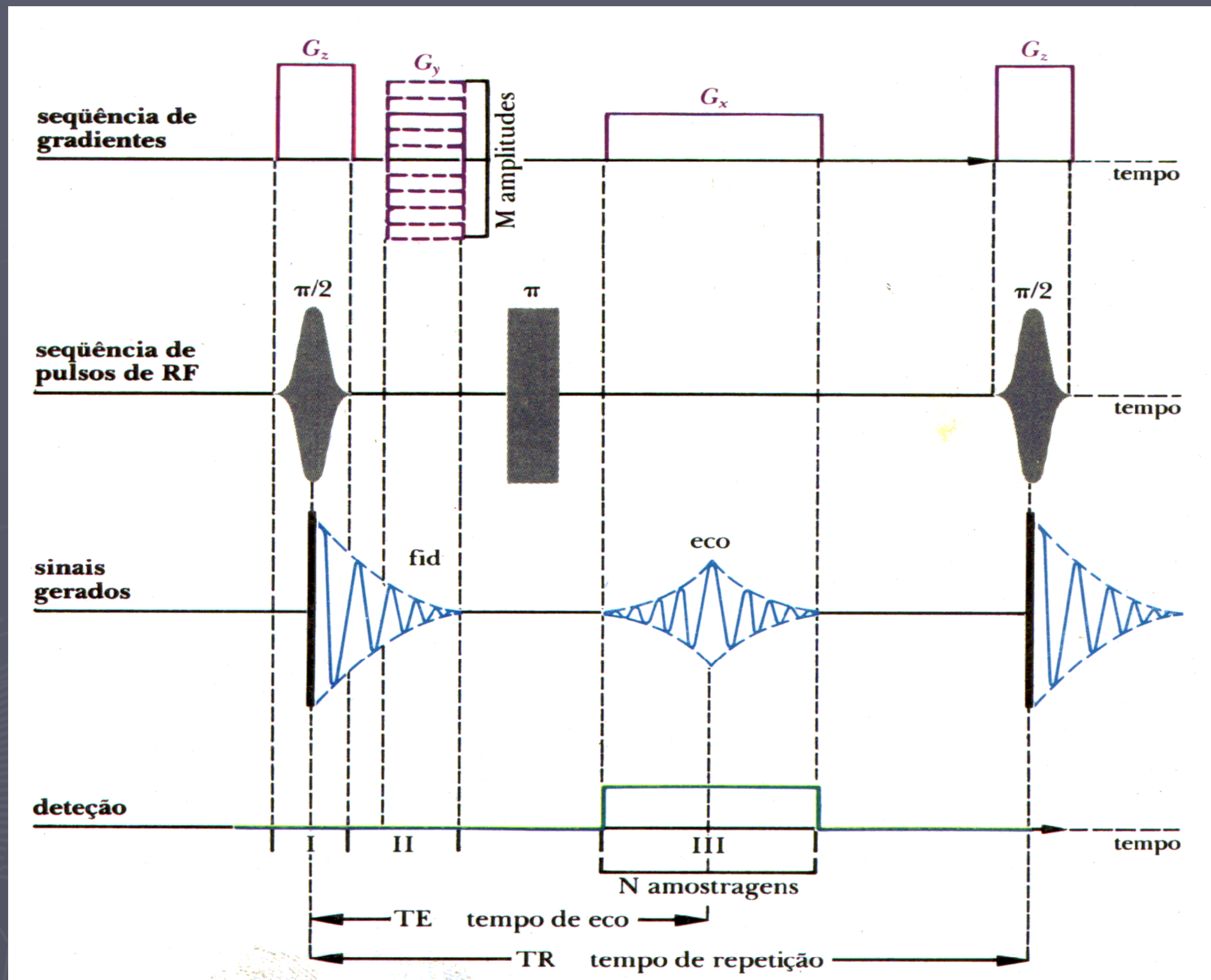
Seleção de planos - tomografia







Seqüência de pulsos – TF 2D

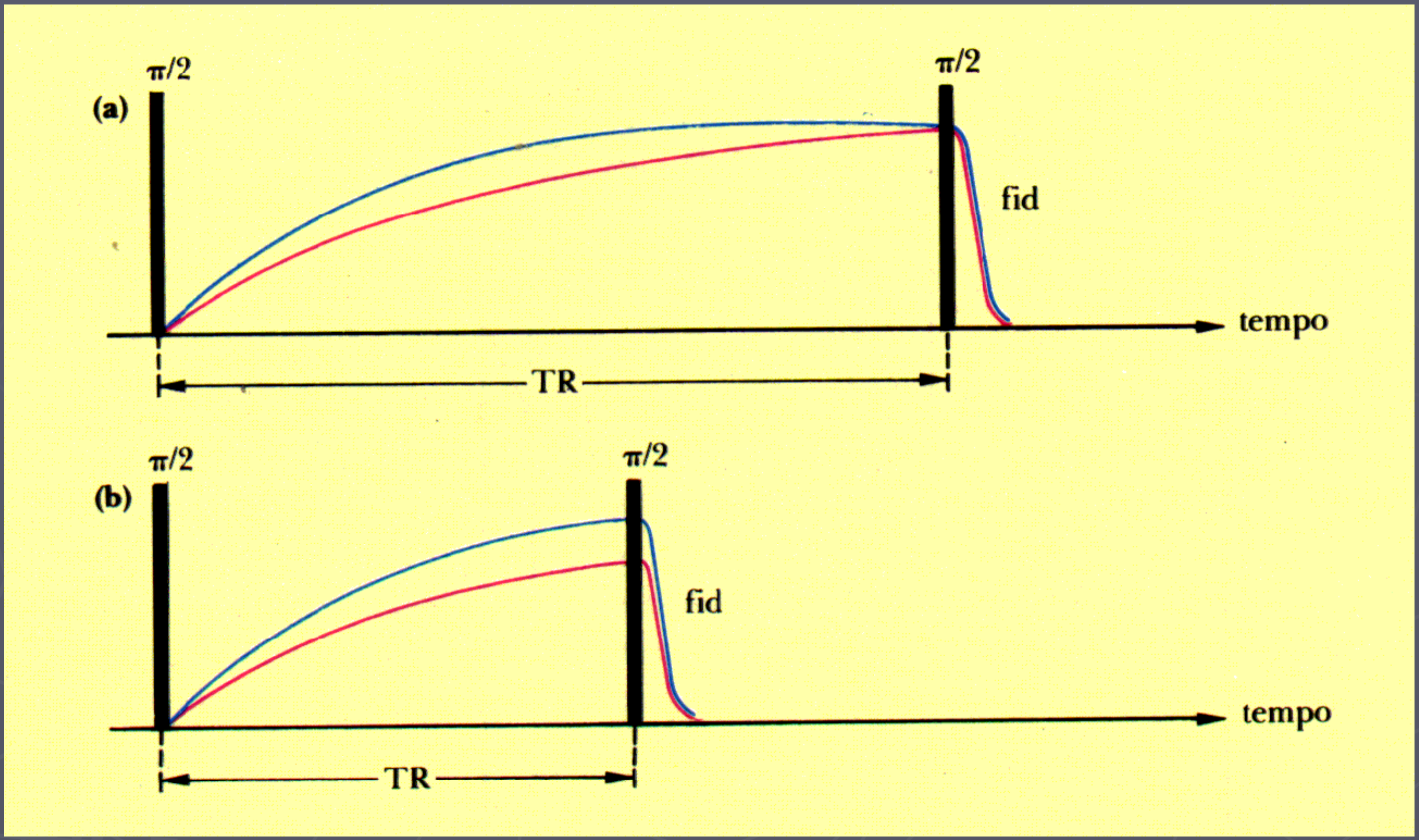


Técnicas de contraste

- Contraste pela densidade de prótons.
- Contraste por T_1 (relaxação longitudinal).
- Contraste por T_2 (relaxação transversal).

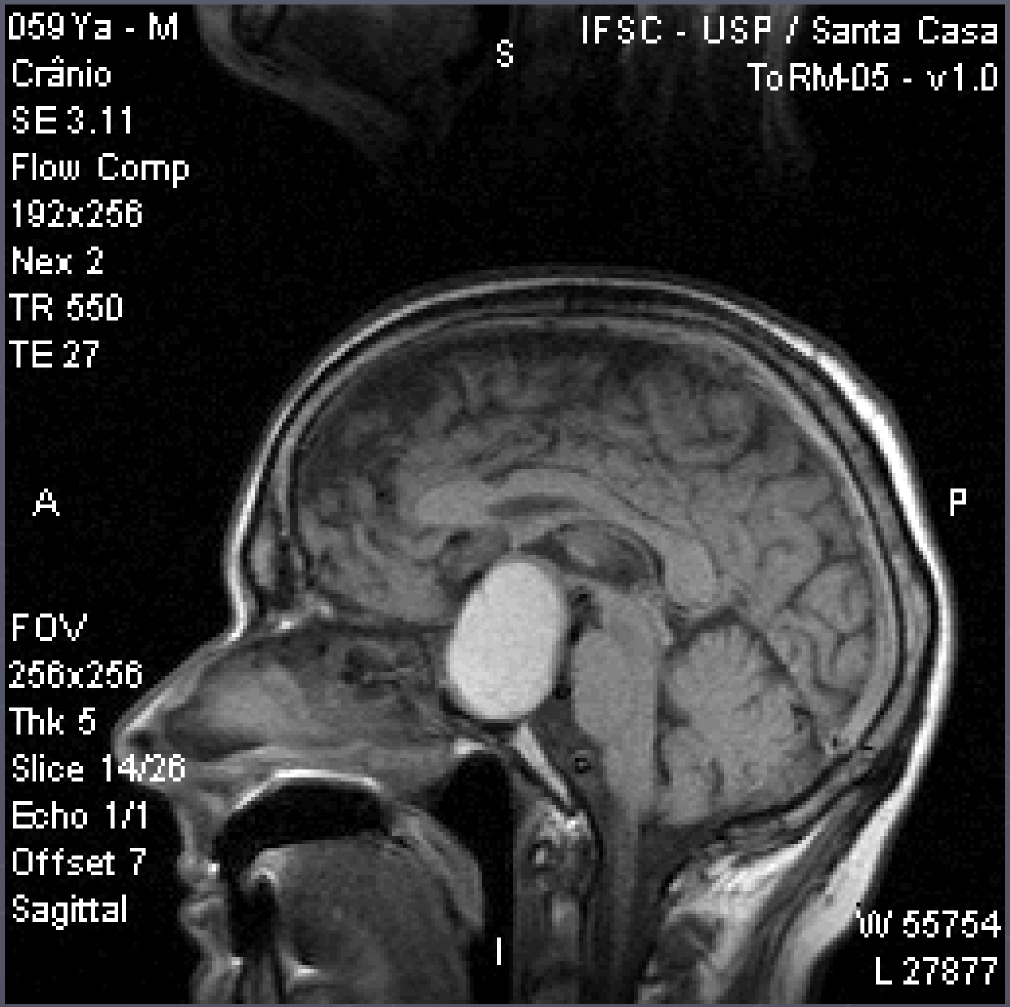
	T_1 (s) Tumoral	T_1 (s) Normal
Tórax	1,08	0,37
Pele	1,05	0,62
Fígado	0,83	0,57
Pulmão	1,11	0,79
Próstata	1,11	0,80
Ossos	1,03	0,55

Contraste por T_1



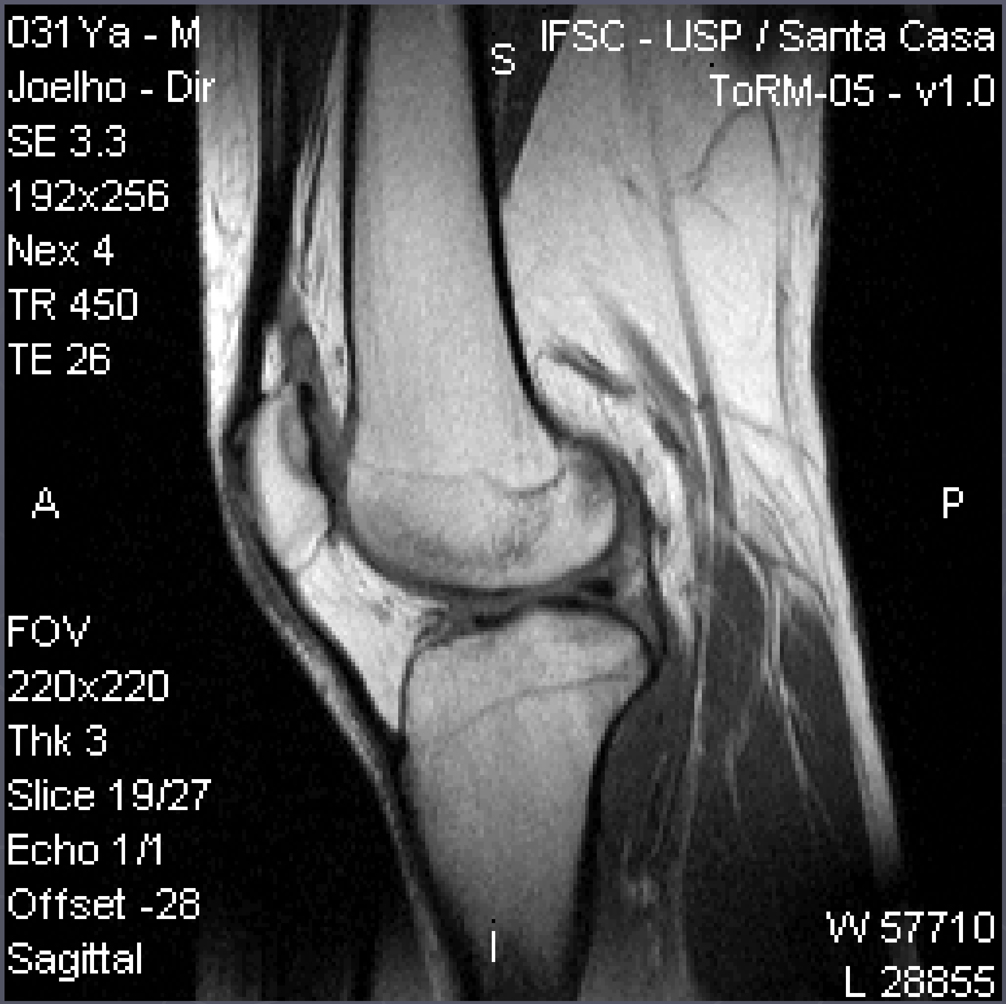
Métodos: saturação/recuperação; inversão/recuperação; spin-eco

Exemplo de contraste por T_1



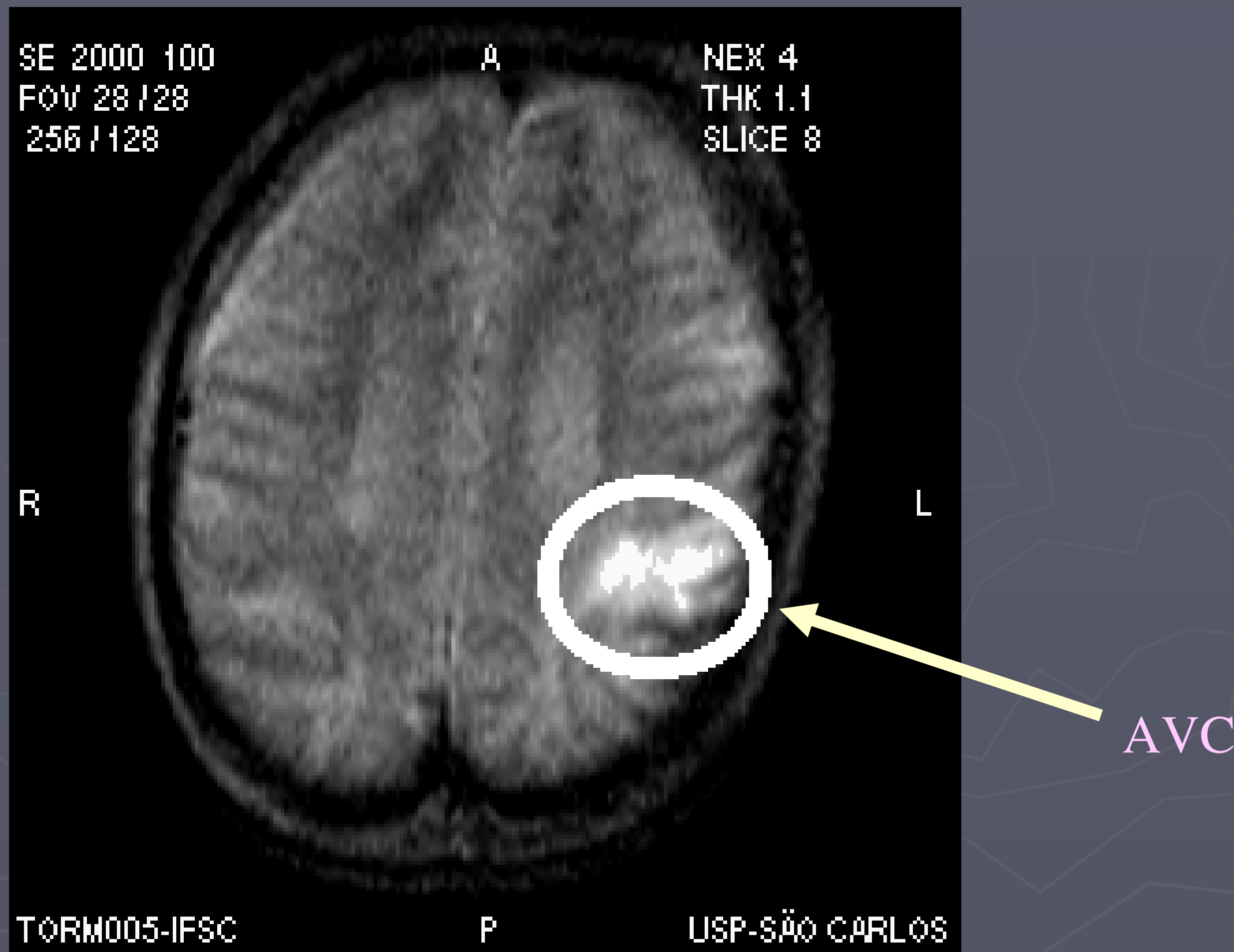
http://mri.if.sc.usp.br

Exemplo de contraste por T_1



http://mri.if.sc.usp.br

Exemplo de contraste por T_2



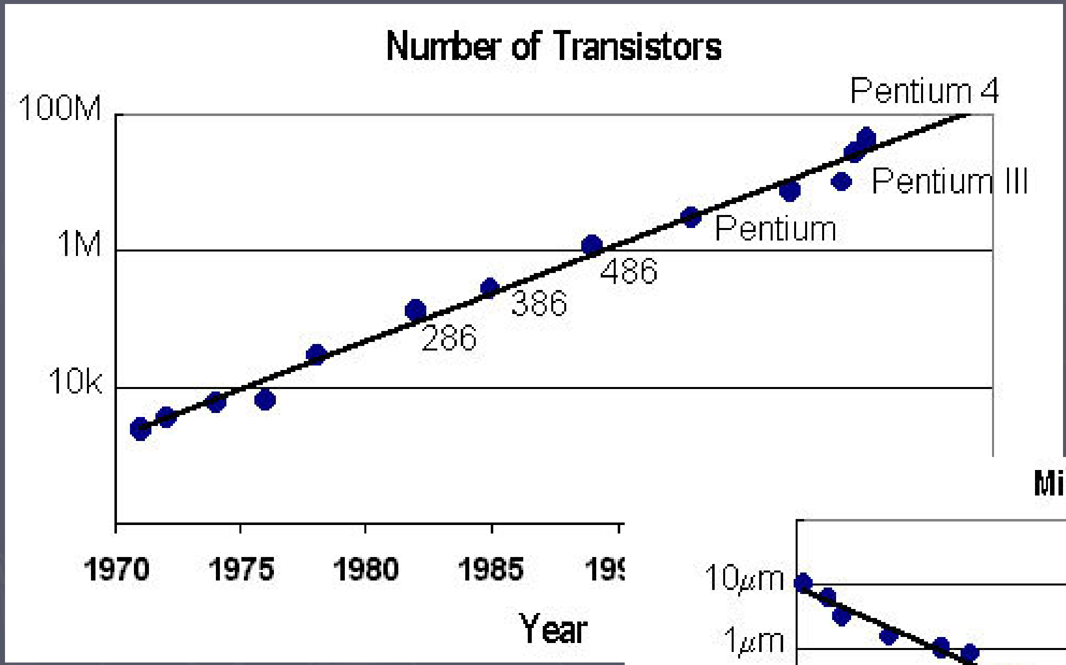
(corte transversal)

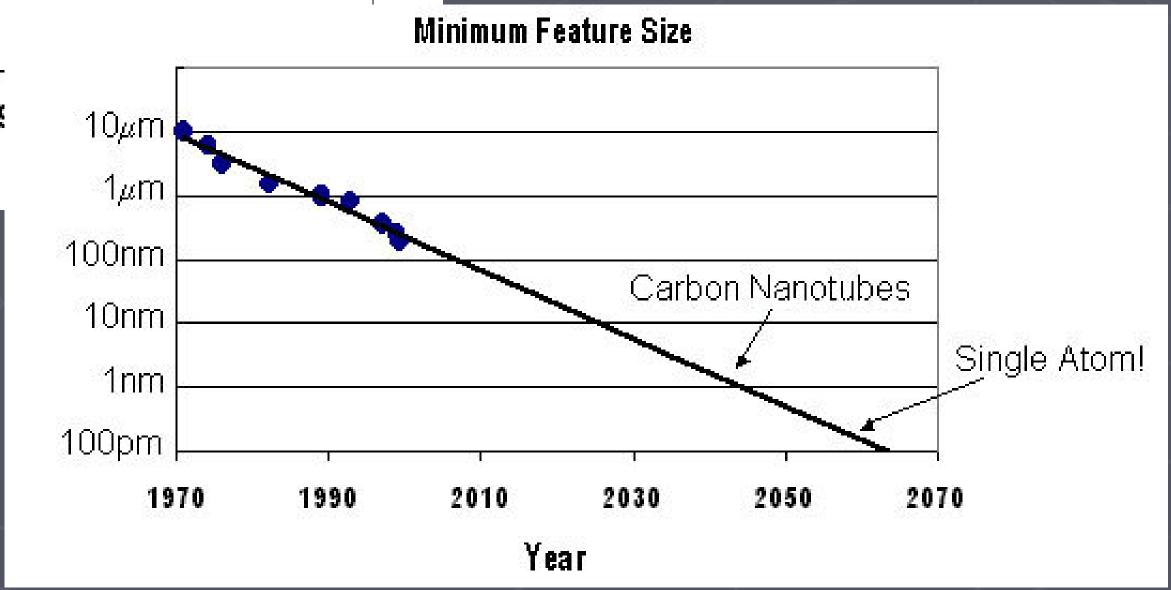
http://mri.if.sc.usp.br

Princípios de Informação Quântica

- Feynman (1980):
  - Dificuldade de simular sistemas quânticos em computadores clássicos.
  - Grupo com N spins 1/2 $\Rightarrow$ $O(2^N)$.
  - Sistemas quânticos “controlados” podem ser usados nas simulações de outros sistemas quânticos.
  - Computadores quânticos “analógicos”.

Lei de Moore: limites da computação clássica





http://barrett-group.mcgill.ca/teaching/nanotechnology/nano03.htm

Algoritmos quânticos

- Algoritmo de Deutsch (1986):
  - Avaliação de funções binárias em apenas uma iteração.
- Algoritmo de Shor (1994):
  - Fatoração de números grandes (milhares de dígitos) em tempo polinomial.
  - N dígitos $\Rightarrow$ $O(N^2)$ quântico $\times$ $O(10^{N/2})$ clássico.
  - Implicação em criptografia de sistemas de segurança.
- Algoritmo de Grover (1997):
  - Busca de itens em uma lista desordenada.
  - N itens $\Rightarrow$ $O(N^{1/2})$ quântico $\times$ $O(N/2)$ clássico.

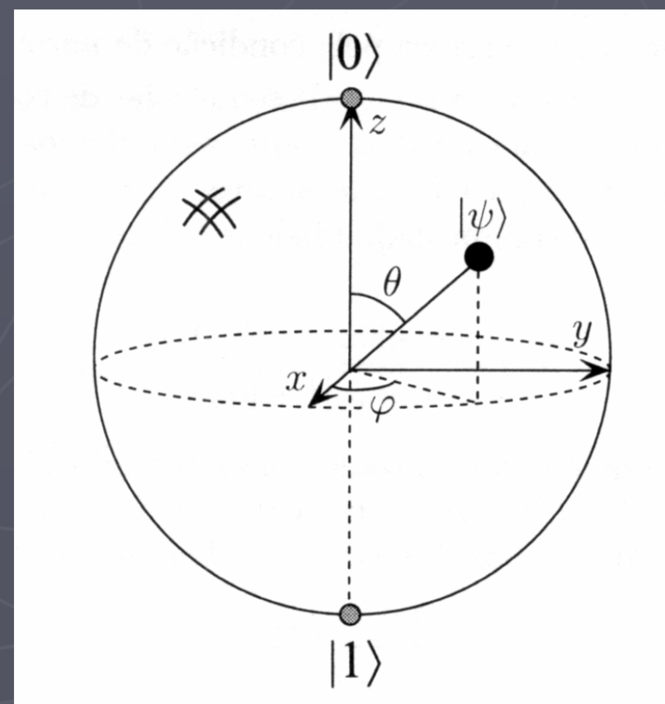
Base computacional

Bits “clássicos” $\begin{cases} 0 \\ 1 \end{cases}$

Bits “quânticos” (q-bits)

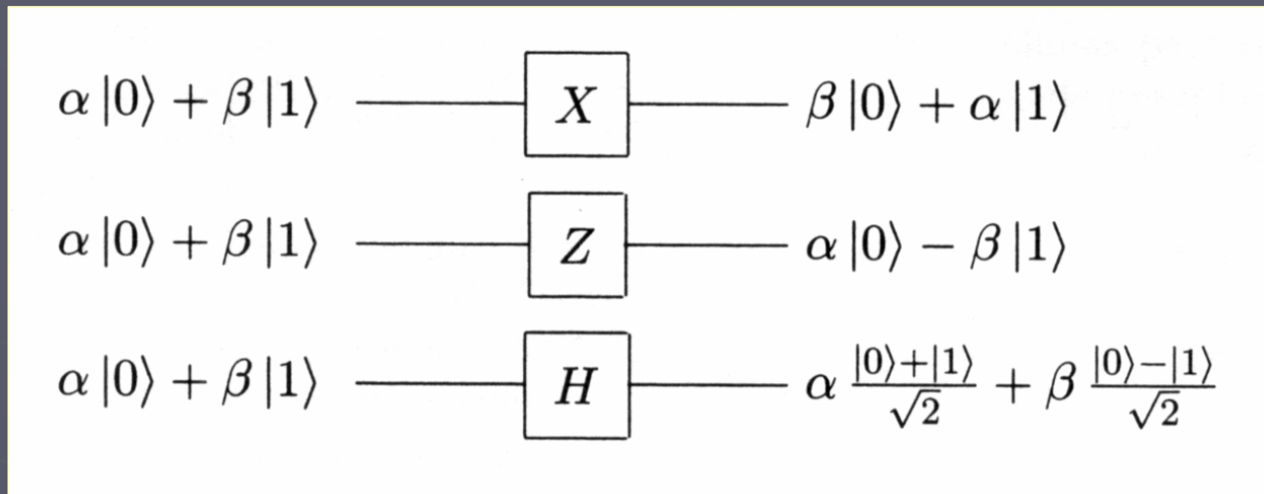
$|0\rangle$ $|1\rangle$ Estados da base

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$ Superposição coerente

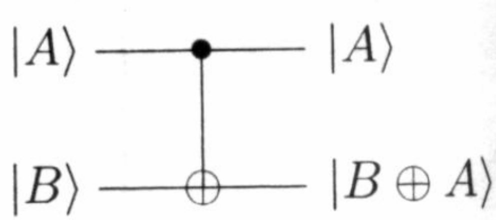


- ✓ Informação “oculta”.
- ✓ Evolução de estados coerentes.
- ✓ Paralelismo quântico.
- ✓ Possibilidade de emaranhamento (“entanglement”).
- ✓ Colapso do estado ao se efetuar uma medida.

Algumas portas lógicas



Não-controlado



$$U_{CN} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$|00\rangle \to |00\rangle$$
$$|01\rangle \to |01\rangle$$
$$|10\rangle \to |11\rangle$$
$$|11\rangle \to |10\rangle$$

Estados emaranhados (estados de Bell)

Tabela 1.1. "Tabela-verdade" quântica do circuito da Figura 1.12

Entrada	**Saída**
$\|00\rangle$	$(\|00\rangle + \|11\rangle)/\sqrt{2} \equiv \|\beta_{00}\rangle$
$\|01\rangle$	$(\|01\rangle + \|10\rangle)/\sqrt{2} \equiv \|\beta_{01}\rangle$
$\|10\rangle$	$(\|00\rangle - \|11\rangle)/\sqrt{2} \equiv \|\beta_{10}\rangle$
$\|11\rangle$	$(\|01\rangle - \|10\rangle)/\sqrt{2} \equiv \|\beta_{11}\rangle$

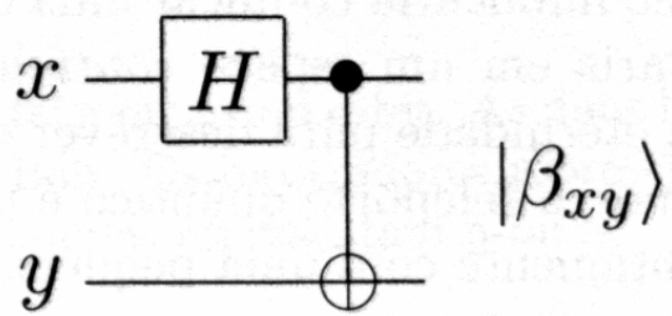


Figura 1.12. Circuito quântico para criar estados de Bell.

O emaranhamento e seus “mistérios”

Vol 454|14 August 2008 nature

NEWS & VIEWS

Swiss speed trap: two Swiss villages separated by 18 kilometres (and Lake Geneva), yet connected by quantum entanglement.

M-SAT LTD/SPL

QUANTUM MECHANICS

The speed of instantly

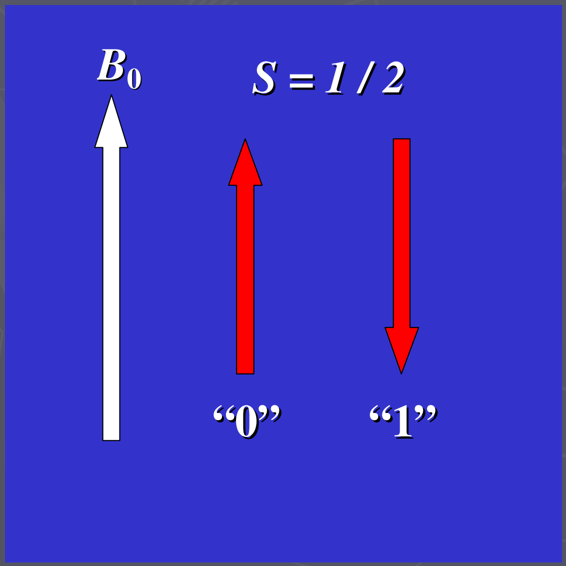
Terence G. Rudolph

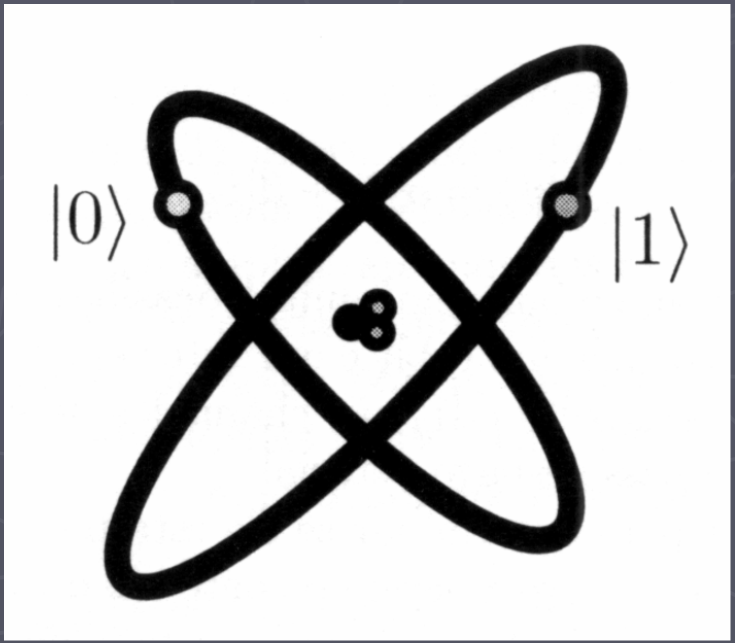
Pairs of quantum-mechanically entangled particles seem to know at once what is happening to each other. Experiments show that even if this signalling is not instantaneous, it must be really, really fast.

Implementações de q-bits

Sistema de dois níveis:

- ✓ Spin nuclear em um campo magnético.
- ✓ Spin eletrônico em um campo magnético.
- ✓ Polarizações de um fóton.
- ✓ Estados eletrônicos em um átomo.





Características de um computador quântico

- Superposição de estados.
- Operações reversíveis.
- Conservação do número de q-bits.
- Portas lógicas $\Rightarrow$ operadores unitários.

Requisitos de um “candidato” a computador quântico

- Sistema de dois níveis (no mínimo) para cada q-bit.
- Atuação sobre os q-bits individualmente.
- Criação de estados puros e de superposições.
- Operações lógicas condicionais.
- Isolamento de interações com o ambiente.

Comparação entre candidatos à implementação de q-bits

Sistema	***Tempo de descoerência*** (s)	***Tempo de operação*** (s)	**Número máximo de operações**
Spin nuclear	$10^{-2} - 10^{8}$	$10^{-3} - 10^{-6}$	$10^{5} - 10^{14}$
Spin eletrônico	10^{-3}	10^{-7}	10^{4}
Armadilha iônica (In^{+})	10^{-1}	10^{-14}	10^{13}
Elétron – Au	10^{-8}	10^{-14}	10^{6}
Elétron – GaAs	10^{-10}	10^{-13}	10^{3}
Ponto quântico	10^{-6}	10^{-9}	10^{3}
Cavidade ótica	10^{-5}	10^{-14}	10^{9}
Cavidade de microondas	10^{0}	10^{-4}	10^{4}

Implementação experimental: armadilha iônica

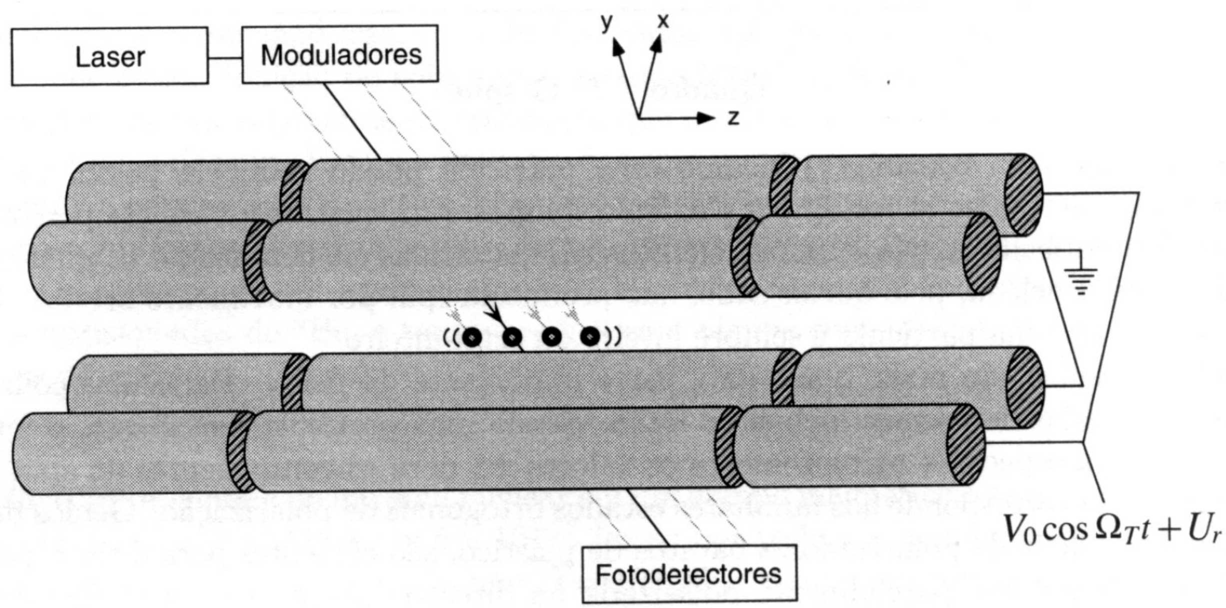


Figura 7.6. Esquema de um computador quântico de armadilha de ions (fora de escala) mostrando quatro ions aprisionados no centro por um potencial criado por quatro eletrodos cilíndricos. O dispositivo permanece em alto vácuo ($\approx 10^{-8}$ Pa), e os ions são inseridos a partir de um forno. Um feixe modulado de *laser* incide sobre os ions através de aberturas na câmara de vácuo e implementa operações, bem como realiza a leitura dos estados atômicos.

Computação quântica via RMN

- Gershenfeld & Chuang (1997):
  - RMN em amostras líquidas macroscópicas.
  - Moléculas contendo *N* núcleos ($I = 1/2$) acoplados.
  - O(10^{20}) "computadores" em paralelo com *N* q-bits.
  - Operações unitárias sobre o *ensemble*.
  - Preparação de estados pseudo-puros.
  - Resultado das operações: espectro com amplitudes e fases relacionadas aos estados de saída.

Descrição com matriz densidade

$$\rho_{\text{eq}} = \frac{e^{-H/kT}}{Z}$$

$$\rho_{\text{eq}} \cong \frac{1}{Z} - \underbrace{\frac{1}{Z}\frac{H}{kT}}_{\text{Desvio}}$$

$$U\rho_{\text{eq}}U^{\dagger} \cong \frac{1}{Z} - \frac{1}{Z}\frac{1}{kT}UHU^{\dagger}$$

Exemplo para $N = 2$:

Equilíbrio térmico

$$\rho_{\text{eq}} \cong \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \frac{10^{-4}}{4}\begin{pmatrix} -0,75 & 0 & 0 & 0 \\ 0 & -0,25 & 0 & 0 \\ 0 & 0 & 0,25 & 0 \\ 0 & 0 & 0 & 0,75 \end{pmatrix}$$

Estado pseudo-puro

$$\rho_{\text{eq}} \cong \left(\frac{1}{4} - 0,75\times 10^{-4}\right)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + 10^{-4}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Implementação de algoritmos via RMN

- Preparação do estado inicial.
- Realização de operações unitárias (portas lógicas).
- Leitura do resultado final (espectro de RMN).

Operadores unitários

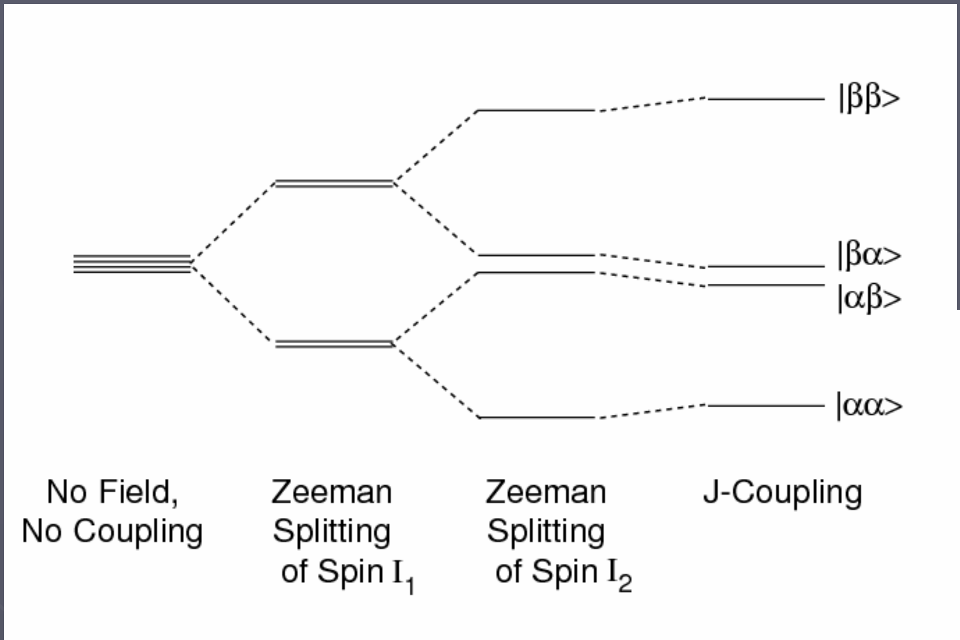
- Operadores de rotação (campos de RF seletivos ou não):

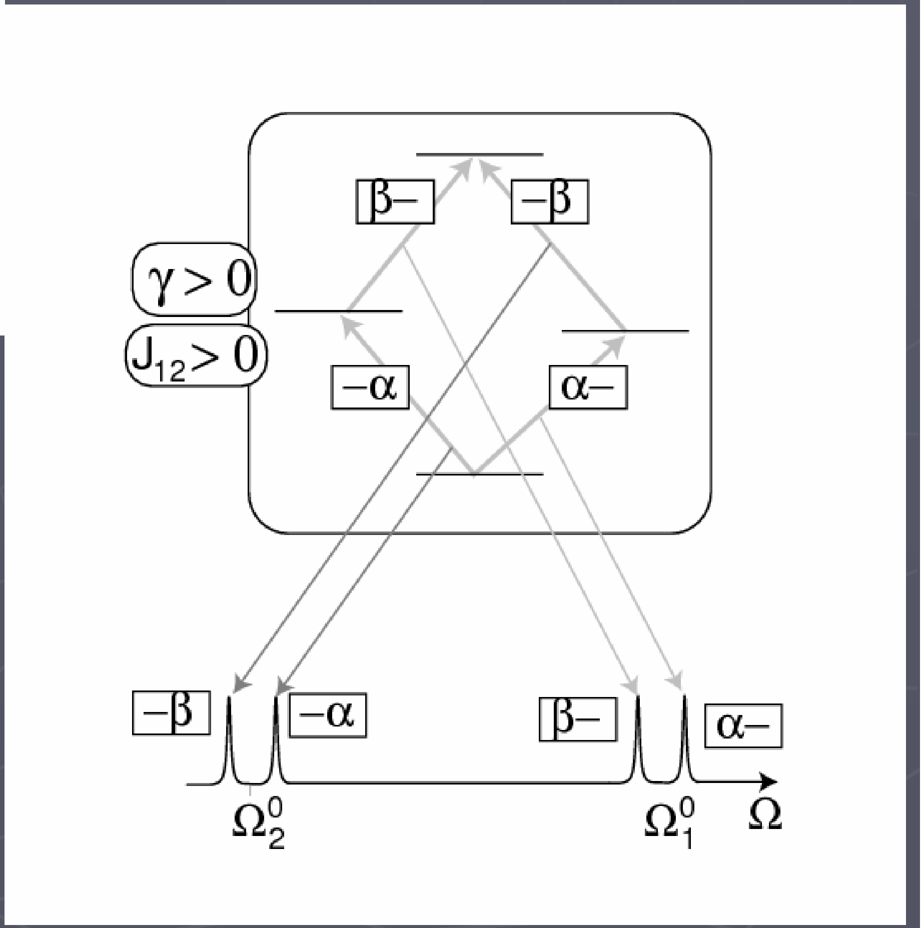
$$R(\theta) = \mathrm{e}^{-i\theta I_{\pm x, \pm y}}$$

- Operadores de evolução temporal:

$$T(t, H_{\text{int}}) = \mathrm{e}^{-iH_{\text{int}} t}$$

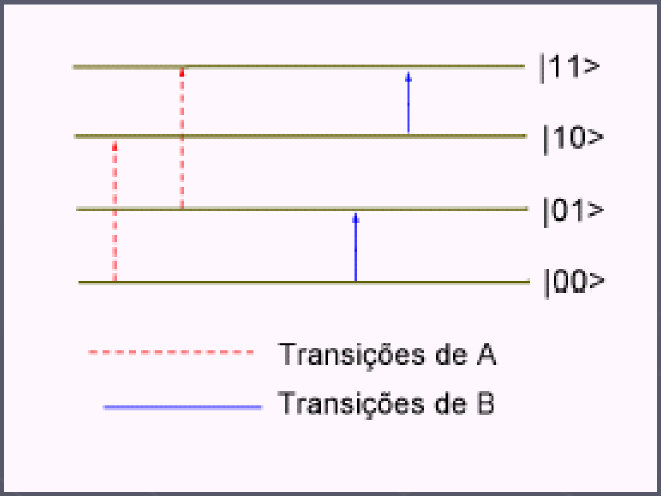
Implementação com 2 núcleos (I = 1/2) acoplados

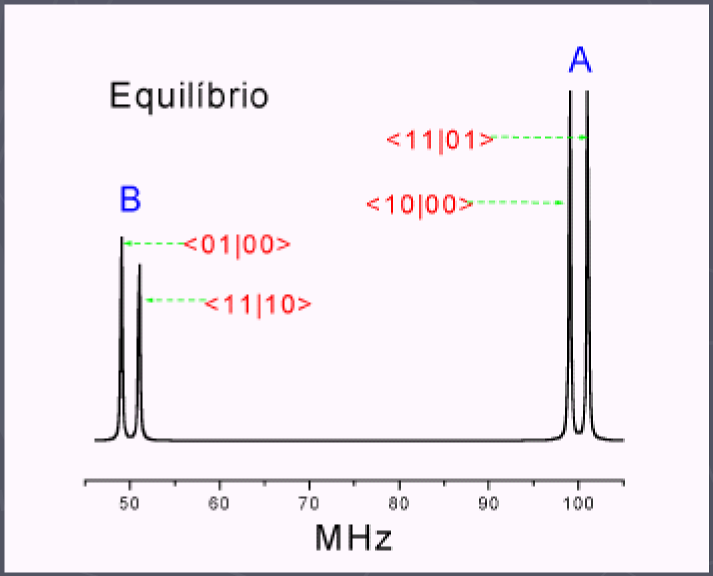




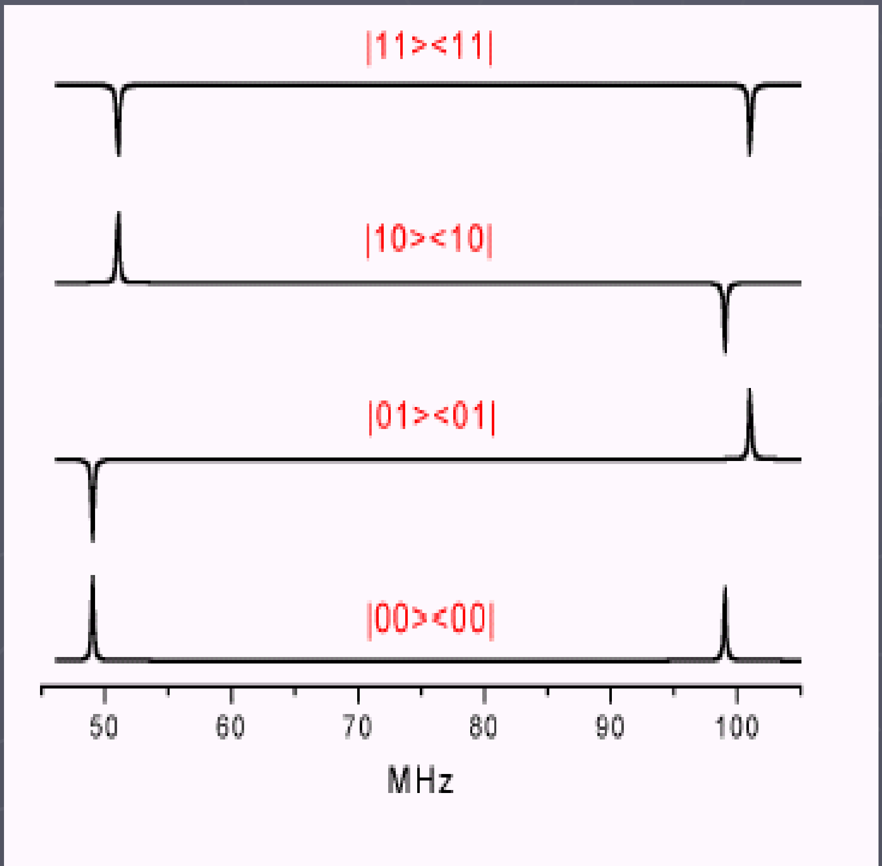
$$H_{\text{int}} \cong \omega_1 I_{1z} + \omega_2 I_{2z} + 2\pi J I_{1z} I_{2z}$$

Exemplo de criação de estados pseudo-puros



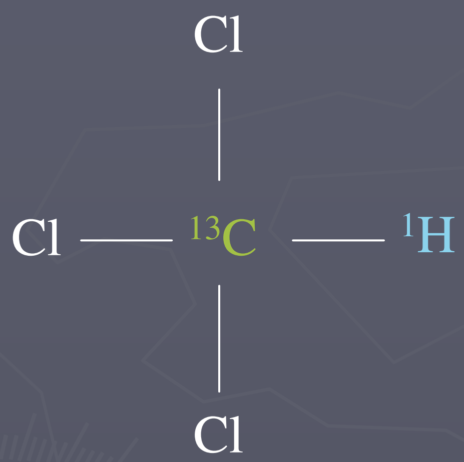


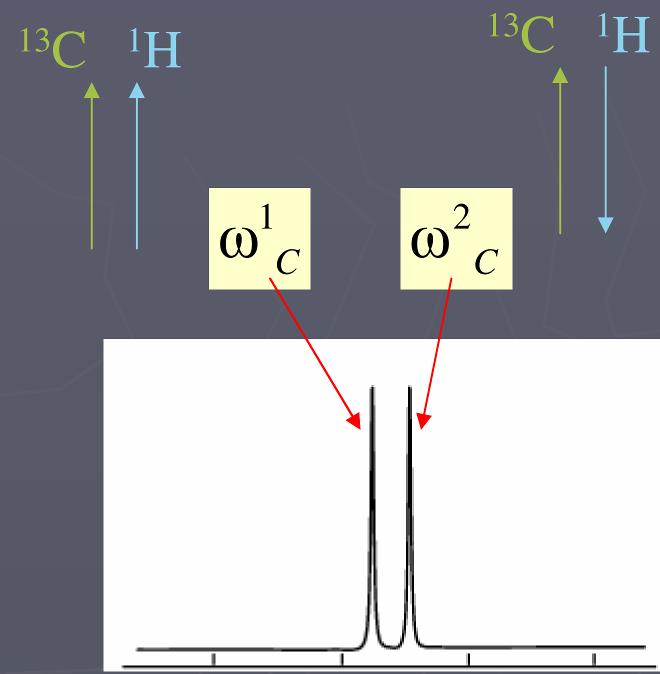
Estados pseudo-puros



Exemplo de sistema com 2 núcleos (I = 1/2) acoplados

Molécula de clorofórmio:





$$H \cong \omega_C I_{Cz} + \omega_H I_{Hz} + 2\pi J_{CH} I_{Cz} I_{Hz}$$

$$\omega^1{}_C = \omega_C + \pi J_{CH}$$

$$\omega^2{}_C = \omega_C - \pi J_{CH}$$

$$B_0 = 11{,}8\ \mathrm{T}$$

$$2\pi\omega_H \cong 500\ \mathrm{MHz}$$

$$2\pi\omega_C \cong 125\ \mathrm{MHz}$$

$$J_{CH} \cong 215\ \mathrm{Hz}$$

$$T_{1C} \cong 25\ \mathrm{s} \quad T_{1H} \cong 18\ \mathrm{s}$$

$$T_{2C} \cong 300\ \mathrm{ms} \quad T_{2H} \cong 7\ \mathrm{s}$$

$$1/2J_{CH} \cong 2{,}3\ \mathrm{ms}$$

Implementação com 2 núcleos (I = 1/2) acoplados

Porta Não-controlado (CNOT)
ou Ou-Exclusivo (XOR):

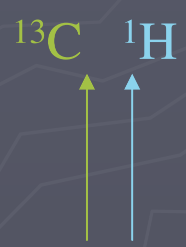
$$|00\rangle \rightarrow |00\rangle$$
$$|01\rangle \rightarrow |01\rangle$$
$$|10\rangle \rightarrow |11\rangle$$
$$|11\rangle \rightarrow |10\rangle$$

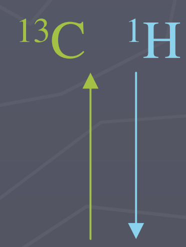
$$\omega^1{}_C = \omega_C + \pi J_{CH}$$
$$\omega^2{}_C = \omega_C - \pi J_{CH}$$

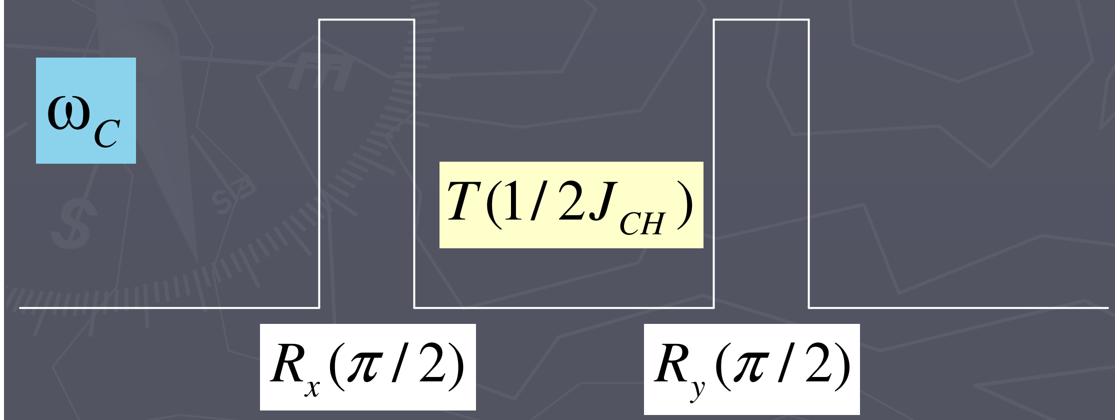
Sistema girante:

$$\Delta\omega^1{}_C = +\pi J_{CH}$$

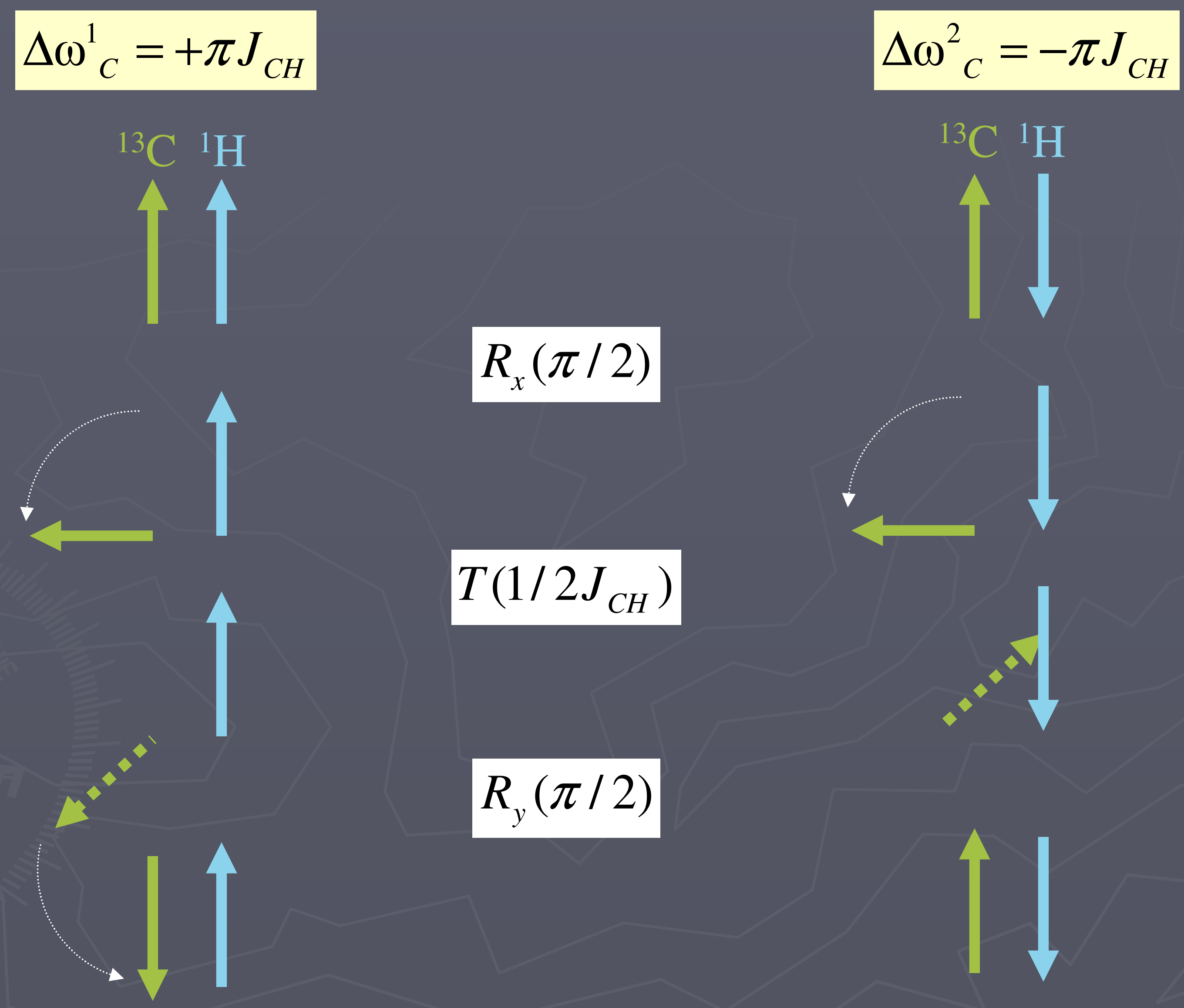
$$\Delta\omega^2{}_C = -\pi J_{CH}$$







Implementação com 2 núcleos (I = 1/2) acoplados

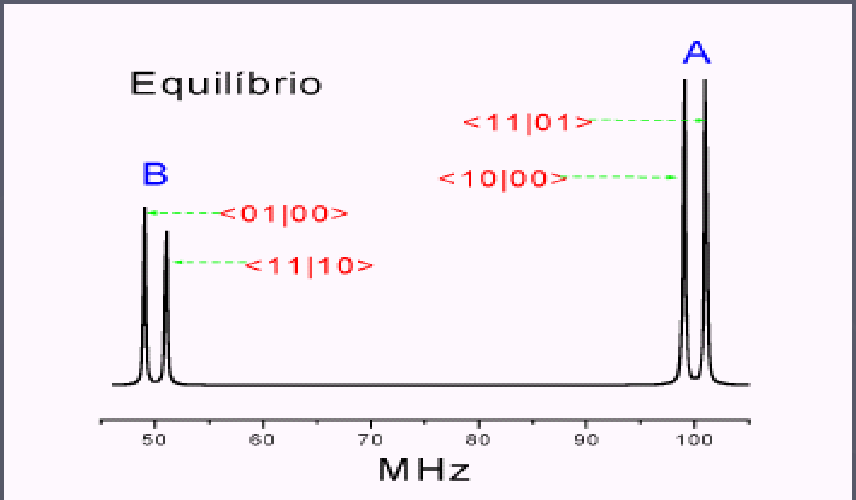


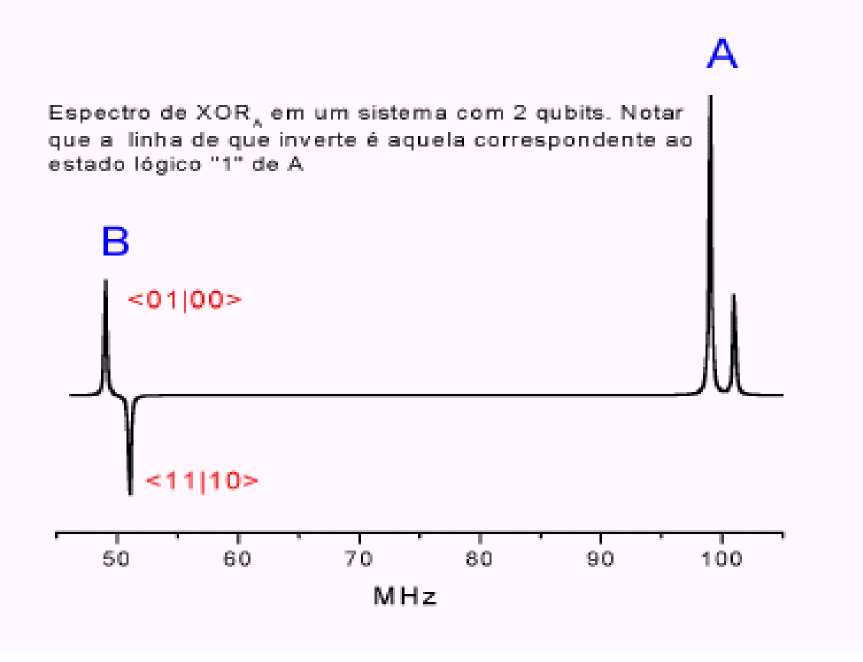
Inversão condicional do spin do núcleo ^{13}C

Exemplo de implementação da porta CNOT

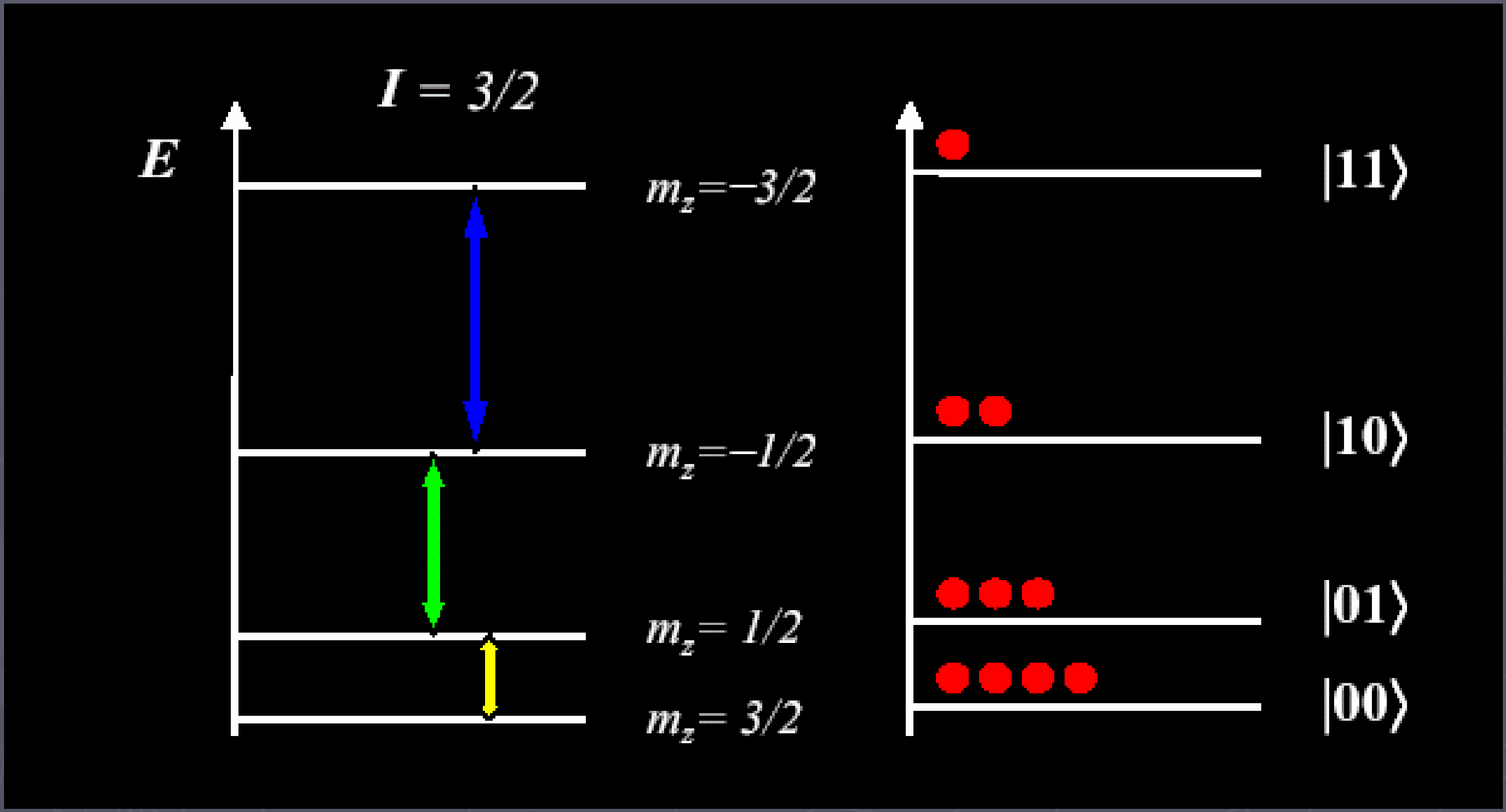
Porta CNOT (ou XOR):

$$|00\rangle \rightarrow |00\rangle$$
$$|01\rangle \rightarrow |01\rangle$$
$$|10\rangle \rightarrow |11\rangle$$
$$|11\rangle \rightarrow |10\rangle$$



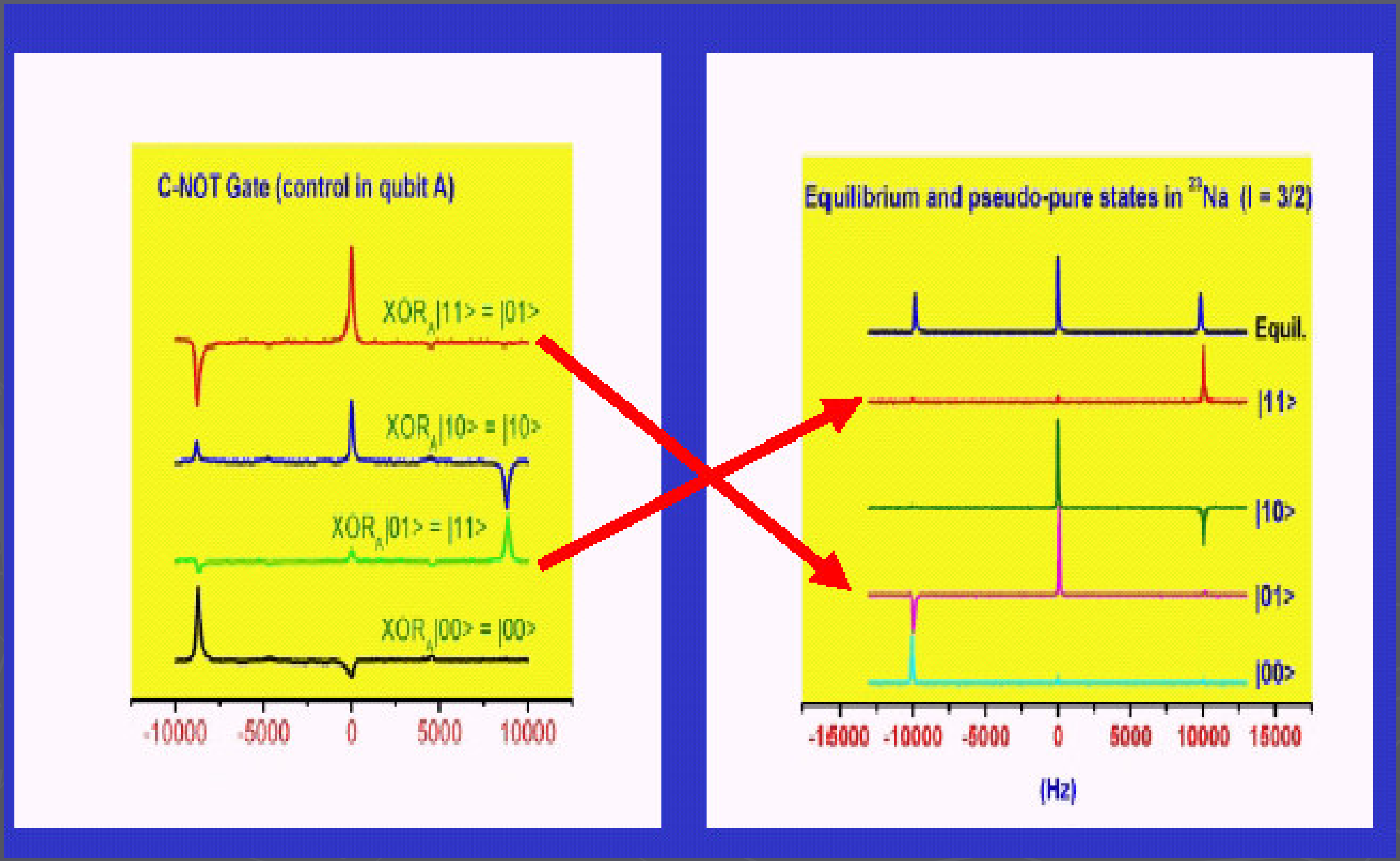


Uso de núcleos quadrupolares (I > 1/2)



RMN de ^{23}Na (I = 3/2) em cristal líquido

Sistema com 2 q-bits por núcleo



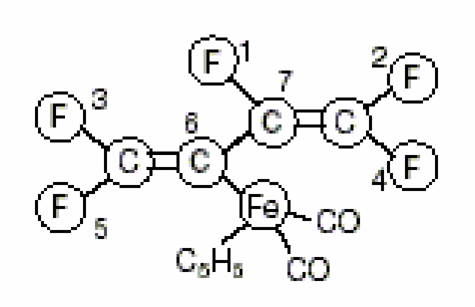
Experimentos em computação quântica via RMN

Algoritmo de Grover:

- Chuang et al., *Phys. Rev. Lett.* (1998).
- 2 q-bits (molécula de clorofórmio, ^{1}H e ^{13}C).

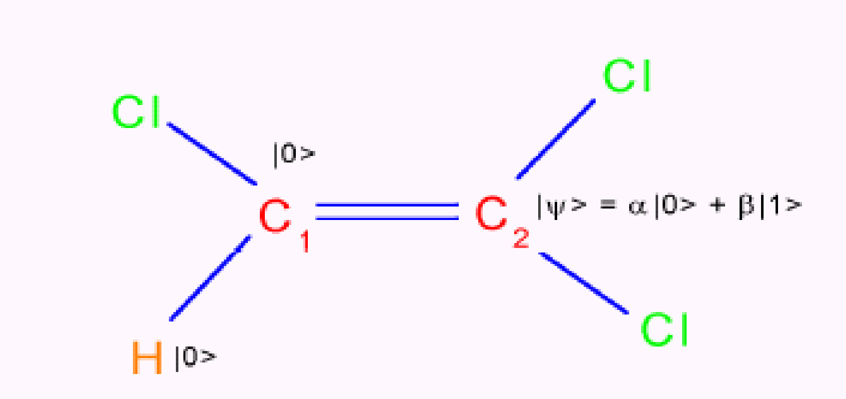
Algoritmo de Shor: $15 = 3 \times 5$

- Vandersypen et al., *Nature* (2001).
- 7 q-bits (^{1}H e ^{13}C).



Teleporte quântico:

- Nielsen et al., *Nature* (1998).
- 3 q-bits (^{1}H e ^{13}C).



Implementação experimental com 12 q-bits

PRL **96,** 170501 (2006) PHYSICAL REVIEW LETTERS week ending 5 MAY 2006

Benchmarking Quantum Control Methods on a 12-Qubit System

C. Negrevergne,[1] T. S. Mahesh,[2] C. A. Ryan,[1] M. Ditty,[1] F. Cyr-Racine,[1] W. Power,[1] N. Boulant,[2]
T. Havel,[2] D. G. Cory,[2] and R. Laflamme[1,3]

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[2]*Department of Nuclear Engineering, MIT, Cambridge, Massachusetts 02139, USA*
[3]*Perimeter Institute for Theoretical Physics, Wa*
(Received 17 December 2005; publi

In this Letter, we present an experimental benchmark o information processors extended up to 12 qubits. We imple space using two complementary approaches and discuss thei ence, we were able to reach a 12-coherence state (or a 12-qub 11 qubit plus one qutrit pseudopure state using liquid s information processors.

DOI: 10.1103/PhysRevLett.96.170501

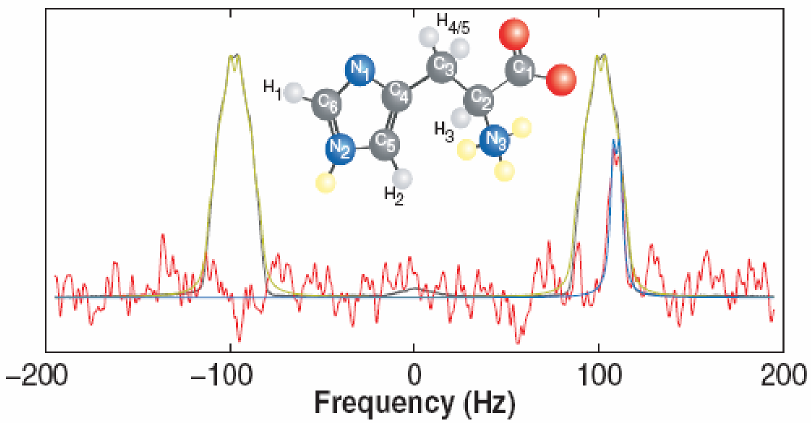

FIG. 2 (color). This *l*-histidine molecule has 14 spin-1/2 nuclei: five ^{1}H, six ^{13}C, and three ^{15}N. See Ref. [24] for a more complete description of the molecule. The two protons H_4 and H_5, are chemically equivalent and indistinguishable. As such, they can be seen as a composite particle with a spin-1 and a spin-0 part. We considered only the spin-1 subspace (qutrit) since the spin-0 does not interact with the other spin-1/2. This molecule is therefore a 12-qubits plus one qutrit quantum register. However,

Proposta experimental: dispositivos microeletrônicos

NATURE | VOL 393 | 14 MAY 1998

A silicon-based nuclear spin quantum computer

B. E. Kane

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Quantum computers promise to exceed the computational efficiency of ordinary classical machines because quantum algorithms allow the execution of certain tasks in fewer steps. But practical implementation of these machines poses a formidable challenge. Here I present a scheme for implementing a quantum-mechanical computer. Information is encoded onto the nuclear spins of donor atoms in doped silicon electronic devices. Logical operations on individual spins are performed using externally applied electric fields, and spin measurements are made using currents of spin-polarized electrons. The realization of such a computer is dependent on future refinements of conventional silicon electronics.

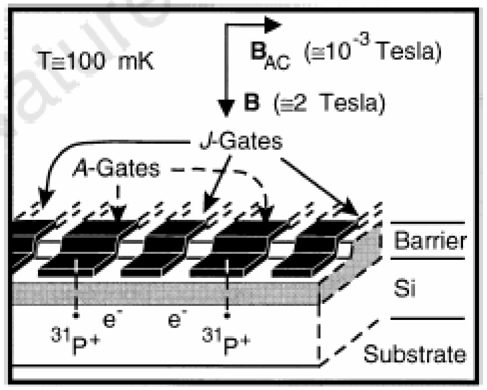


Figure 1 Illustration of two cells in a one-dimensional array containing ^{31}P donors and electrons in a Si host, separated by a barrier from metal gates on the surface. 'A gates' control the resonance frequency of the nuclear spin qubits; 'J gates' control the electron-mediated coupling between adjacent nuclear spins. The ledge over which the gates cross localizes the gate electric field in the vicinity of the donors.

Proposta experimental: dispositivos microeletrônicos

Techniques

NMR on a chip

Robert Tycko

If a nanoscale gallium arsenide structure is excited with an oscillating magnetic field, superpositions of nuclear spin states can be created and detected electrically. Quantum computing could be the beneficiary.

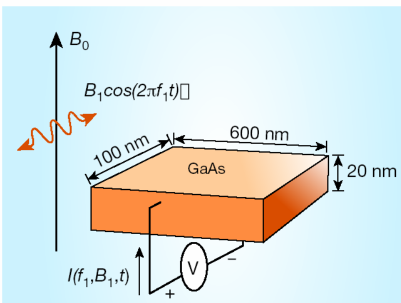
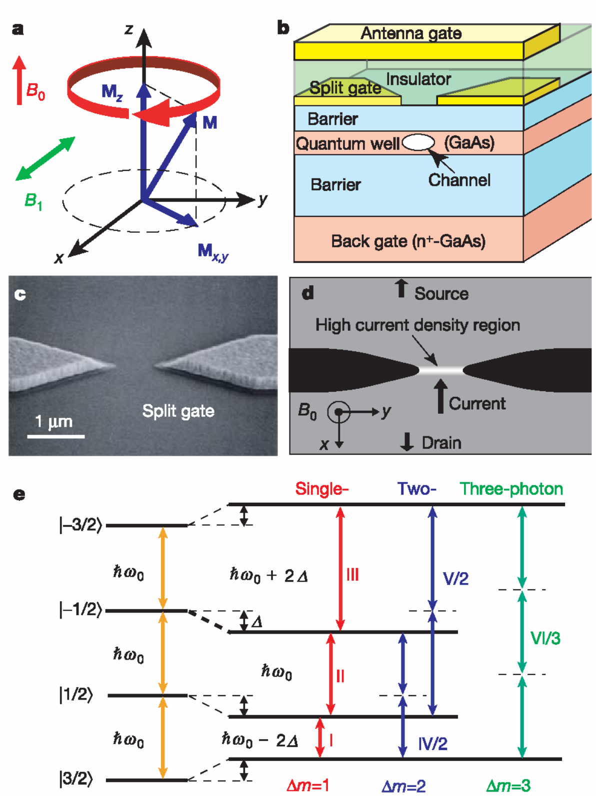


Figure 1 **Nanoscale resonator. Current *I* passing through a gallium arsenide nanostructure as described by Yusa *et al.*[1] produces a large polarization in nuclear spin in the presence of a static magnetic field B_0. Applying a second magnetic field B_1, which varies sinusoidally with a frequency f_1 close to an NMR frequency, causes the spin polarization, and thus the resistance, in the GaAs channel to oscillate. Varying the frequency of this field allows the spectrum of all allowed NMR transitions to be mapped out electrically.**



Controlled multiple quantum coherences of nuclear spins in a nanometre-scale device

Go Yusa[1], Koji Muraki[1], Kei Takashina[1], Katsushi Hashimoto[2*] & Yoshiro Hirayama[1,2]

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[2]*SORST Program, Japan Science and Technology Agency (JST), 4-1-8 Honmachi, Kawaguchi, Saitama 331-0012, Japan*

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The analytical technique of nuclear magnetic resonance (NMR[1,2]) is based on coherent quantum mechanical superposition of nuclear spin states. Recently, NMR has received considerable renewed interest in the context of quantum computation and information processing[3–11], which require controlled coherent qubit operations. However, standard NMR is not suitable for the implementation of realistic scalable devices, which would require all-electrical control and the means to detect microscopic quantities of coherent nuclear spins. Here we present a self-contained NMR semiconductor device that can control nuclear spins in a nanometre-scale region. Our approach enables the direct detection of (otherwise invisible) multiple quantum coherences between levels separated by more than one quantum of spin angular momentum. This microscopic high sensitivity NMR technique is especially suitable for probing materials whose nuclei contain multiple spin levels, and may form the basis of a versatile multiple qubit device.

Proposta experimental: dispositivos microeletrônicos

PHYSICAL REVIEW B **80**, 115326 (2009)

Nuclear spin coherence in a quantum wire

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(Received 6 April 2009; revised manuscript received 31 August 2009; published 29 September 2009)

We have observed millisecond-long coherent evolution of nuclear spins in a quantum wire at 1.2 K. Local, all-electrical manipulation of nuclear spins is achieved by dynamic nuclear polarization in the breakdown regime of the integer quantum Hall effect combined with pulsed nuclear magnetic resonance. The excitation thresholds for the breakdown are significantly smaller than what would be expected for our sample and the direction of the nuclear polarization can be controlled by the voltage bias. As a four-level spin system, the device is equivalent to two qubits.

DOI: 10.1103/PhysRevB.80.115326 PACS number(s): 76.70.Fz, 73.43.Fj, 73.63.Nm, 76.60.Es

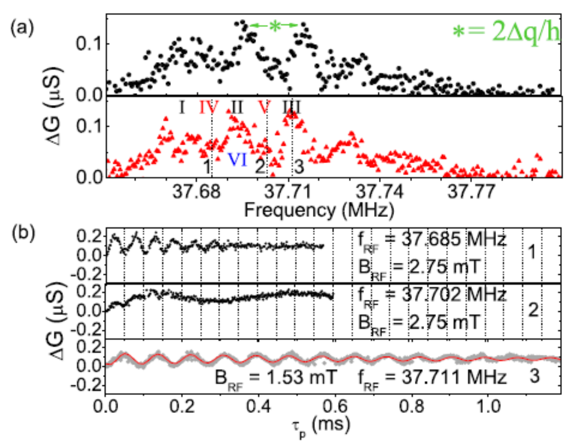

FIG. 6. (Color online) (a) Frequency spectrum of ^{75}As at T = 1.2 K using 312 μs long pulses and B_{RF}=1.53 mT with (triangles) and without (circles) electron-nuclear coupling, showing a 4 kHz Knight shift. Resonance frequencies for the different transitions in Fig. 5(c) are indicated; (b) Rabi oscillations corresponding to the frequencies 1, 2, and 3 in (a).

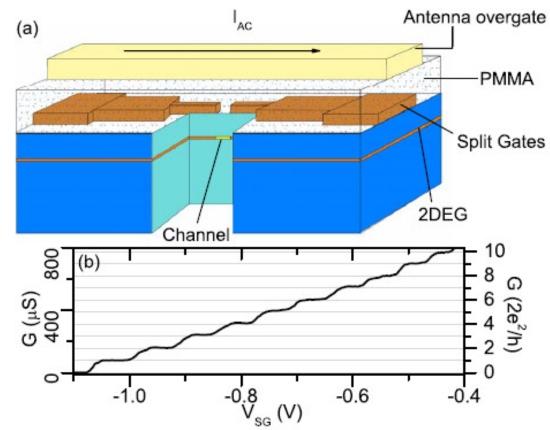

FIG. 1. (Color online) (a) Schematic view of the device (not to scale). Two split gates define the one-dimensional channel. A layer of PMMA isolates the split gates from the antenna overgate used to apply the RF magnetic field; (b) one-dimensional subbands as a function of gate voltage V_{SG} at 50 mK and zero magnetic field. The conductance is shown in μS (left-hand vertical axis) and in units of $2e^2/h$ (right-hand vertical axis)

Proposta experimental: detecção por MRFM

Single spin detection by magnetic resonance force microscopy

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IBM Research Division, Almaden Research Center, 650 Harry Rd, San J
California 95120, USA

NATURE | VOL 430 | 15 JULY 2004 | www.nature.com/nature

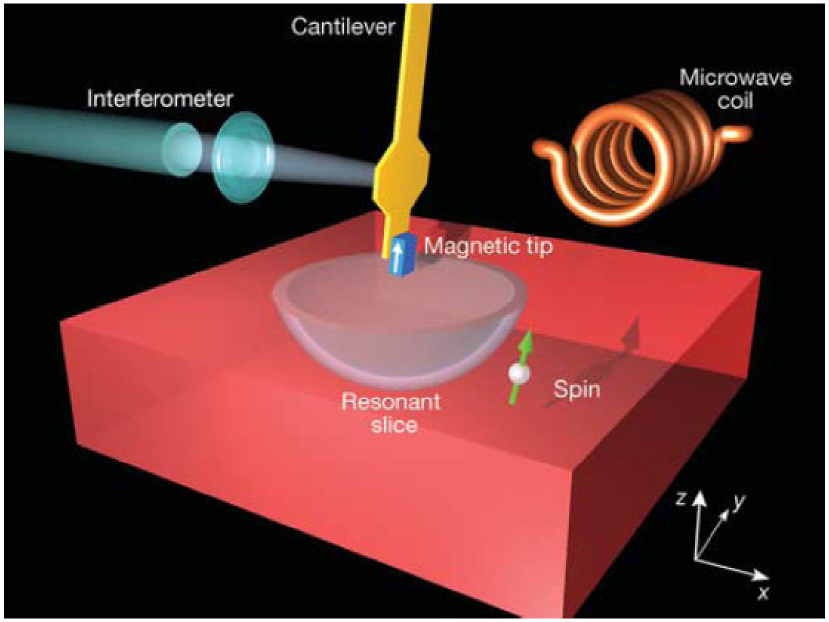

Figure 1 Configuration of the single-spin MRFM experiment. The magnetic tip at the end of an ultrasensitive silicon cantilever is positioned approximately 125 nm above a polished SiO_2 sample containing a low density of unpaired electron spins. The resonant slice represents those points in the sample where the field from the magnetic tip (plus an external field) matches the condition for magnetic resonance. As the cantilever vibrates, the resonant slice swings back and forth through the sample causing cyclic adiabatic inversion of the spin. The cyclic spin inversion causes a slight shift of the cantilever frequency owing to the magnetic force exerted by the spin on the tip. Spins as deep as 100 nm below the sample surface can be probed.

Proposta experimental: detecção por MRFM

PHYSICAL REVIEW B VOLUME 61, NUMBER 21 1 JUNE 2000-I

Solid-state nuclear-spin quantum computer based on magnetic resonance force microscopy

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V. I. Tsifrinovich
IDS Department, Polytechnic University, Six Metrotech Center, Brooklyn, N

(Received 13 September 1999)

We propose a nuclear-spin quantum computer based on magnetic resonance force r
is shown that an MRFM single-electron spin measurement provides three essential re
computation in solids: (a) preparation of the ground state, (b) one- and two-qubit quar
a measurement of the final state. The proposed quantum computer can operate at tem

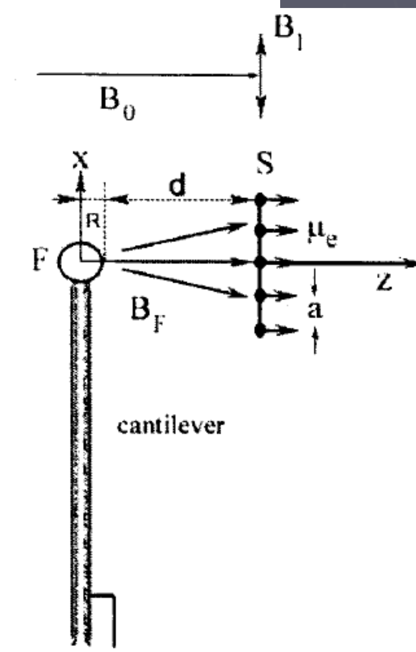


FIG. 1. A nuclear-spin quantum computer based on MRFM using single-spin measurement: B_0 is the permanent magnetic field, B_1 is the radio-frequency magnetic field, $\vec{B}_F$ is the nonuniform magnetic field produced by a ferromagnetic particle F in the sample S, R is the radius of the ferromagnetic particle, d is the distance between the ferromagnetic particle and the targeted atom, and a is the distance between neighboring impurity atoms. The origin is placed at the equilibrium position of the center of the ferromagnetic particle. Arrows on the sample S show the direction of electron magnetic moments μ_e.

Computação quântica via RMN

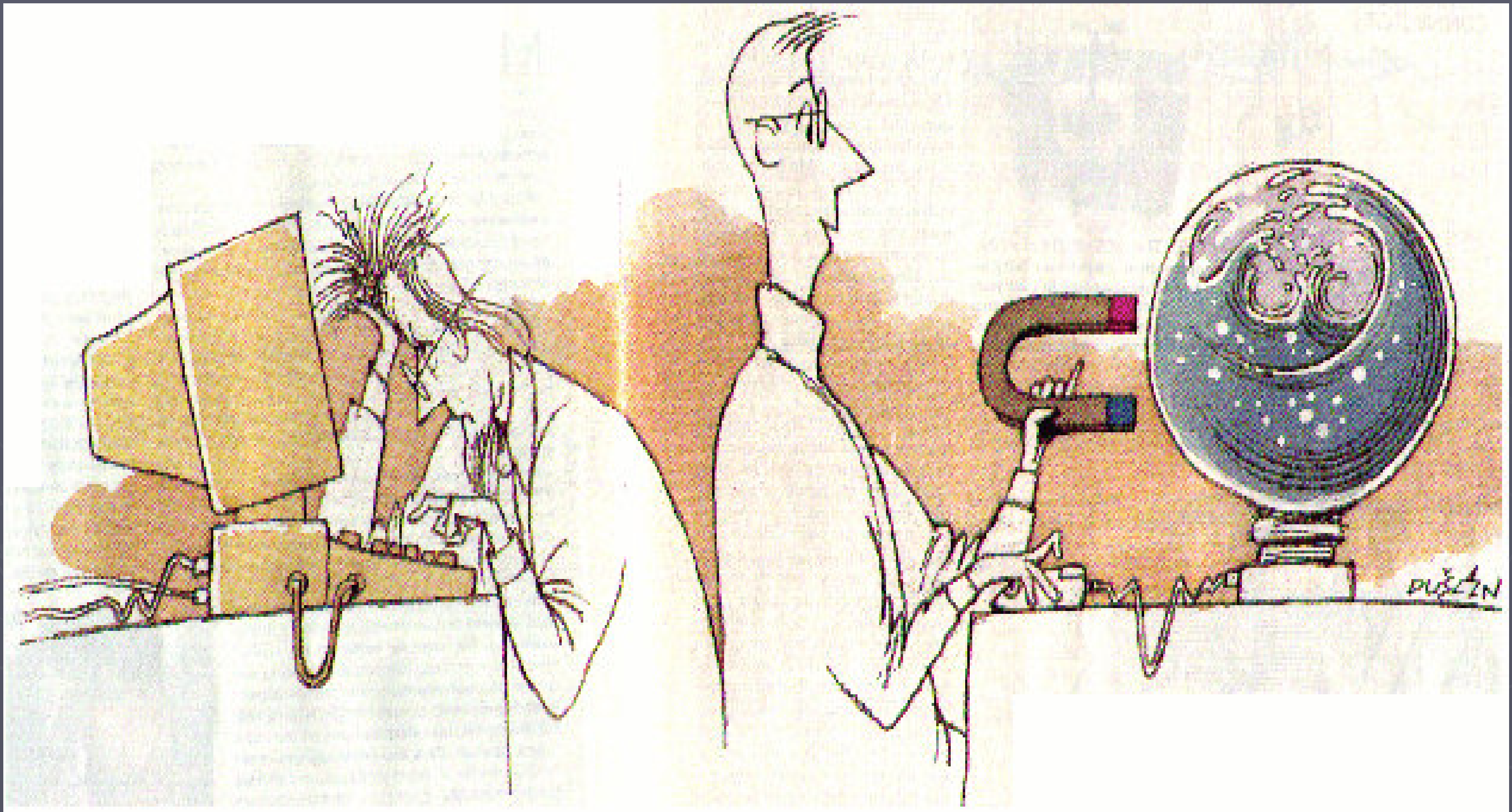
Vantagens e Perspectivas

- Manipulação de q-bits com técnicas bem estabelecidas.
- Implementação com sucesso de algoritmos em sistemas simples (única!!).
- Simulação bem sucedida de sistemas quânticos.
- É possível aumentar o número de q-bits...

Limitações

- ...número máximo de q-bits limitado.
- Tempos de coerência curtos (relaxação).
- É possível criar emaranhamento ("entanglement") em estados pseudo-puros??

Computadores do futuro = Espectrômetros de RMN?



Sci. Amer., Junho 1998

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    (Excelentes figuras!!!)
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