NMR: Formalism & Techniques

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Why NMR?

- Local microscopic & bulk probe

- Can be performed on relatively small samples (~1 mg +)
  & no contacts on the sample

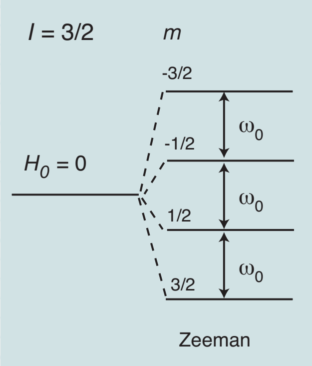
- $\omega_{NMR} \approx 0$ (μeV), partial q info, $r \approx$ constant

- Extreme conditions: high field, dilution refrigerator, pressure cell

NMR Principles

The basic steps of NMR are as follows:

1. A sample is placed in a high magnetic field environment. This breaks the degeneracy of the nuclear Zeeman spin state.



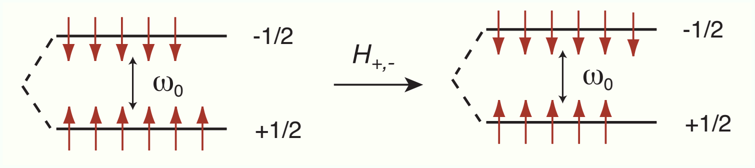
Nuclear spin I in a magnetic field H_0 ⇒ $\mathcal{H} = -\gamma\hbar I \cdot H_0$

$$\Delta E = \omega_0\hbar = \gamma\hbar H_{loc} \propto H_{loc}$$

2. A coil around the sample generates a low amplitude, high frequency oscillating magnetic field transverse to the main field. This excites nuclei from one state to another.

$$\mathcal{H}_\perp = \gamma\hbar H_j I_j e^{i\omega_0 t}$$

$$\mathcal{H}_\perp \propto h_{+,-}(\omega)$$

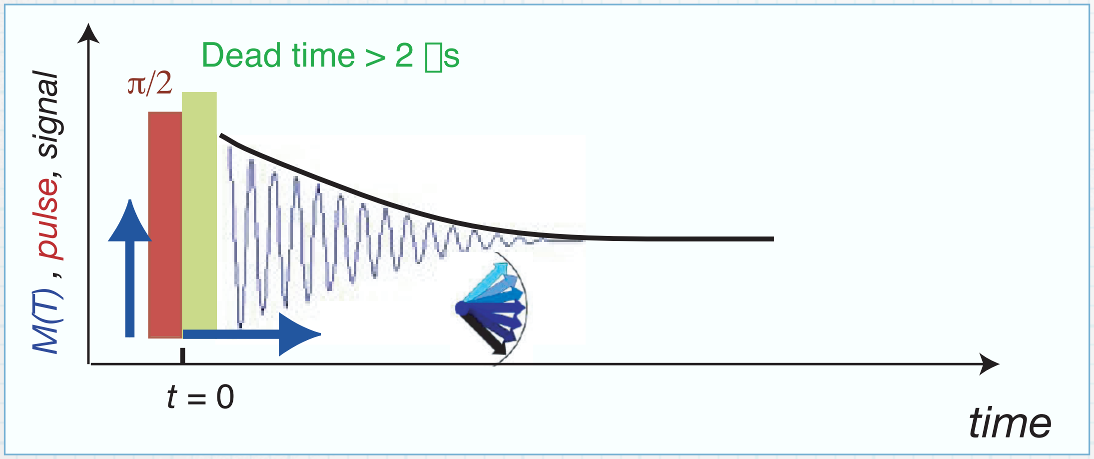


$$\frac{n_\downarrow}{n_\uparrow} = e^{\frac{\hbar\omega_0}{k_B T}} \quad \& \quad \hbar\omega_0 \ll k_B T \Rightarrow \Delta n \approx \frac{\hbar\omega_0}{k_B T}$$

NMR Principles

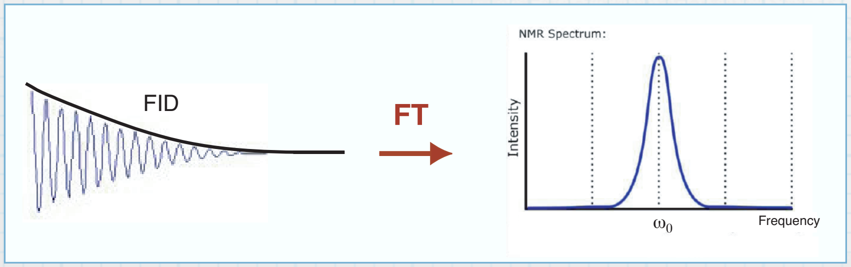
The basic steps of NMR *cnt*:

3. The oscillating field is removed, and the nuclei begin to relax back to their original state.



4. As the nuclei relax, a small current is induced in the coil that generated the original oscillating field.

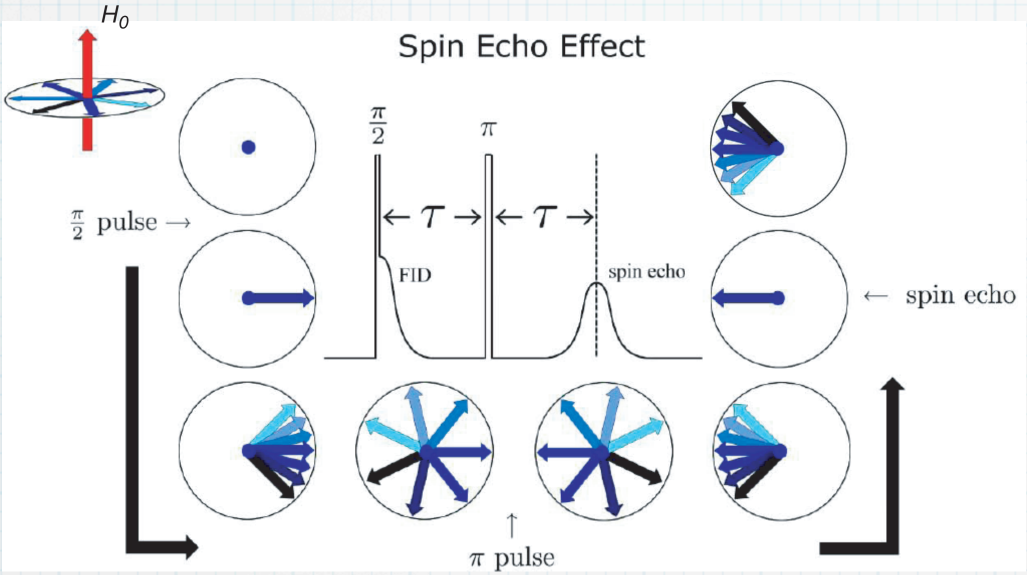
5. This current is amplified and analyzed, yielding information about the energy eigenstates of the sample.



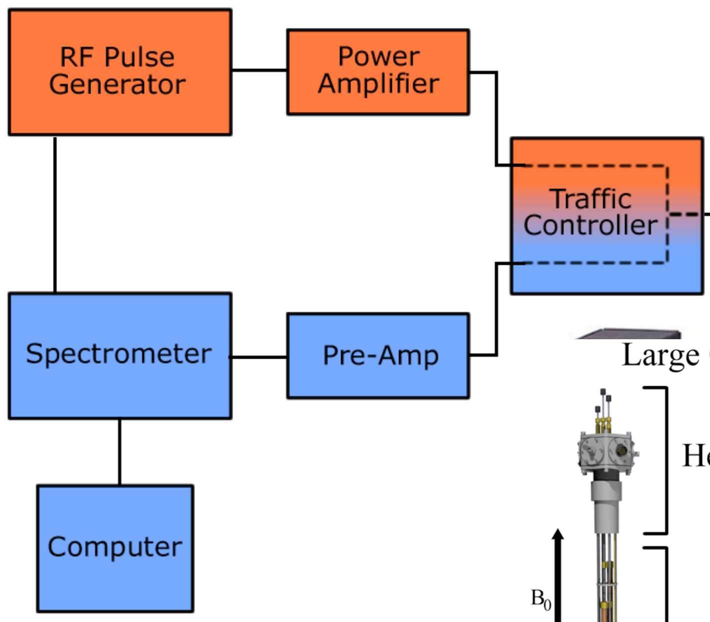
$$\omega_0 \propto H_{loc}$$

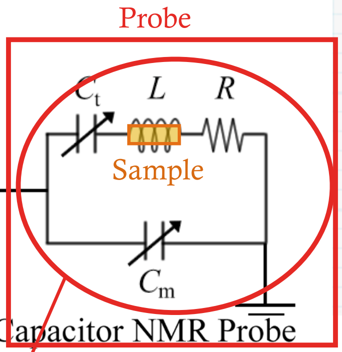
NMR Principles

Spin Echo (*Hahn, Phys. Rev.* ***80****, 5801 (1950)*)

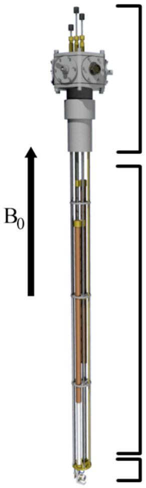


How is it done?





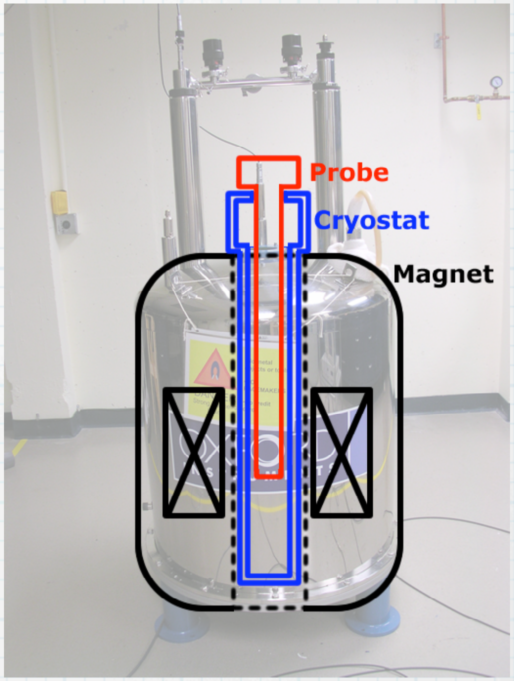
Large Capacitor NMR Probe

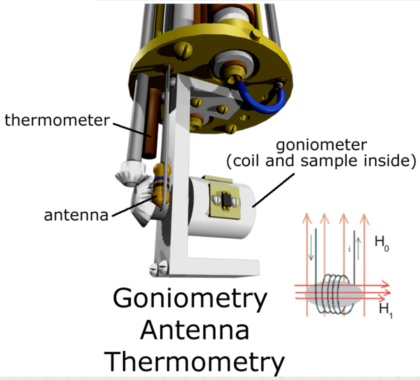


Head - BNC and multipin connections
Capacitor tuning
Goniometer control
Height adjustment

Body - Capacitor Housing

Sample Housing
Goniometry
Foot - Thermometry





Goniometry
Antenna
Thermometry

Canister
Heater

Static NMR Measurements

Static NMR Spectrum Measurements ⇒

Local Magnetic Field Probability Distribution

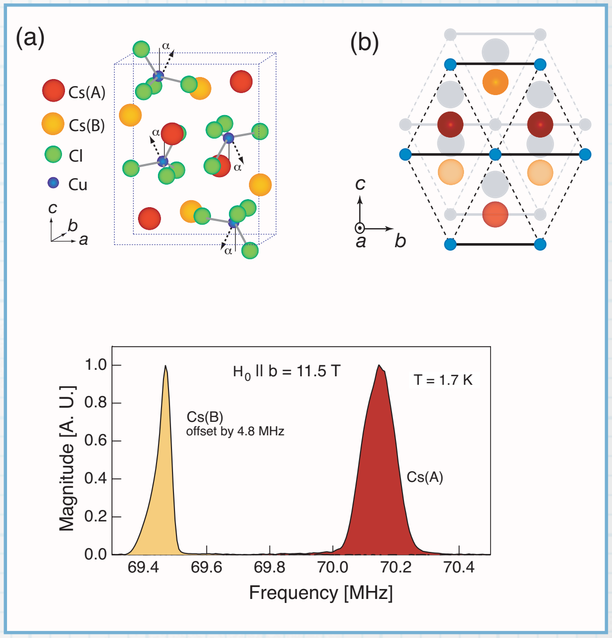
$$\omega_n = \gamma_n H_{loc} = \gamma_n \left(H_0 + \langle H_{hf} \rangle\right)$$

$$\langle H_{hf} \rangle = \sum_n -A_{n,k} \langle S_k \rangle$$

Hyperfine tensor

e^- spin operator || H_0
averaged over ~ 10 µs

Contributions to hyperfine coupling constant (A):
- on-site: A = strong & ~ known
- transferred: A can be anything
- dipole: A can be calculated & weak



$$\langle H_{hf} \rangle = \sum_n -A_{n,k} \langle S_k \rangle = \sum_n -A_{n,k} \frac{1}{g_k \mu_B} \chi_k(T)$$

χ = magnetic susceptibility per site

$$\frac{\omega_n - \omega_0}{\omega_0} = K(T) \propto \chi(T) = \chi(q = 0, \omega \to 0)$$

⇒ Magnetic hyperfine shift

Static NMR Measurements

Static NMR Spectrum Measurements ⇒
Local Magnetic Field Probability Distribution

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$$\langle H_{hf} \rangle = \sum_n -A_{n,k} \langle S_k \rangle$$

Width of an NMR spectrum ⇒ **Distribution of** $\langle \vec{S}_z(r) \rangle$

$$K(T) \propto \chi'(q=0, \omega \rightarrow 0)$$

Shift of an NMR spectrum ⇒ **Magnetic susceptibility**

In metals:

$$K(T) \propto N(E_F)$$

Quadrupolar Interactions - NQR

For *I* > 1/2 ⇒ nuclei have nuclear **quadrupole moment *Q***

For *I* > 1/2 & non-cubic local symmetry ⇒ ***Q*** interacts with the electric field gradient (EFG) arising from the surrounding electronic charge distribution.

The EFG = 2nd rank tensor with components along its principal axes *(i= X, Y,Z)* :

$$V_{i,j} = \partial^2 V/\partial x_i \partial x_j \quad \& \quad |V_{ZZ}| \geq |V_{YY}| \geq |V_{XX}|$$

Quadrupolar Hamiltonian:

$$\mathcal{H}_Q = \frac{h\nu_Q}{2}\left[I_Z^2 - \frac{I(I+1)}{3} + \frac{\eta}{6}(I_+^2 + I_-^2)\right] \Rightarrow$$

$$\nu_Q = \frac{3eQ}{2I(2I-1)h} V_{ZZ} \quad \& \quad \eta = \frac{|V_{XX} - V_{YY}|}{V_{ZZ}}$$

$$H_0 \neq 0$$

NMR line spilts into ***2I*** lines

$$H_0 = 0$$

NQR lines with $\omega_Q \propto \nu_Q$

Quadrupolar Interactions - NQR

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$$\mathcal{H}_Q = \frac{h\nu_Q}{2}\left[I_Z^2 - \frac{I(I+1)}{3} + \frac{\eta}{6}(I_+^2 + I_-^2)\right] \Rightarrow H_0 \neq 0$$

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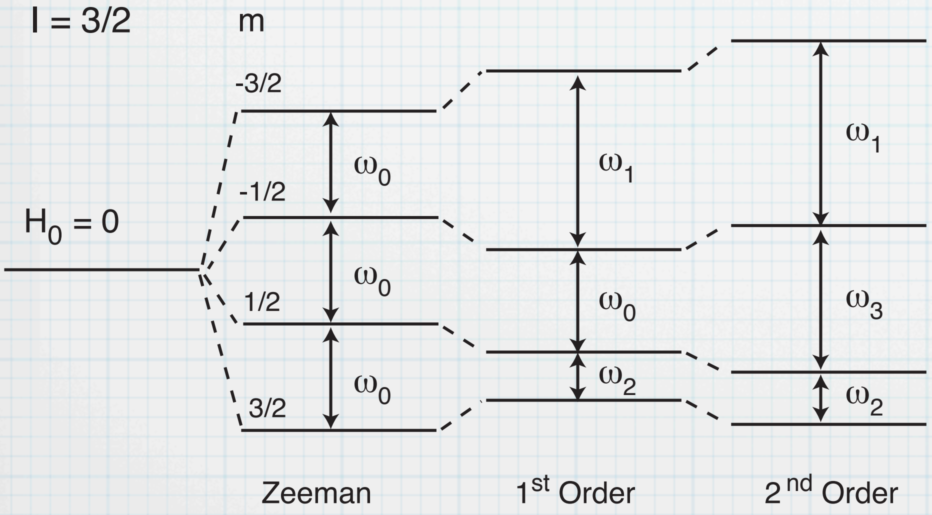
$$\nu_Q = \frac{3eQ}{2I(2I-1)h}V_{ZZ} \quad \& \quad \eta = \frac{|V_{XX} - V_{YY}|}{V_{ZZ}}$$

$$H_0 = 0$$

NQR lines with $\omega_Q \propto \nu_Q$



Good for study of lattice deformations....

Dynamic NMR Measurements

Dynamic NMR Spectrum Measurements ⇒
Measure of Fluctuations of Local Magnetic Field

Spin decoherence ***(spin-spin relaxation)*** rate: $T_2^{-1} \propto h_{||}(t)$

(no energy loss for nuclear system)

Spin lattice relaxation rate: $T_1^{-1} \propto h_{\perp}(t) = h_{+,-}(t)$

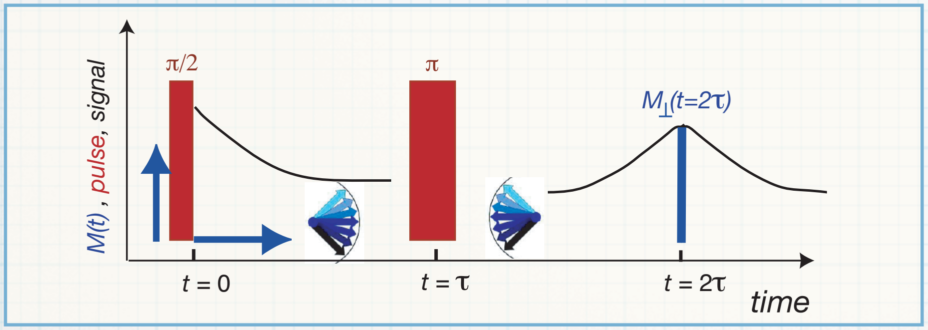
The nuclear spin-lattice relaxation time measures the time that it takes for excited nuclear spins to return to thermal equilibrium with the lattice (electrons). The nuclei relax to equilibrium (the state in which the population of the nuclear Zeeman levels is described by the Boltzmann population function) by exchanging energy with the electronic system.

$$T_1^{-1} \propto \chi''(q, \omega \rightarrow 0)$$

$$T_2^{-1} \propto \chi'(q, \omega \rightarrow 0)$$

How to measure rates?

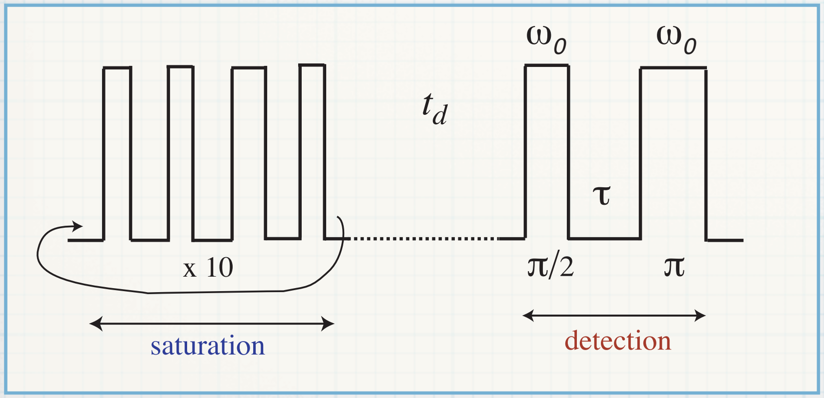
Spin-spin relaxation rate, T_2^{-1}:

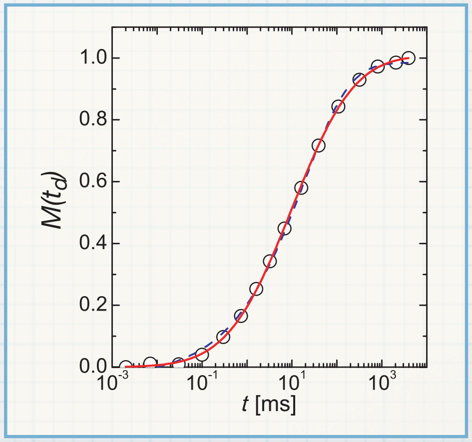


- Record $M_\perp(2\tau)$ as a function of $t = \tau$

Spin-lattice relaxation rate, T_1^{-1}:

- Record $M_\perp(2\tau)$ as a function of $t = t_d$





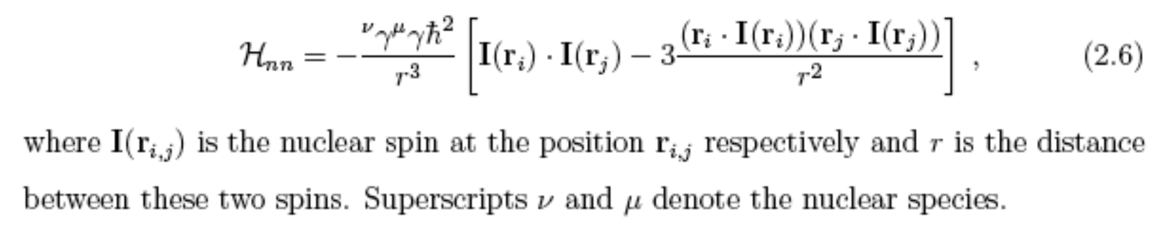
Spin-Spin Relaxation

$T_2^{-1} \propto h_{||}(t)$

The nuclear spin–spin relaxation time T_2 is the characteristic time for the decay of the $M_\perp$ component of the nuclear magnetisation M. Can be a poverfull tool for probing e.g. vortex dynamics.

In correlated electron systems 3 main sources of the decay of the $M_\perp$ **:**

1. Nuclear-nuclear interaction - the spin exchange between two nuclear spins (nuclear dipole-dipole interaction):



$$\mathcal{H}_{nn} = -\frac{{}^{\nu}\gamma^{\mu}\gamma\hbar^2}{r^3}\left[\mathbf{I}(\mathbf{r}_i)\cdot\mathbf{I}(\mathbf{r}_j) - 3\frac{(\mathbf{r}_i\cdot\mathbf{I}(\mathbf{r}_i))(\mathbf{r}_j\cdot\mathbf{I}(\mathbf{r}_j))}{r^2}\right], \qquad (2.6)$$

where $\mathbf{I}(\mathbf{r}_{i,j})$ is the nuclear spin at the position $\mathbf{r}_{i,j}$ respectively and r is the distance between these two spins. Superscripts ν and μ denote the nuclear species.

In most solids T_2 arises from nuclear dipole-dipole interaction to give :

$$M_\perp(t) \propto \exp^{-t^2/\left(2(T_{2G})^2\right)}$$

& $(T_{2G})^{-2}$ = 2nd moment of the homogeneous lineshape (excluding the broadening due to the finite lifetime of a spin in an eigenstate).

Spin-Spin Relaxation

$$T_2^{-1} \propto h_{||}(t)$$

2. ``T_1'' or the Redfield processes - the fluctuations of the nearby e$^-$ spin cause T_1 relaxation & provide a decay of $\boldsymbol{M}_\perp$:

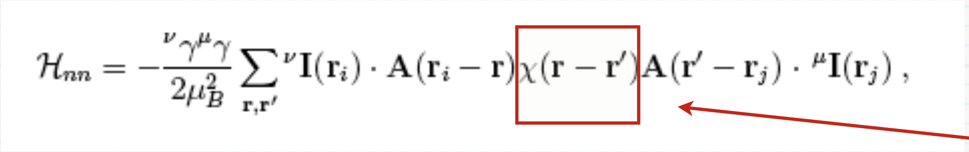
$$M_\perp(t) \propto \exp^{-t/(T_{2R})}$$

Can be removed from the raw experimental data after T_1 is measuremed.

Spin-Spin Relaxation

$T_2^{-1} \propto h_{||}(t)$

3. Indirect nuclear interaction: (C. Kittel, Quantum Theory of Solids)



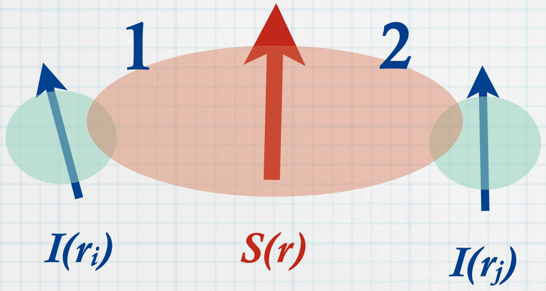
$$\mathcal{H}_{nn} = -\frac{{}^{\nu}\gamma\,{}^{\mu}\gamma}{2\mu_B^2}\sum_{\mathbf{r},\mathbf{r}'} {}^{\nu}\mathbf{I}(\mathbf{r}_i)\cdot\mathbf{A}(\mathbf{r}_i-\mathbf{r})\boxed{\chi(\mathbf{r}-\mathbf{r}')}\mathbf{A}(\mathbf{r}'-\mathbf{r}_j)\cdot{}^{\mu}\mathbf{I}(\mathbf{r}_j)\,,$$

$$\frac{1}{T_2} \propto \chi(q)$$

$\chi(r-r') =$ the real part of the e^- spin susceptibility

$A(r'-r) =$ describes the strength of the contact interaction between a nucleaus and e^-s

Indirect nuclear interaction = 2 step process



1. $\mathcal{H}_{ne} \propto \sum_{r} I(r_i)A(r_i-r)S(r)$

2. $\mathcal{H}_{en} \propto \sum_{r'} S(r')A(r'-r_j)I(r_j)$

1\. + 2. => $\mathcal{H}_{nn} \propto \sum_{rr'} I(r_i)A(r_i-r)S(r)S(r')A(r-r_j)I(r_j)$

$\langle S(r)S(r')\rangle$ = e^- spin density correlation function = the real part of the retarded susceptibility $\chi'(r-r')$

Spin Lattice Relaxation

Hyperfine Hamiltonian -

interaction between conduction electrons and nucleus of species ν at position $\mathbf{R}_{\nu}$:

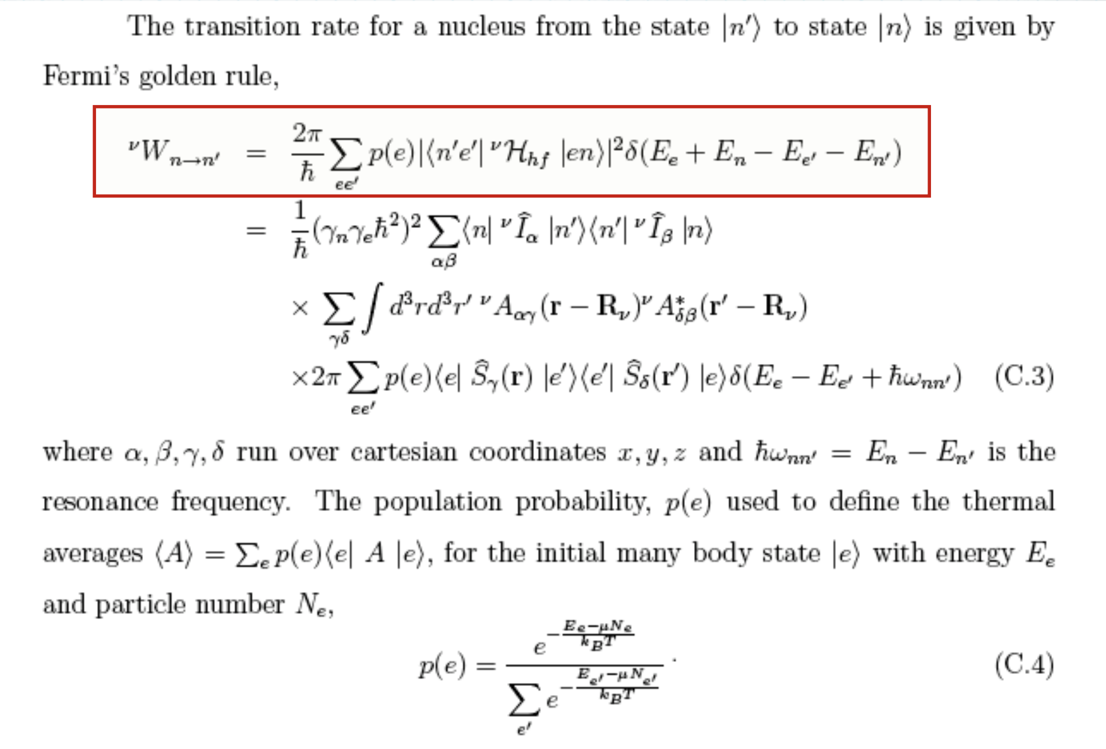
$$\begin{aligned} {}^{\nu}\mathcal{H}_{hf} &= \int d^3r \left(\gamma_n \hbar\, {}^{\nu}\hat{\mathbf{I}}\right) \cdot {}^{\nu}\overleftrightarrow{\mathbf{A}}(\mathbf{r}-\mathbf{R}_{\nu}) \cdot \left(\gamma_e \hbar \hat{\mathbf{S}}(\mathbf{r})\right) \\ &= (\gamma_n \gamma_e \hbar^2) \int d^3r\, {}^{\nu}\hat{\mathbf{I}} \cdot {}^{\nu}\overleftrightarrow{\mathbf{A}}(\mathbf{r}-\mathbf{R}_{\nu}) \cdot \hat{\mathbf{S}}(\mathbf{r}) . \end{aligned}$$

I = nuclear spin operator

S = e^{-} spin operator

A = hyperfine matrix element

$$\hat{\mathbf{S}}(\mathbf{r}) = \sum_{\alpha,\beta} \Psi_{\alpha}^{+}(\mathbf{r}) \frac{\sigma_{\alpha\beta}}{2} \Psi_{\beta}(\mathbf{r}) ,$$



The transition rate for a nucleus from the state $|n'\rangle$ to state $|n\rangle$ is given by Fermi's golden rule,

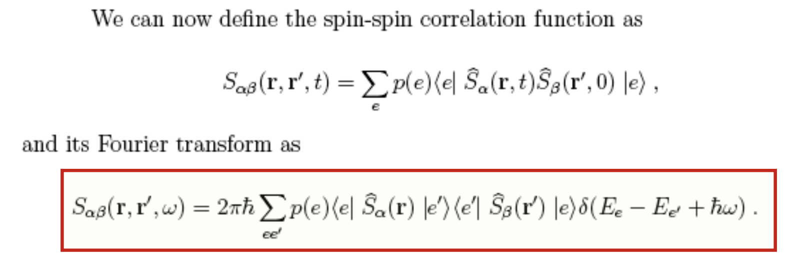
$$\boxed{{}^{\nu}W_{n\to n'} = \frac{2\pi}{\hbar}\sum_{ee'} p(e) |\langle n'e'|\, {}^{\nu}\mathcal{H}_{hf}\, |en\rangle|^2 \delta(E_e + E_n - E_{e'} - E_{n'})}$$

$$\begin{aligned} &= \frac{1}{\hbar}(\gamma_n\gamma_e\hbar^2)^2 \sum_{\alpha\beta} \langle n|\, {}^{\nu}\hat{I}_{\alpha}\, |n'\rangle\langle n'|\, {}^{\nu}\hat{I}_{\beta}\, |n\rangle \\ &\times \sum_{\gamma\delta} \int d^3r d^3r'\, {}^{\nu}A_{\alpha\gamma}(\mathbf{r}-\mathbf{R}_{\nu})^{\nu}A^{*}_{\delta\beta}(\mathbf{r}'-\mathbf{R}_{\nu}) \\ &\times 2\pi \sum_{ee'} p(e)\langle e|\, \hat{S}_{\gamma}(\mathbf{r})\, |e'\rangle\langle e'|\, \hat{S}_{\delta}(\mathbf{r}')\, |e\rangle \delta(E_e - E_{e'} + \hbar\omega_{nn'}) \end{aligned} \tag{C.3}$$

where $\alpha, \beta, \gamma, \delta$ run over cartesian coordinates x, y, z and $\hbar\omega_{nn'} = E_n - E_{n'}$ is the resonance frequency. The population probability, $p(e)$ used to define the thermal averages $\langle A\rangle = \sum_e p(e)\langle e|\, A\, |e\rangle$, for the initial many body state $|e\rangle$ with energy E_e and particle number N_e,

$$p(e) = \frac{e^{-\frac{E_e - \mu N_e}{k_B T}}}{\sum_{e'} e^{-\frac{E_{e'} - \mu N_{e'}}{k_B T}}} . \tag{C.4}$$

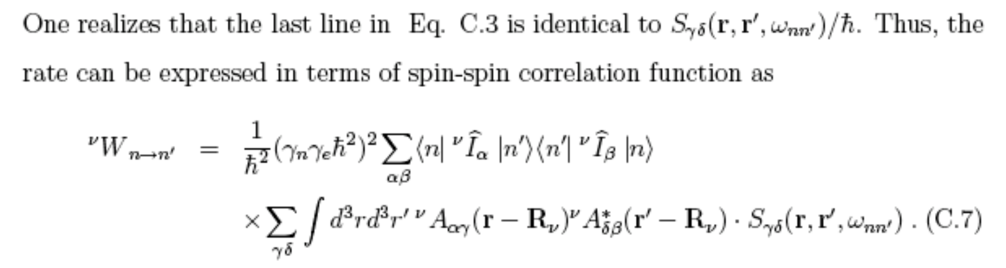
Spin Lattice Relaxation


We can now define the spin-spin correlation function as

$$S_{\alpha\beta}(\mathbf{r},\mathbf{r}',t) = \sum_e p(e)\langle e|\,\hat{S}_\alpha(\mathbf{r},t)\hat{S}_\beta(\mathbf{r}',0)\,|e\rangle\,,$$

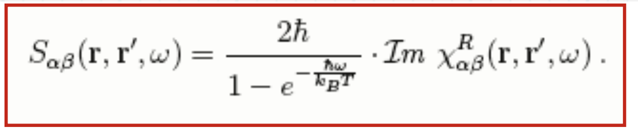
and its Fourier transform as

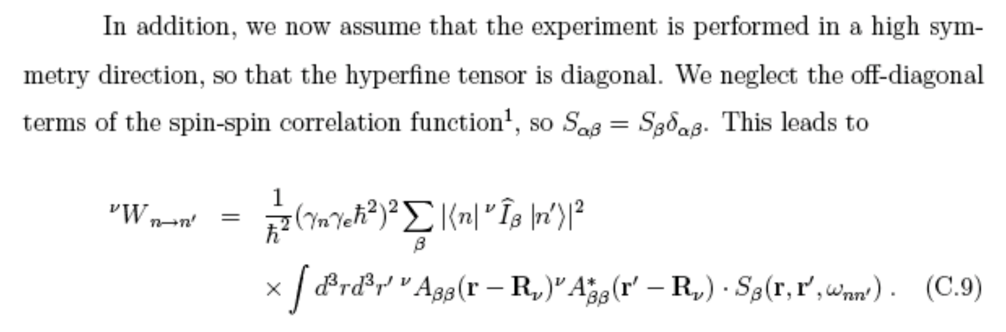
$$\boxed{S_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = 2\pi\hbar\sum_{ee'} p(e)\langle e|\,\hat{S}_\alpha(\mathbf{r})\,|e'\rangle\langle e'|\,\hat{S}_\beta(\mathbf{r}')\,|e\rangle\delta(E_e - E_{e'} + \hbar\omega)\,.}$$


One realizes that the last line in Eq. C.3 is identical to $S_{\gamma\delta}(\mathbf{r},\mathbf{r}',\omega_{nn'})/\hbar$. Thus, the rate can be expressed in terms of spin-spin correlation function as

$$\begin{aligned} {}^{\nu}W_{n\to n'} &= \frac{1}{\hbar^2}(\gamma_n\gamma_e\hbar^2)^2\sum_{\alpha\beta}\langle n|\,{}^{\nu}\hat{I}_\alpha\,|n'\rangle\langle n'|\,{}^{\nu}\hat{I}_\beta\,|n\rangle \\ &\quad\times\sum_{\gamma\delta}\int d^3r d^3r'\,{}^{\nu}A_{\alpha\gamma}(\mathbf{r}-\mathbf{R}_\nu)^{\nu}A^*_{\delta\beta}(\mathbf{r}'-\mathbf{R}_\nu)\cdot S_{\gamma\delta}(\mathbf{r},\mathbf{r}',\omega_{nn'})\,. \quad (C.7) \end{aligned}$$

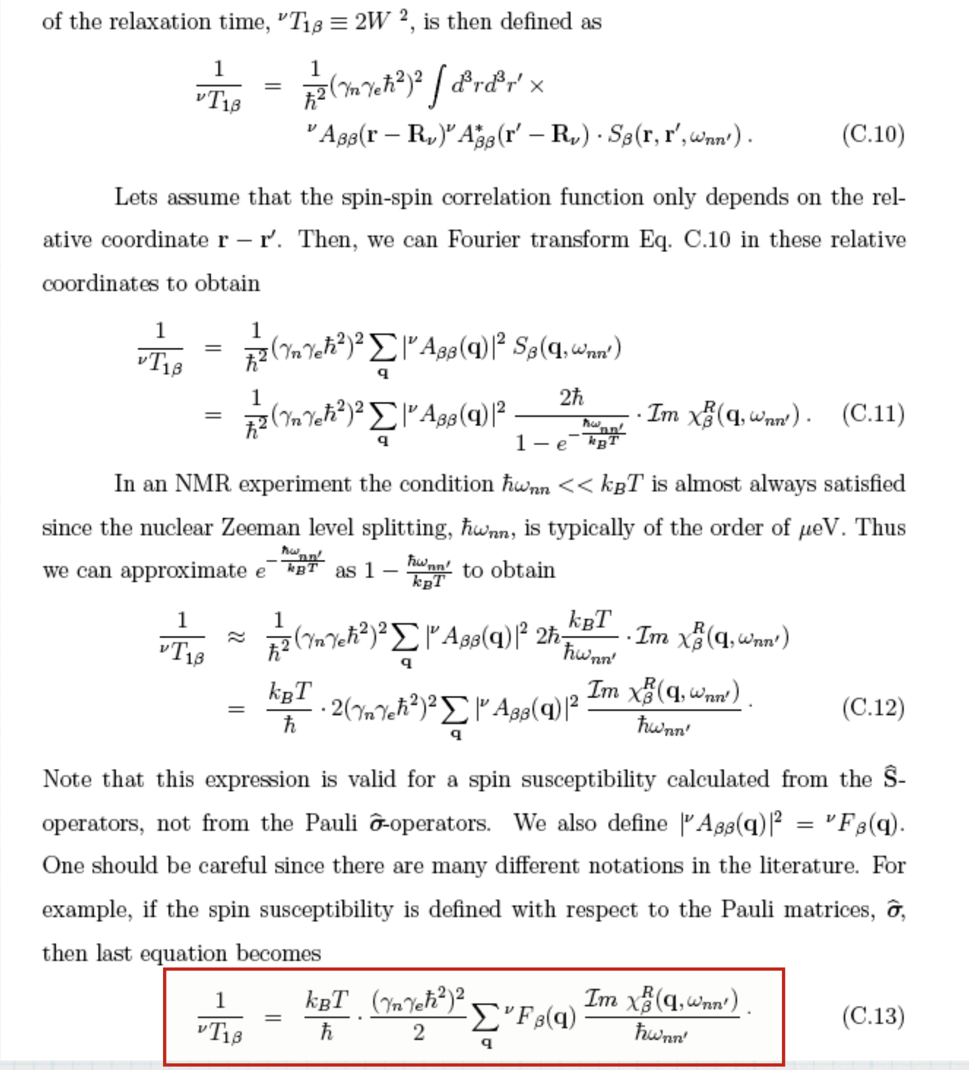
From the fluctuation-dissipation theorem =>


$$\boxed{S_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = \frac{2\hbar}{1-e^{-\frac{\hbar\omega}{k_BT}}}\cdot\mathcal{Im}\ \chi^R_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)\,.}$$


In addition, we now assume that the experiment is performed in a high symmetry direction, so that the hyperfine tensor is diagonal. We neglect the off-diagonal terms of the spin-spin correlation function[1], so $S_{\alpha\beta} = S_\beta\delta_{\alpha\beta}$. This leads to

$$\begin{aligned} {}^{\nu}W_{n\to n'} &= \frac{1}{\hbar^2}(\gamma_n\gamma_e\hbar^2)^2\sum_{\beta}|\langle n|\,{}^{\nu}\hat{I}_\beta\,|n'\rangle|^2 \\ &\quad\times\int d^3r d^3r'\,{}^{\nu}A_{\beta\beta}(\mathbf{r}-\mathbf{R}_\nu)^{\nu}A^*_{\beta\beta}(\mathbf{r}'-\mathbf{R}_\nu)\cdot S_\beta(\mathbf{r},\mathbf{r}',\omega_{nn'})\,. \quad (C.9) \end{aligned}$$

Spin Lattice Relaxation



of the relaxation time, ${}^{\nu}T_{1\beta} \equiv 2W^{\ 2}$, is then defined as

$$\frac{1}{{}^{\nu}T_{1\beta}} = \frac{1}{\hbar^2}(\gamma_n\gamma_e\hbar^2)^2 \int d^3r d^3r' \times$$
$${}^{\nu}A_{\beta\beta}(\mathbf{r}-\mathbf{R}_\nu){}^{\nu}A^*_{\beta\beta}(\mathbf{r}'-\mathbf{R}_\nu) \cdot S_\beta(\mathbf{r},\mathbf{r}',\omega_{nn'})\,. \tag{C.10}$$

Lets assume that the spin-spin correlation function only depends on the relative coordinate $\mathbf{r}-\mathbf{r}'$. Then, we can Fourier transform Eq. C.10 in these relative coordinates to obtain

$$\begin{aligned}\frac{1}{{}^{\nu}T_{1\beta}} &= \frac{1}{\hbar^2}(\gamma_n\gamma_e\hbar^2)^2 \sum_{\mathbf{q}} |{}^{\nu}A_{\beta\beta}(\mathbf{q})|^2\, S_\beta(\mathbf{q},\omega_{nn'}) \\ &= \frac{1}{\hbar^2}(\gamma_n\gamma_e\hbar^2)^2 \sum_{\mathbf{q}} |{}^{\nu}A_{\beta\beta}(\mathbf{q})|^2\, \frac{2\hbar}{1-e^{-\frac{\hbar\omega_{nn'}}{k_BT}}} \cdot \mathcal{I}m\ \chi^R_\beta(\mathbf{q},\omega_{nn'})\,. \end{aligned} \tag{C.11}$$

In an NMR experiment the condition $\hbar\omega_{nn} << k_BT$ is almost always satisfied since the nuclear Zeeman level splitting, $\hbar\omega_{nn}$, is typically of the order of μeV. Thus we can approximate $e^{-\frac{\hbar\omega_{nn'}}{k_BT}}$ as $1-\frac{\hbar\omega_{nn'}}{k_BT}$ to obtain

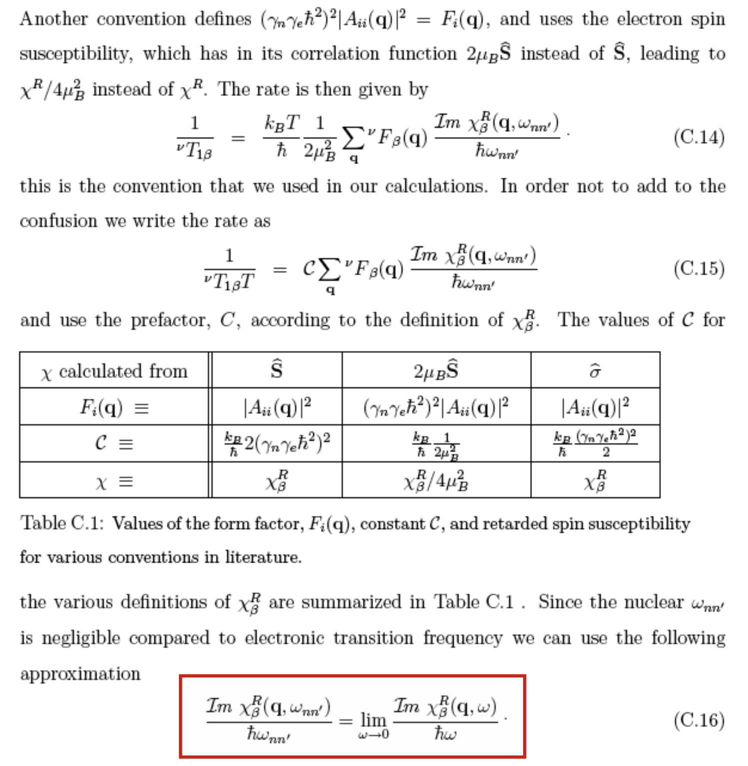
$$\begin{aligned}\frac{1}{{}^{\nu}T_{1\beta}} &\approx \frac{1}{\hbar^2}(\gamma_n\gamma_e\hbar^2)^2 \sum_{\mathbf{q}} |{}^{\nu}A_{\beta\beta}(\mathbf{q})|^2\, 2\hbar\frac{k_BT}{\hbar\omega_{nn'}} \cdot \mathcal{I}m\ \chi^R_\beta(\mathbf{q},\omega_{nn'}) \\ &= \frac{k_BT}{\hbar} \cdot 2(\gamma_n\gamma_e\hbar^2)^2 \sum_{\mathbf{q}} |{}^{\nu}A_{\beta\beta}(\mathbf{q})|^2\, \frac{\mathcal{I}m\ \chi^R_\beta(\mathbf{q},\omega_{nn'})}{\hbar\omega_{nn'}}\,. \end{aligned} \tag{C.12}$$

Note that this expression is valid for a spin susceptibility calculated from the $\hat{\mathbf{S}}$-operators, not from the Pauli $\hat{\boldsymbol{\sigma}}$-operators. We also define $|{}^{\nu}A_{\beta\beta}(\mathbf{q})|^2 = {}^{\nu}F_\beta(\mathbf{q})$. One should be careful since there are many different notations in the literature. For example, if the spin susceptibility is defined with respect to the Pauli matrices, $\hat{\boldsymbol{\sigma}}$, then last equation becomes

$$\boxed{\frac{1}{{}^{\nu}T_{1\beta}} = \frac{k_BT}{\hbar} \cdot \frac{(\gamma_n\gamma_e\hbar^2)^2}{2} \sum_{\mathbf{q}} {}^{\nu}F_\beta(\mathbf{q})\, \frac{\mathcal{I}m\ \chi^R_\beta(\mathbf{q},\omega_{nn'})}{\hbar\omega_{nn'}}\,.} \tag{C.13}$$

T. Moriya, J. Phys. Soc. Jpn **18**, 516 (1963).

Spin Lattice Relaxation



Another convention defines $(\gamma_n\gamma_e\hbar^2)^2|A_{ii}(\mathbf{q})|^2 = F_i(\mathbf{q})$, and uses the electron spin susceptibility, which has in its correlation function $2\mu_B\hat{\mathrm{S}}$ instead of $\hat{\mathrm{S}}$, leading to $\chi^R/4\mu_B^2$ instead of χ^R. The rate is then given by

$$\frac{1}{{}^{\nu}T_{1\beta}} = \frac{k_BT}{\hbar}\frac{1}{2\mu_B^2}\sum_{\mathbf{q}}{}^{\nu}F_\beta(\mathbf{q})\,\frac{\mathcal{I}m\ \chi_\beta^R(\mathbf{q},\omega_{nn'})}{\hbar\omega_{nn'}}\,. \tag{C.14}$$

this is the convention that we used in our calculations. In order not to add to the confusion we write the rate as

$$\frac{1}{{}^{\nu}T_{1\beta}T} = \mathcal{C}\sum_{\mathbf{q}}{}^{\nu}F_\beta(\mathbf{q})\,\frac{\mathcal{I}m\ \chi_\beta^R(\mathbf{q},\omega_{nn'})}{\hbar\omega_{nn'}} \tag{C.15}$$

and use the prefactor, C, according to the definition of χ_β^R. The values of $\mathcal{C}$ for

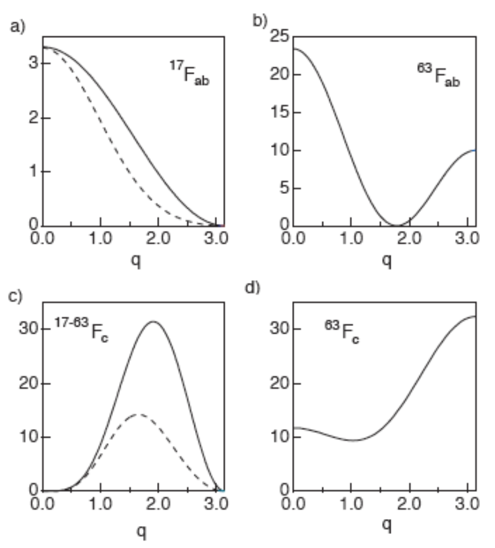
χ calculated from	$\hat{\mathrm{S}}$	$2\mu_B\hat{\mathrm{S}}$	$\hat{\sigma}$
$F_i(\mathbf{q})\ \equiv$	$\lvert A_{ii}(\mathbf{q})\rvert^2$	$(\gamma_n\gamma_e\hbar^2)^2\lvert A_{ii}(\mathbf{q})\rvert^2$	$\lvert A_{ii}(\mathbf{q})\rvert^2$
$\mathcal{C}\ \equiv$	$\frac{k_B}{\hbar}2(\gamma_n\gamma_e\hbar^2)^2$	$\frac{k_B}{\hbar}\frac{1}{2\mu_B^2}$	$\frac{k_B}{\hbar}\frac{(\gamma_n\gamma_e\hbar^2)^2}{2}$
$\chi\ \equiv$	χ_β^R	$\chi_\beta^R/4\mu_B^2$	χ_β^R

Table C.1: Values of the form factor, $F_i(\mathbf{q})$, constant $\mathcal{C}$, and retarded spin susceptibility for various conventions in literature.

the various definitions of χ_β^R are summarized in Table C.1 . Since the nuclear $\omega_{nn'}$ is negligible compared to electronic transition frequency we can use the following approximation

$$\boxed{\frac{\mathcal{I}m\ \chi_\beta^R(\mathbf{q},\omega_{nn'})}{\hbar\omega_{nn'}} = \lim_{\omega\to 0}\frac{\mathcal{I}m\ \chi_\beta^R(\mathbf{q},\omega)}{\hbar\omega}\,.} \tag{C.16}$$

A(q) and/or ***F(q)*** = form factors => partial ***q*** dependence

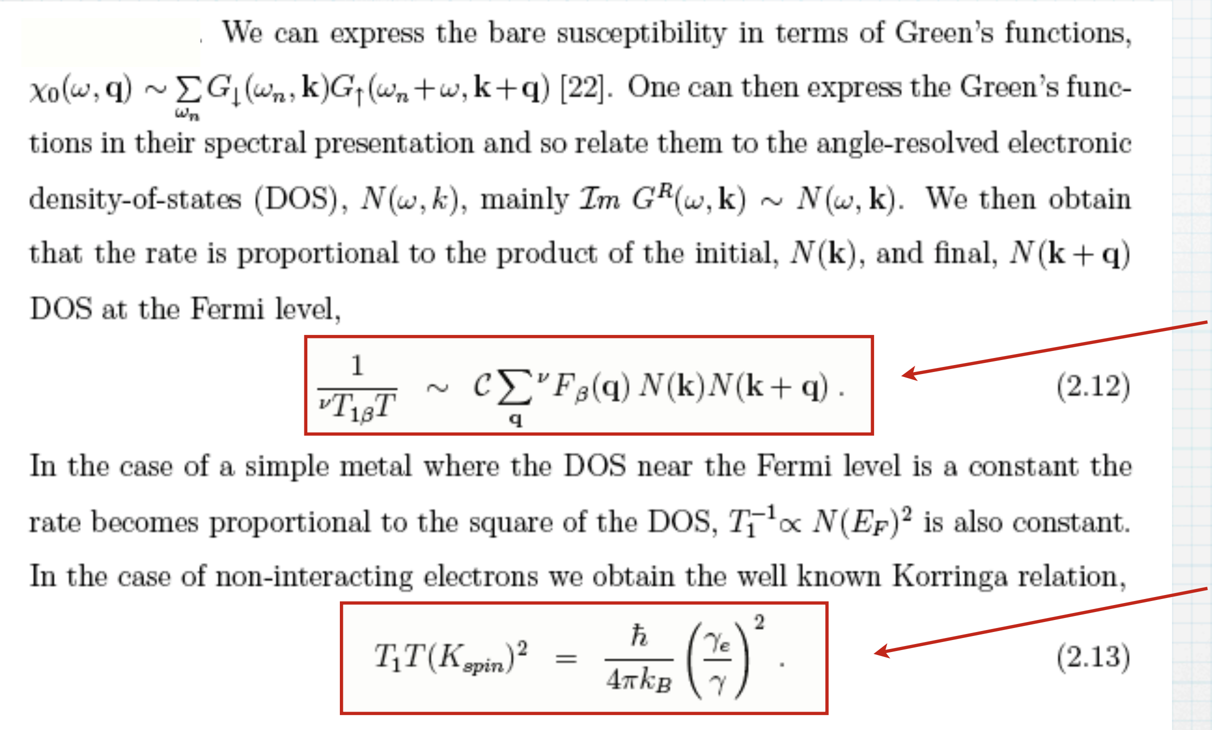


Shastry-Mila-Rice form factors for HTS, Physica C **157**, 561 (1989).

In general case - for non-diagonal hyperfine tensor =>

$$\boxed{\frac{1}{{}^{\nu}T_{1z}T} = C\sum_q\sum_{\beta=x,y,z}\left(A_{x\beta}^2(q) + A_{y\beta}^2(q)\right)\frac{\Im m\,\chi_{\beta\beta}(q,\omega_{nn'})}{\hbar\omega_{nn'}}}$$

Spin Lattice Relaxation



We can express the bare susceptibility in terms of Green's functions, $\chi_0(\omega,\mathbf{q}) \sim \sum_{\omega_n} G_\downarrow(\omega_n,\mathbf{k})G_\uparrow(\omega_n+\omega,\mathbf{k}+\mathbf{q})$ [22]. One can then express the Green's functions in their spectral presentation and so relate them to the angle-resolved electronic density-of-states (DOS), $N(\omega,k)$, mainly $\mathcal{I}m\ G^R(\omega,\mathbf{k}) \sim N(\omega,\mathbf{k})$. We then obtain that the rate is proportional to the product of the initial, $N(\mathbf{k})$, and final, $N(\mathbf{k}+\mathbf{q})$ DOS at the Fermi level,

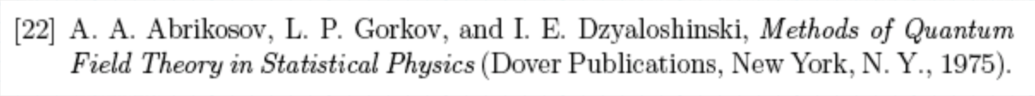
$$\boxed{\frac{1}{{}^{\nu}T_{1\beta}T} \sim \mathcal{C}\sum_{\mathbf{q}}{}^{\nu}F_\beta(\mathbf{q})\,N(\mathbf{k})N(\mathbf{k}+\mathbf{q})\ .} \qquad (2.12)$$

In the case of a simple metal where the DOS near the Fermi level is a constant the rate becomes proportional to the square of the DOS, $T_1^{-1} \propto N(E_F)^2$ is also constant. In the case of non-interacting electrons we obtain the well known Korringa relation,

$$\boxed{T_1T(K_{spin})^2 = \frac{\hbar}{4\pi k_B}\left(\frac{\gamma_e}{\gamma}\right)^2 .} \qquad (2.13)$$

$$\frac{1}{T_1} \propto N^2(E_F)$$

Korringa relation



[22] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover Publications, New York, N. Y., 1975).

To Remember

Static NMR Spectrum Measurements ⇒

Local Magnetic Field Probability Distribution

$$\omega_n = \gamma_n H_{loc} = \gamma_n \left(H_0 + \langle H_{hf} \rangle \right)$$

$$\langle H_{hf} \rangle = \sum_n -A_{n,k} \langle S_k \rangle$$

Width of an NMR spectrum ⇒ **Distribution of** $\langle \vec{S}_z(r) \rangle$

$$K(T) \propto \chi'(q = 0, \omega \rightarrow 0)$$

Shift of an NMR spectrum ⇒ **Magnetic susceptibility**

In metals:

$$K(T) \propto N(E_F)$$

$$T_1^{-1} \propto \chi''(q, \omega \rightarrow 0)$$

$$T_2^{-1} \propto \chi'(q, \omega \rightarrow 0)$$