The dipolar relaxation of multiple quantum coherences as a model for an investigation of decoherence processes in many-qubit clusters in multiple-quantum NMR

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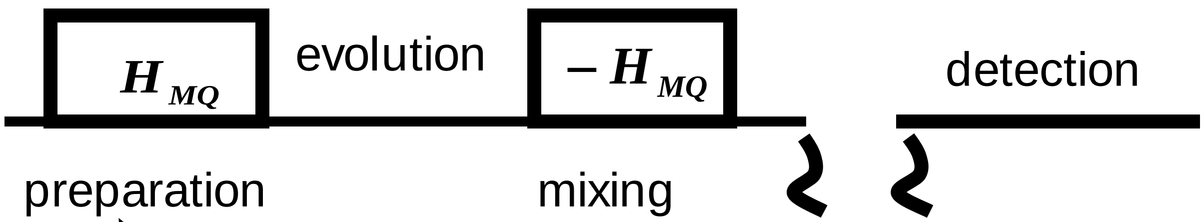
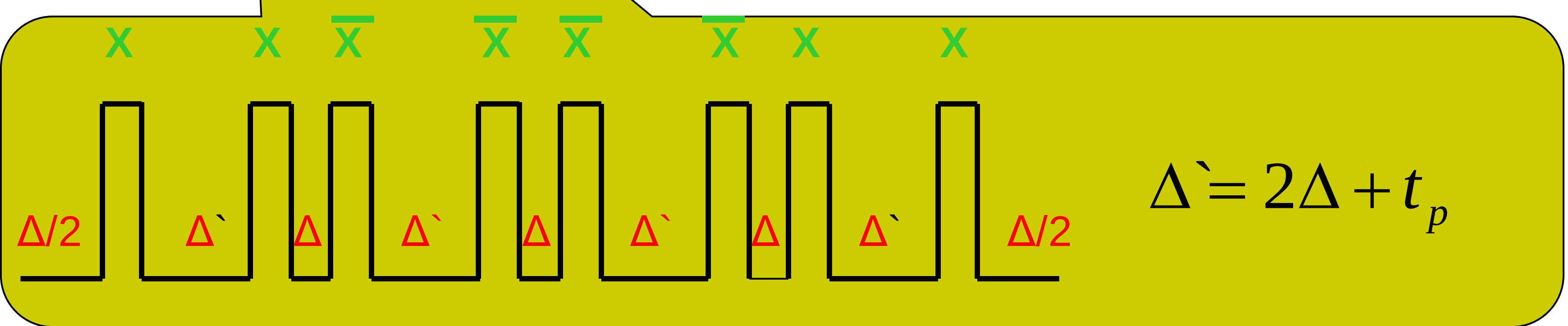
MQ NMR EXPERIMENT IN SOLIDS

$$\rho_2 \sim I_{1z} I_2^+ I_3^+ I_{4z} I_5^+ I_6^-$$



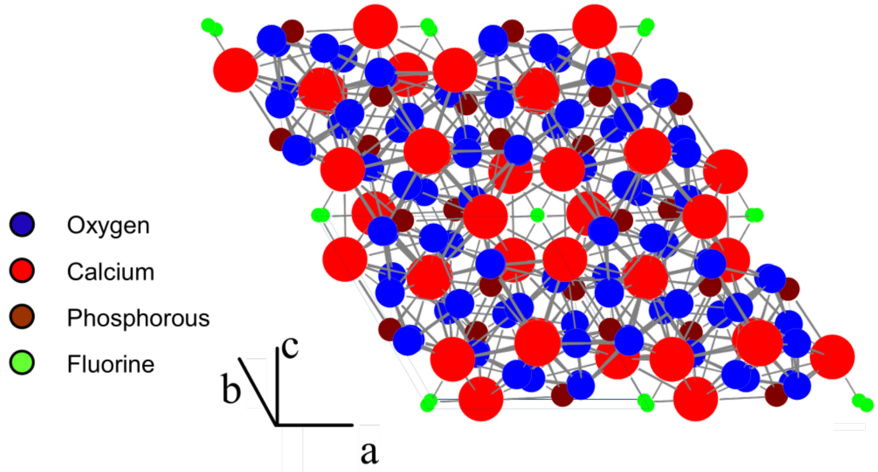
J.Baum, M.Munovitz, A.N.Garroway, A.Pines, J.Chem.Phys.**83**, 2015 (1985)



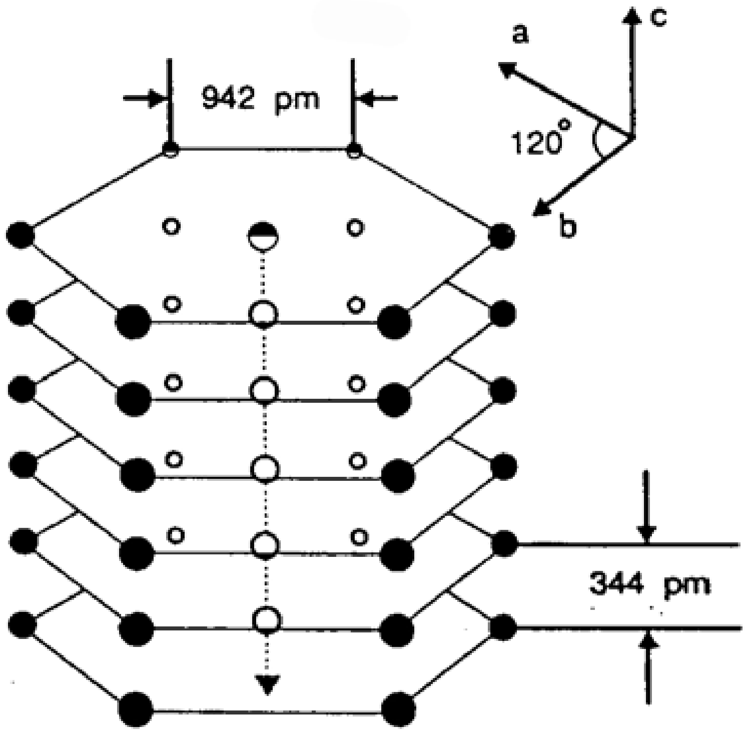
$$\Delta` = 2\Delta + t_p$$

One-dimensional spin chains

Fluorapatite – $Ca_5(PO_4)_3F$

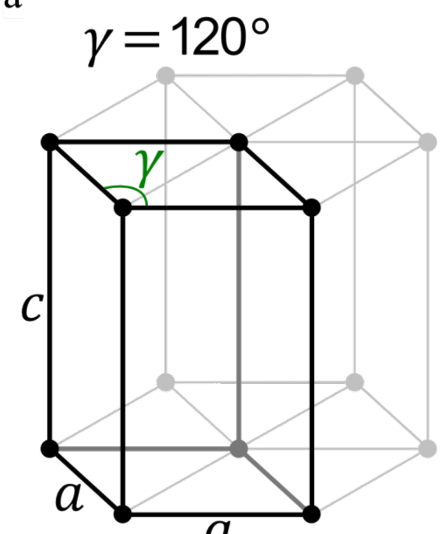


$Ca_5(PO_4)_3F$



a = 942 pm

c = 344 pm



EXACT SOLUTION FOR MQ NMR DYNAMICS ON THE PREPARATION PERIOD

$$\sigma(\tau) = \sigma_0(\tau) + \sigma_2(\tau) + \sigma_{-2}(\tau)$$

$$\sigma_0(\tau) = \frac{1}{2}\sum_k \cos[2D\tau \sin k](1 - a_k^+ a_k)$$

$$\sigma_2(\tau) = -\frac{1}{2}\sum_k \sin[2D\tau \sin k] a_k a_{-k}$$

$$\sigma_{-2}(\tau) = \frac{1}{2}\sum_k \sin[2D\tau \sin k] a_k^+ a_{-k}^+$$

$$N >> 1$$

$$k = \frac{2\pi n}{N}\left(n = -\frac{N}{2}, -\frac{N}{2}+1, \ldots \frac{N}{2}-1\right)$$

$$a_k = \frac{1}{\sqrt{N}}\sum_m \Psi_m e^{-ikm} \qquad a_k^+ = \frac{1}{\sqrt{N}}\sum_m \Psi_m^+ e^{ikm}$$

Jordan-Wigner transformation

$$\Psi_m = 2^{m-1} I_1^z I_2^z \ldots I_{m-1}^z I_m^+; \qquad \Psi_m^+ = 2^{m-1} I_1^z I_2^z \ldots I_{m-1}^z I_m^-$$

ZZ MODEL FOR RELAXATION OF MQ NMR COHERENCES

$$H_{dz} = \sum_{i<j} D_{ij}(3I_i^z I_j^z - \vec{I}_i \vec{I}_j) = \sum_{i<j} D_{ij}(2I_i^z I_j^z - I_i^x I_j^x - I_i^y I_j^y)$$

$$H_{zz} = 2\sum_{i<j} D_{ij} I_i^z I_j^z = \sum_{i \neq j} D_{ij} I_i^z I_j^z$$

$$F_0(\tau, t) = \frac{\mathrm{Tr}\left[e^{-iH_{zz}t}\sigma_0(t)e^{iH_{zz}t}\sigma_0(t)\right]}{\mathrm{Tr}(I_z^2)}$$

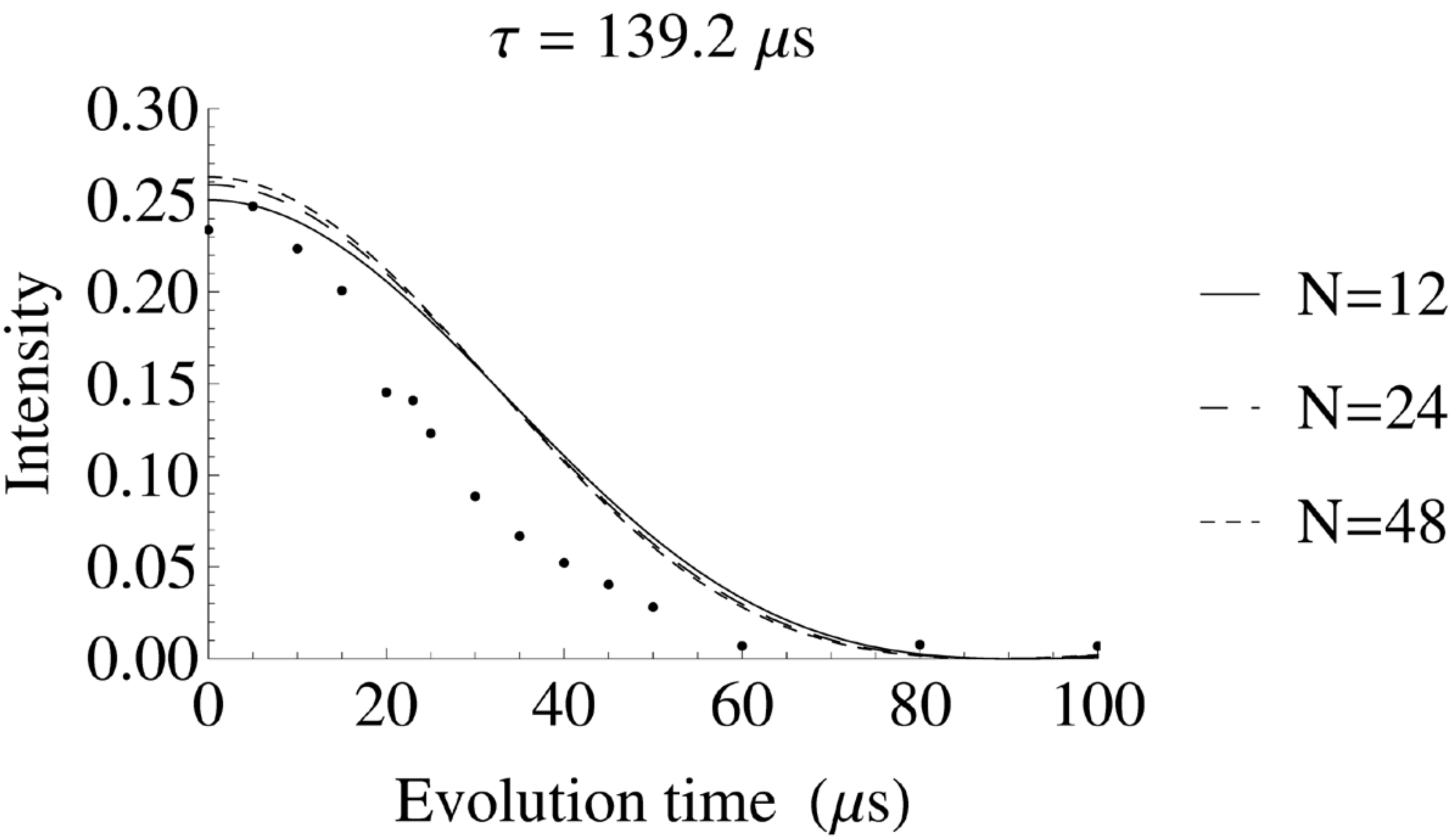
$$F_{\pm 2}(\tau, t) = \frac{\mathrm{Tr}\left[e^{-iH_{zz}t}\sigma_2(t)e^{iH_{zz}t}\sigma_{-2}(t)\right]}{\mathrm{Tr}(I_z^2)}$$

RELAXATION OF THE MQ NMR COHERENCES OF THE SECOND ORDER

$$F_2(\tau,t) = -\frac{4}{N(N+1)^2} \sum_{\substack{l=1,3,\ldots N-1 \\ l'=2,4,\ldots N}} \prod_{\substack{m \\ m\neq l, m\neq l'}} \cos[(D_{ml}+D_{ml'})t] \cdot \left(\sum_k \sin kl \sin kl' e^{-2iD\tau\cos k} \right)^2$$

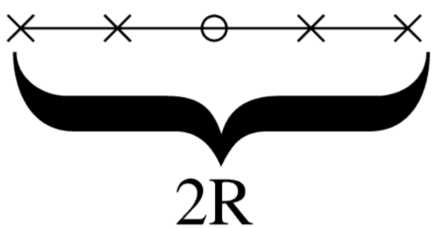
$$M_2(\tau) = -\frac{1}{G_2(\tau)} \left. \frac{d^2 F_2(\tau,t)}{dt^2} \right|_{t=0}$$

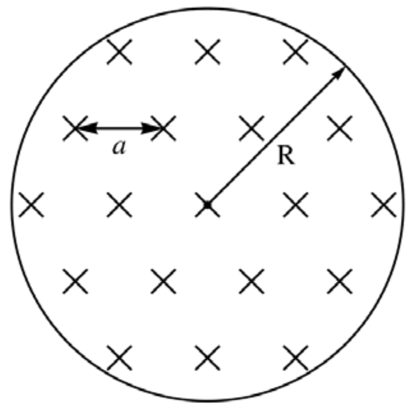
$$S(t) = e^{-\frac{1}{2} M_2(\tau) t^2} \qquad t_e = \sqrt{\frac{2}{M_2(\tau)}}$$

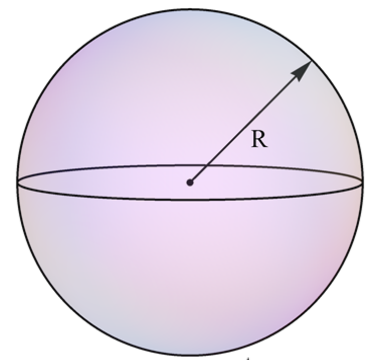


The experimental and theoretical intensities of the MQ NMR coherence of the second order on the evolution period *t* for the duration of the preparation period τ=139.2 μs. The lines are the theoretical plots for various N.

$$\omega_d \tau = 1 \qquad \omega_d = \frac{\gamma^2 \hbar}{R^3} \qquad V_d = \frac{\pi^{D/2} R^D}{\Gamma\left(D/2+1\right)}$$

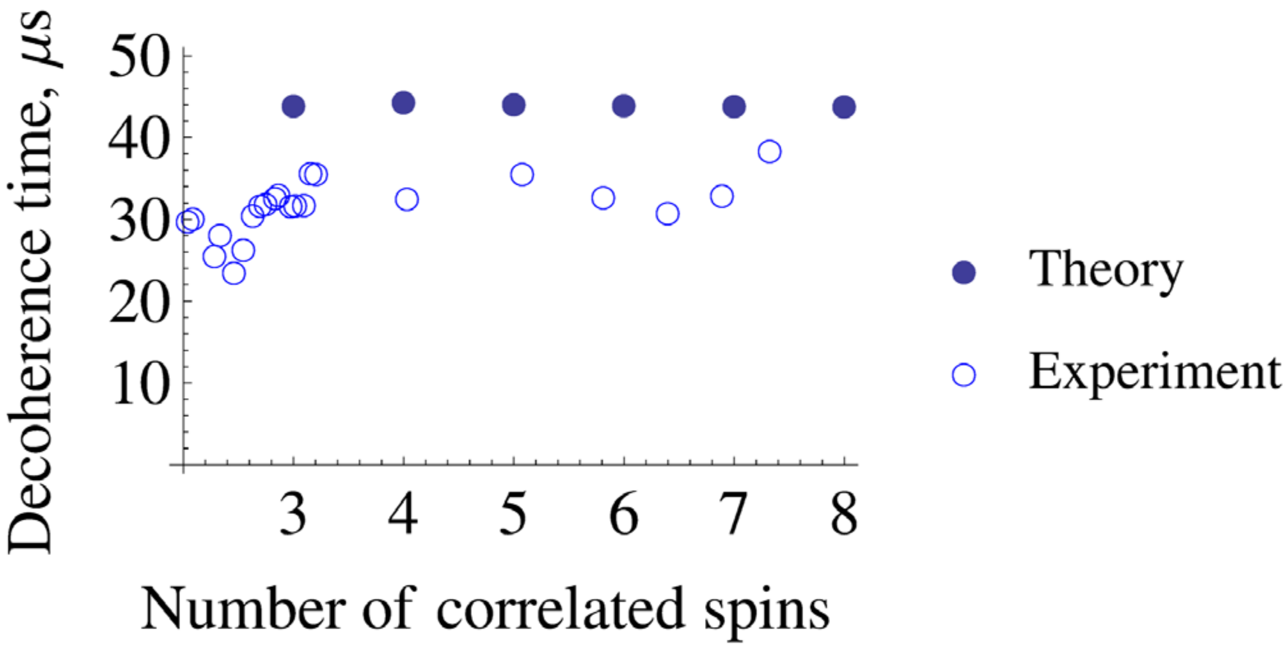






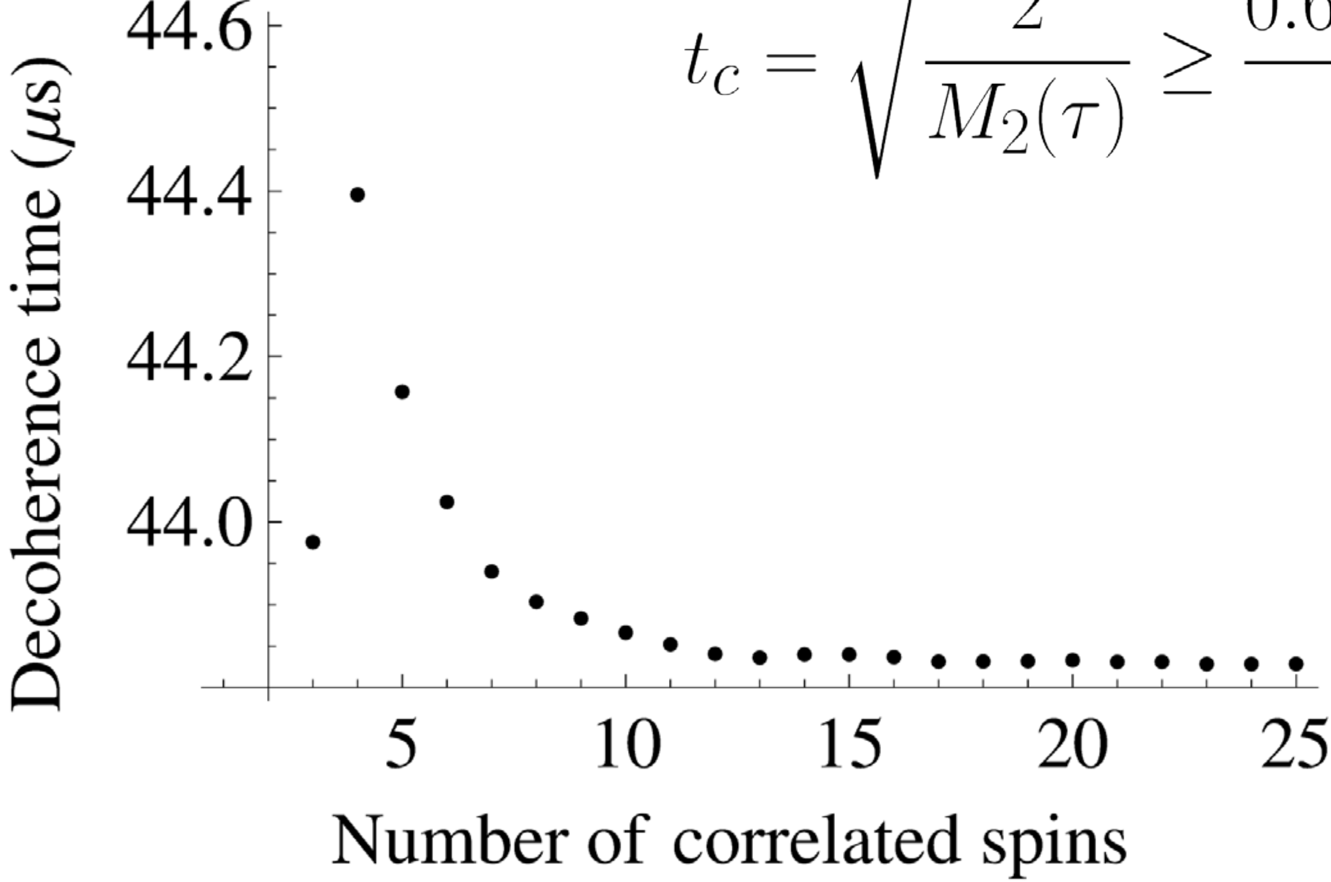
$$V_1 = 2R \qquad V_2 = \pi R^2 \qquad V_3 = \frac{4}{3}\pi R^3$$

$$N = \frac{V_d}{a^D} = \frac{\pi^{D/2} R^D}{a^D \Gamma(D/2+1)} = \underbrace{\frac{\pi^{D/2}\left(\gamma^2\hbar\right)^{D/3}}{a^D \Gamma(D/2+1)}}_{k} \tau^{D/3}$$



The experimental and theoretical times of dipolar relaxation of the MQ NMR coherence of the second order versus the cluster size.

$$t_c = \sqrt{\frac{2}{M_2(\tau)}} \geq \frac{0.61595}{D}$$



The theoretical times of dipolar relaxation of the MQ NMR coherence of the second order versus the cluster size, for larger cluster sizes.

Conclusions

- A theory of the dipolar relaxation of multiple quantum NMR coherences is developed for one dimensional spin systems.
- It is shown that relaxation of the multiple quantum NMR coherence of the second order can be considered as a model for investigations of decoherence processes
- The decoherence (relaxation) time of the MQ NMR coherence of the second order decreases only slowly when the cluster size increased in our model.
- A lower bound of decoherence time does not depend on the number of qubits in correlated clusters.

Thank You for attention !

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