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Effect of intramolecular interaction on time growth of second moment of multiple quantum NMR in solids

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Abstract. The time dependence of the NMR multiple quantum spectrum in solids containing methyl groups is investigated. We studied both of types of the nuclear spin systems: namely linking by secular part of the mutual dipole-dipole interaction and linking by effective double quantum Hamiltonian. It is revealed for the first type of systems the rate with the time of the growing up of the second moment when intramolecular interaction is present becomes less in compare with situation when a strong intramolecular interaction is absent. On the contrary for the second type of Hamiltonian the above rate increases.

1. Introduction

Multiple quantum (MQ) NMR spectroscopy of solids [1-6] is unique and very suitable method of studying multiple spin correlation dynamics involving thousands spins [6]. In principle the field of applications of MQ spectroscopy extremely vast: from the medicine to superconductivity [3]. In particular, MQ spectroscopy presents the high-usage tool for the special study: what a type of particle distribution does explorer sees: uniform distribution or with clusters one (including the analysis of the type and structure of cluster)? Frequently this study provides by the means of exploring of the time dependence of the average number of correlated spins. Seems it has been done for the first time in ref. [2]. The experimental method evolved in ref. [2] has been working out for primarily using in molecular crystals and the theory developed there based on supposition that intra- and intermolecular dipole-dipole interactions are reciprocally independent. At the same time in conventional NMR for crystallohydrates the “principle 5/6 effect” is well known [7]. For example the width of Pake’s doublet component stipulated by intermolecular interaction decreases by 5/6 factor.

In this paper we theoretically investigate the influence of a strong intramolecular interaction at the process of growing correlation.

2. Brief remarks on MQ NMR spectroscopy

The intensity of multiple-quantum coherences observed experimentally is determined by the time correlation function [1-6]:

$$\Gamma_{\varphi\alpha}(t, \tau) = Sp\{U^+(\tau)U_{\varphi\alpha}U(t)S_{\alpha}U^+(t)U_{\varphi\alpha}^+U(\tau)S_{\alpha}\} / Sp\{S_{\alpha}^2\}. \quad (1)$$

Here we have, $U_{\varphi\alpha} = \exp(i\varphi S_{\alpha})$ is the rotation operator by an angle φ about the z axis (if $\alpha=z$) or x axis (if $\alpha=x$); $S_{\alpha} = \sum_i S_{\alpha i}$, where S_{α} is the α component of the total spin of a nuclear spin system; $S_{\alpha i}$ is α – component of the spin $S=1/2$ vector operator in the lattice site “ i ” and $U(t)$ is the evolution operator with the secular part of the dipole-dipole interaction Hamiltonian H_d [8]

$$H_d = \sum_{i \neq j} b_{ij} S_{zi} S_{zj} + \sum_{i \neq j} a_{ij} S_{+i} S_{-j} = H_{zz} + H_{ff}, \quad (2)$$

or the evolution operator with this interaction but transformed by certain radiofrequency pulses into a new nonsecular effective Hamiltonian H_{eff} with double quantum interaction [1-6]:

$$H_{eff} = - \sum_{i < j} c_{ij} (S_{+i} S_{+j} + S_{-i} S_{-j}). \quad (3)$$

Here we have $b_{ij} = \gamma^2 \hbar (1 - 3 \cos^2 \theta_{ij}) / 2r_{ij}^3$, $a_{ij} = -b_{ij} / 2$, $c_{ij} = b_{ij} / 2$, \vec{r}_{ij} - is the vector connecting spins i and j , θ_{ij} is the angle formed by vector \vec{r}_{ij} and the external constant magnetic field, $S_{\pm} = S_x \pm iS_y$. For the use in the microscopic theory, we introduced the designation τ for the evolution with “time reversal.” Experimental conditions $t = \tau$ will be fulfilled in the final equations.

As the consequence of the generalized form of the equation (1) we can describe as ordinary experiment with the Hamiltonian (3) and with rotation by angle φ around z-axis (let’s name this one by z-basis [1]), as also the new type of experiment introduced recently [4] which contains rotation by angle φ around x-axis (let’s name that one by x-basis). It is possible in the x-basis to observe multiple spin correlations appeared under influence ordinary secular dipole-dipole interaction in the process of the free induction decay (FID) [5].

We shall have the intensity of n order by Fourier transforming equation (1) (to say by other words by the using of the integration on variable $n\varphi$). Based on the simplest statistical model [1], a Gaussian shape is usually assumed in the experiment for the distribution of coherences of different orders in the MQ spectrum:

$$g_n(\tau) \sim \exp(-n^2/N(\tau)). \quad (4)$$

The variance of the distribution in this model ($N(\tau)/2$) is determined by the number of spins $N(\tau)$ among which dynamical correlation due to the spin-spin interaction is settled during the preparation time τ . This number, called the number of correlated spins or the effective cluster size, grows as the preparation time increases.

Whether the spin system of many spins consists of groups with closed spins (e.g. molecules) it was proposed to describe MQ intensities by the sum of two independent Gaussian distributions [2]:

$$g_n(\tau) = m_c \exp(-n^2/N_c(\tau)) + m_2 \exp(-n^2/N_2(\tau)). \quad (5)$$

Here $N_c(\tau)$ describes the increasing intramolecular correlations while $N_2(\tau)$ describes the intermolecular ones. The increasing of $N_c(\tau)$ restricts by the number of spins in molecule whereas $N_2(\tau)$ has no restriction.

3. Second moment of the intensity distribution for coherences of different orders in a multiple-quantum spectrum

As it has been shown in [9], the principle attribute of a number of correlated spins (quite the same is effective cluster size) what can be worked even for arbitrary form of a distribution function, is the second moment of the intensities of multiple quantum coherences of a different orders $\langle n^2(\tau) \rangle$. For example, for Gaussian distribution this moment really coincides with the variance $N(\tau)/2$ in eq. (4) and there is no necessity to execute the Fourier- transformation because as it was shown in [9] actually anybody has the relation:

$$\langle n^2(t) \rangle = -d^2 \Gamma_{\varphi\alpha}(t, t) / d\varphi^2 \Big|_{\varphi=0} = -Sp\{[S_{\alpha}, S_{\alpha}(t)]^2\} / Sp\{S_x^2\}, \quad (6)$$

$$S_{\alpha}(t) = U(t) S_{\alpha} U^+(t) \quad (\alpha = z, x).$$

Let us generalize this formula for situation $t \neq \tau$ (if $t = \tau$, $\langle\langle n^2(t, t) \rangle\rangle = \langle n^2(t, t) \rangle = \langle n^2(t) \rangle$)

$$\begin{aligned} & \langle\langle n^2(t, \tau) \rangle\rangle = \langle n^2(t, \tau) \rangle / 2 + \langle n^2(\tau, t) \rangle / 2; \\ \langle n^2(t, \tau) \rangle & = 2 \sum_{i,j,f,q} \{Sp\{S_{\alpha_j} S_{\alpha_f} S_{\alpha_i}(t) S_{\alpha_q}(\tau)\} / Sp\{S_x^2\} - Sp\{S_{\alpha_j} S_{\alpha_i}(t) S_{\alpha_f} S_{\alpha_q}(\tau)\} / Sp\{S_x^2\}\}. \end{aligned} \quad (7)$$

Now we can rewrite the second summand from (7) in a form

$$\begin{aligned} Sp\{S_{\alpha_j} (4S_{\alpha_f} S_{\alpha_f}) S_{\alpha_i}(t) S_{\alpha_f} S_{\alpha_q}(\tau)\} / Sp\{S_x^2\} & = Sp\{S_{\alpha_j} S_{\alpha_f} \sigma_{\alpha_f} S_{\alpha_i}(t) \sigma_{\alpha_f} S_{\alpha_q}(\tau)\} / Sp\{S_x^2\} = \\ & = Sp\{S_{\alpha_j} S_{\alpha_f} \overline{S_{\alpha_i}(t)}^{(f)} S_{\alpha_q}(\tau)\} / Sp\{S_x^2\}, \end{aligned}$$

because of $4S_{\alpha_f} S_{\alpha_f} = 1$ for $S = 1/2$. The notation $\overline{S_{\alpha_i}(t)}^{(f)}$ means that in the time evolution operator we are using the Hamiltonian $\sigma_{\alpha_f} H \sigma_{\alpha_f}$ with the inverted spin f . So from (7) we get:

$$\langle n^2(t, \tau) \rangle = \sum_{i,j,f,q} Sp\{S_{\alpha_j} S_{\alpha_f} \{S_{\alpha_i}(t) - \overline{S_{\alpha_i}(t)}^{(f)}\} S_{\alpha_q}(\tau)\} / Sp\{S_x^2\}, \quad (\alpha = z, x). \quad (8)$$

Whether we are starting to find the solution of our problem via expanding into series on the powers of a time the correlation function from (8), we shall see (as it has been shown in [10]), that the principle contributions into the second moment defined by equation (8) is carrying out by diagrams consisting of the chains with double connections starting with the lattice site i and ending with the site f . For the both of studying of interactions if we want to construct the require chains, we have to exploit two positions for the chain links (sections) with j and k sites (see figure 1):

1. Sequentially by the chain (see figure 1a)
2. Transversal relatively the chain (see figure 1b)

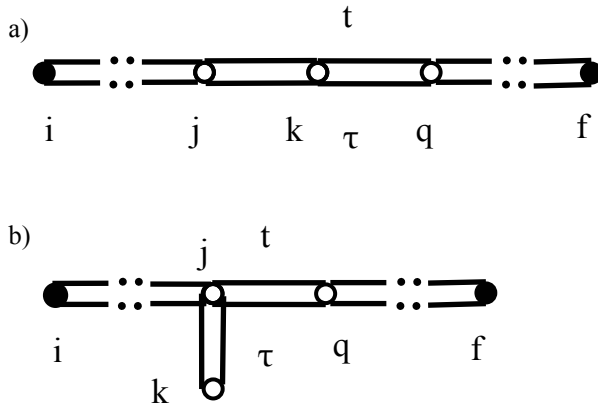


Figure 1. The location of the chain links at the lattice. The lattice points notates as i, j, k, q, f , correspond to the diagram vertexes and the lines at the figure present the interaction between spins occupied of these lattice points.

For the both of the above positions of the chain links (sections of the chain) (see figure 1) the diagrams with fixing locations of commutators and spin operators in the process of developing with the time are shown at figure 2 via chain with five links as example. Because of diagram construction laws we have to take one connection from the $\overline{S_{\alpha_i}(t)}^{(f)}$ operator and the second one from the $S_{\alpha_q}(\tau)$ ($q=i$) operator and we have to do so for the every double connection. As the consequence of integration by every of different variables t_m (τ_m) with the limits from 0 up to t_{m-1} (or τ_{m-1}) every skeleton diagram having the form of the chain with m links is giving us the time dependence as $(t^2 \tau^2)^m$. We can take into account the interaction of spins belongs to chain with the rest of spins of a crystal by the dressing of the diagram lines. By the last process the decay with the time of the lines appears having quite sophisticated dependence. We have done the estimation of that dependence in [10]. In what follows we shall estimate the changing the account of the mentioned links of chain if the strong intramolecular interaction is taking place.

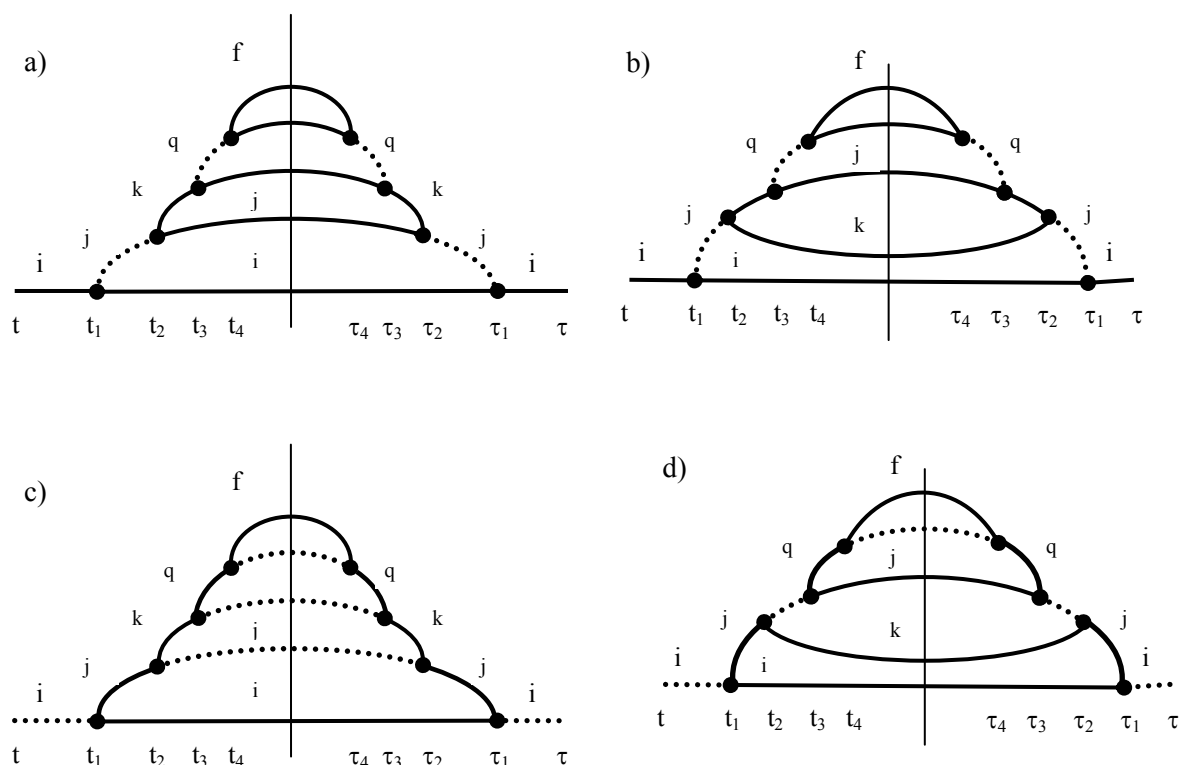


Figure 2. The examples of the diagram for the chains contain 5 spins. At the figures a) and b) it is shown the evolution with H_d interaction while figures c) and d) shows the occasion with H_{eff} interaction. The vertical line means the border between the forward and reversed evolution with the time (see (1) and (8)). The vertexes of diagram correspond to the acts of interaction between spins (actually it means the commutation of spin operator with the acting Hamiltonian) at the noted moments of time. Namely: t_m are on the left from the line mentioned above and τ_m are on the right from that line. Lines of the diagrams correspond to the $S_{\pm p}$ spin components (solid lines) or S_{zp} (dotted lines) at the indicated sites i, j, f, k etc.

4. Effect of intramolecular secular dipole-dipole interaction in methyl groups on the time growth of the second moment

Let us divide the Hamiltonian (2) on two divisions with the first of one reflects intramolecular interaction $H_M^{(d)}$ while the second one describes intermolecular interaction $H_{MM}^{(d)}$. Let us also mark that methyl groups usually expose oneself to rapid rotations about the axis of the third order. As a typical example we can point out at the Hexamethylbenzene [11] the MQ spectra of which were substantially studied in articles [1,2]. We shall describe the average intramolecular interaction by only one constant b_1 while the average intermolecular interaction depends only of the reference number of the methyl group. So we have:

$$H_M^{(d)} = \sum_i b_{i1} (S_{zi1}S_{zi2} + S_{zi1}S_{zi3} + S_{zi3}S_{zi2}), \quad (9)$$

$$H_{MM}^{(d)} = \sum_{i \neq j} b_{ij} S_{zi} S_{zj} + \sum_{i \neq j} a_{ij} S_{+i} S_{-j} = H_{zz} + H_{ff}, \quad (10)$$

$$S_{zi} = S_{zi1} + S_{zi2} + S_{zi3}, \quad S_{\pm i} = S_{\pm i1} + S_{\pm i2} + S_{\pm i3}.$$

Because of the permutation proton spins symmetry in the methyl group, anybody has to use only zz-part of intramolecular interaction $H_M^{(d)}$ as far as the exchange (or scalar) part of that interaction becomes unobservable [8]. The flip-flop processes between spins situated in a different methyl groups is getting registered only if the frequencies in the local field of the both of flipping spins coincide reciprocally. As the spectrum of alone methyl group is a triplet with frequencies $-b_1, 0, b_1$ and with the respective intensities $\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$, for the probabilities of frequencies coincidence (if we suppose $b_{11}=b_{21}$) we can find

$$\left(\frac{1}{4}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{4}\right)^2 = \frac{3}{8}.$$

The calculated constant fixes the reduction of the square of flip-flop interaction between two different methyl groups: $A_1^2 = 3A^2/8$. Here $A^2 = 3\sum_j a_{ij}^2$ is the origin constant corresponds to situation $b_1=0$.

Whether $b_{11}\neq b_{21}$ it can be found $A_1^2 = A^2/4$.

For the sake of simplicity we shall assuming in what follows below that all of a methyl groups has the same intramolecular interaction described by only one constant b_1 for the secular dipole-dipole interaction (see equation (9)).

If the secular dipole-dipole interaction produces the above described chains on diagrams, which combines the inverse spin with the number of $\{f\}$ with the central (fixing) spin having the number of i , the chains has to be built with the help of flip-flop - processes connecting by zz -interaction (see figures 2 a and 2 b). Their contributions into skeleton diagrams are $2A^2B^2$ for the both of types chain links shown at figure 1 and these contributions has to be just sum. As it was revealed in [10] by summing the entire long chains the dependence of the second moment of MQ spectrum on a time takes a form

$$\langle n^2(t) \rangle_d \sim \exp(a_d t) \frac{-b \pm \sqrt{b^2 - 4ac}}{2a},$$

where we got $a_d = 2(A^2 B \sqrt{\pi})^{1/3}$. Whether to take into account the flip-flop processes rate reduction, the exponent decreasing comes to $\sqrt[3]{\frac{8}{3}} \approx 1,39$ times if $b_1^2 \gg M_{2MM}$ in compare with situation $b_1 = 0$ and it becomes

$$a_{Md} = (3A^2 B \sqrt{\pi})^{1/3}. \quad (11)$$

At last we should mark that $B^2 = 3\sum_j b_{ij}^2$ and $A^2 = 3\sum_j a_{ij}^2$. Also because of in the intermolecular contribution into the second moment of the conventional NMR spectrum one has to sum only by protons of the different methyl groups CH_3 , (where 3 means the number of protons in one group) it can be got for the mentioned contribution:

$$M_{2MM} = 9 \cdot 3 \sum_j b_{ij}^2.$$

5. Effect of intramolecular interaction describes double quantum effective Hamiltonian in methyl groups on the time growth of the second moment

As in the previous section let us divide the Hamiltonian (3) on two divisions with the first of one reflects intramolecular interaction $H_M^{(eff)}$ while the second one describes intermolecular interaction

$H_{MM}^{(eff)}$:

$$H_M^{(eff)} = -\sum_i c_{i1}(S_{+i1}S_{+i2} + S_{+i1}S_{+i3} + S_{+i3}S_{+i2}) - \sum_i c_{i1}(S_{-i1}S_{-i2} + S_{-i1}S_{-i3} + S_{-i3}S_{-i2}), \quad (12)$$

$$H_{MM}^{(eff)} = -\sum_{i<j} c_{ij}(S_{+i}S_{+j} + S_{-i}S_{-j}) \leq, \quad (13)$$

As it was found in [12] the eigenvectors of isolated methyl group are:

$$\Psi_{\pm} = \pm \frac{1}{\sqrt{2}}|++\rangle + \frac{1}{\sqrt{6}}(|+-\rangle + |-+\rangle + |--\rangle), \quad (14)$$

$$\varphi_1 = \frac{1}{\sqrt{2}}|+-\rangle - \frac{1}{\sqrt{2}}|--\rangle, \quad \varphi_2 = \frac{2}{\sqrt{6}}|+-\rangle - \frac{1}{\sqrt{6}}|--\rangle - \frac{1}{\sqrt{6}}|-+\rangle. \quad (15)$$

with eigenvalues: $\mp\sqrt{3}c_1$, 0, 0 respectively. Four other functions $\bar{\Psi}_{\pm}$, $\bar{\varphi}_1$ and $\bar{\varphi}_2$ one can get by inversion of all spins. For eigenvectors of a single spin operator S_z in above formula notations $|\pm\rangle$ been used for spin projections $\pm 1/2$. Functions Ψ are symmetrical relatives to spin permutations while φ are antisymmetrical ones. So matrices of symmetric operators sums $S_{zi} = S_{zi1} + S_{zi2} + S_{zi3}$, $S_{\pm i} = S_{\pm i1} + S_{\pm i2} + S_{\pm i3}$ become as a block forms:

$$S_z = \begin{pmatrix} S_{z,\Psi} & 0 \\ 0 & S_{z,\varphi} \end{pmatrix}, \quad S_{\pm} = \begin{pmatrix} S_{\pm,\Psi} & 0 \\ 0 & S_{\pm,\varphi} \end{pmatrix}. \quad (16)$$

Here 4x4 matrices been introduced.

Let us construct four effective spins $1/2$ with the help of basic functions set: $(\Psi_+, \bar{\Psi}_+)$, $(\Psi_-, \bar{\Psi}_-)$, $(\bar{\varphi}_1, \varphi_1)$ and $(\bar{\varphi}_2, \varphi_2)$. By the means of the Pauli matrices of these spins we can rewrite three matrices introduced above

$$S_{z,\varphi} = \begin{pmatrix} \sigma_1^z/2 & 0 \\ 0 & \sigma_2^z/2 \end{pmatrix}, \quad S_{\pm,\varphi} = \begin{pmatrix} -\sigma_1^{\pm} & 0 \\ 0 & -\sigma_2^{\pm} \end{pmatrix}, \quad (17)$$

and also the remaining of third other matrices secular parts in respect to strong intramolecular interaction.

$$S_{z,(sec)\Psi} = \begin{pmatrix} \sigma_{(+)}^z/2 & 0 \\ 0 & \sigma_{(-)}^z/2 \end{pmatrix}, \quad S_{\pm,(sec)\Psi} = \begin{pmatrix} \sigma_{(+)}^{\pm} + \sqrt{3}\sigma_{(+)}^{\pm} & 0 \\ 0 & \sigma_{(-)}^{\pm} - \sqrt{3}\sigma_{(-)}^{\pm} \end{pmatrix}. \quad (18)$$

To execute the calculations one needs to put (17) and (18) into (13). By exploiting of the well known features of the Pauli matrixes, commutators, what corresponds to vertexes of diagrams in new representation with $H_{MM}^{(eff)}$ operator can be found and also the traces of matrices for every diagram can be computed.

For the systems with effective Hamiltonian (3) the simplest chain between origin spin and “inverse” one “ f ” (see figures 1a and 2c) has to be constructed by the alternation of $c_{ij}S_{+i}S_{+j}$ and $c_{ij}S_{-i}S_{-j}$ interactions. The choice of the first connection linking to S_{zi} defines of all the other ones. As we have only two possibilities e.g.: $(+-+--+ \dots$ or $-+--+--+ \dots)$ the combinatorial factor equal to number 2. Operators remain when commuting procedure is over has to be couple in the centre of

diagram and the results of traces computations of a different methyl groups has to be mutually multiplied. So we get that if a new section adds to a simplest chain one has to add a new factor $C_s^2 = 2,5 \sum_j c_{ij}^2$ instead of $C^2 = 3 \sum_j c_{ij}^2$ what is adequate when intramolecular interaction is absent. So the contribution diminishes by the factor 5/6.

At the same time we can build the chain by some other way (see figure 1b and figure 2d). Really in section number j of the chain we can links $c_{ij}S_{+i}S_{+j}$ or $c_{ij}S_{-i}S_{-j}$ connections to S_{-j} operator and to begin new simple chain. Via this reason we are getting two novel possibilities. So by this way and in compliance with our calculations, if the strong intramolecular interaction is taking place and when all operations has to be done in the representation defined by functions from (14)-(15) the contribution from the diagram grows up by a factor $p = 3,4$ in comparing with the situation when intramolecular interaction is absent. In general situation for complete chain consisting of q simple parts the weight factor has to be taken as $(2p)^q$. If one needs in all weights N_{pm} of different chains with m section in each chain and with their weights it is necessary to review and then sum $(2p)^q$ analogues factors for all of the possible splitting of the section numbers between q simple segments and taking into account the condition $m = \sum_{i=1}^q m_i$. For doing the above operation let us use the generating functions respectively for the needs weights, the weights of simple chain (the ending parts of chains) and for their internal parts:

$$F = \sum_{m=1}^{\infty} N_{pm} \theta^m, \quad F_1 = \sum_{m=1}^{\infty} 2\theta^m = \frac{2\theta}{1-\theta}, \quad F_2 = p \sum_{m=2}^{\infty} 2\theta^m = \frac{2p\theta^2}{1-\theta}.$$

Where θ is a formal parameter. By exploit above described rules of the diagram construction we have the expression

$$F_p(\theta) = \sum_{q=0}^{\infty} (F_{2p}(\theta))^q F_1(\theta) = \frac{F_1(\theta)}{1 - F_2(\theta)} = \frac{\theta}{p(\theta_+ - \theta)(\theta - \theta_-)} \quad (19)$$

where we get

$$\theta_{\pm} = \frac{1}{4p} \left(-1 \pm \sqrt{1 + 8p} \right).$$

If $p = 3,4$ we get $\theta_+ \cong 1/3,155$ instead of 0.5 when $p=1$. In principle multiplying series by θ powers in (19) one can find the needing coefficient N_{pm} in front of θ^m . But because of we are interesting in the exponent constant for the asymptotically long times we shall not do it. The fact is that the changing of the exponent constant what we actually need defines by changing of the amount θ_+ . So for the chains with the large number of sections the average number of the weighting factor for one section is $1/\theta_+ \cong 3,16$ and not 2 when $p=1$.

Thereby if the intramolecular interaction averages up to zero we are getting with the help of theory from [10] the estimation for the MQ second moment growing up:

$$\langle n^2(t) \rangle_e \sim \exp(a_e t),$$

The exponent above is $a_e \approx 1,5C \approx 0,5\sqrt{M_{2MM}}$ and it was formed by the constant $C^2 = 3 \sum_j c_{ij}^2$ where

index "j" runs all of the methyl groups. Strong intramolecular interaction involves the changing of this constant to other amount

$$C_M^2 = \frac{5}{6} \cdot \frac{3,16}{2} \cdot C^2 = 1,32C^2 . \quad (20)$$

It means that the exponent a_e grows up to $\sqrt{1,32} = 1.15$ if the exponent a_e is taken by amount $\sqrt{M_{2MM}}$.

6. Summary

Using the methyl groups contains three nuclear spins as example the estimation of the influence of a strong intramolecular interaction on the rate of the growing up of a number of correlated spins has been done. This rate defines the growing up of the second moment of MQ spectra (quite the same is the parameter $N_2(\tau)$ in equation (5)). As one can see the rate reduces in ~ 1.4 times in occasions when the dipole-dipole interaction H_d governs by the evolution of a system, and increases in ~ 1.2 times when H_{eff} interaction controls our system. The trends marked above reveals in compare with situation when intramolecular interaction is absent.

Certainly mentioned effects realizes in all different systems consist of molecules or clusters of spins and this effect has to be taken into account for any exploiting of the MQ NMR spectroscopy in solids contains quite isolated groups of spins.

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