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The NMR line shape of magneto-active nanoclusters in moveable nano-containers with self-similar stochastic dynamics

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Abstract. NMR line shape of isolated spin clusters in moving nanocontainers with self-similar correlation law was calculated. It was shown that taking into account self-similarity in stochastic dynamics of pores leads to new shapes of NMR lines which differ from traditional shapes of Gauss and Lorentz types. Fractal dimension of spatial-temporal ensemble can serve as convenient fitting parameter for experimental data interpretation.

1. Introduction

In last decade one can see sharp increase of interest to study materials with nanometer pores and there are two reasons for it. In the first place synthesis of materials with pores with dimensions of several nanometers is the part of nanotechnology projects along with synthesis of nanoparticles. Laboratory research directed to obtaining homogeneous pores is conditioned by dependence of porous material properties from dimensions, shape and dimension distribution of pores [1]. For example, materials with ordered pores in the form of nanotubes (zeolite, aluminum silicates and so on) with constant section of tube mouth serve as molecular sieves for separation of mixture of gases molecules by their dimensions. Zeolite microcontainers are used as shells for dye molecules in dye lasers, as vessels for gases, electrolytes, as containers for toxic molecules of contrast medium for magnetic-resonance tomography and so on. In all cases nanocontainers affect the operation of the whole system container + filling. In the second place progress in the field of the nanotechnology have lead to the appearance of the spin physics of nanostructures and particularly to NMR spectroscopy of the gases in nanocavity [2]. High resolution of the NMR spectra and possibility of the precise analytic description of the NMR line shapes of the gases with molecules with nuclear spins in nanocavities [3] allow to get from experimental data the information about structure and dynamics of the nanocontainers investigated [3, 4].

Nanometer range of measurements opens the world of new material properties [5-9]. In comparison with bulk solid substance there are changes in parameters of crystal lattice and atomic dynamics, thermal and electronic properties; magnetic properties is changed, magnetic clusters become one-dimensional, for several metals increase and even appear magnetic moments on atom, abrupt magnetic phase transitions are observed and superparamagnetism occurs. All these effects have dimension character and strongly depend on nanocluster surface state, interactions between clusters and interaction of clusters with matrix. The properties of the isolated clusters differ from properties of

the clusters that are forming nanosystems. Weakly interacting or isolated nanoclusters can be obtained in the form molecular clusters in gas-phase reactions by means of laser induced evaporation with consequent study in time-of-flight mass spectrometer and with application of photoelectron spectroscopy (see for example [11]), or by means of matrix isolation at solid-state and colloidal synthesis under condition of the weak interaction of clusters with matrix. Interactions between clusters and interactions of clusters with matrix allow not only change the properties of isolated clusters but also create complex crystal and supramolecular structures in which clusters play role of the atoms like regular crystal.

Success of analytic calculation of the NMR spectra of the gases and nanoclusters with fast configuration rebuilding in nanocavities was due to presence in system the small adiabatic parameter $\varepsilon = \tau_m / \tau_f << 1$, where τ_m - characteristic time of changing the spin-spin interactions of the particles as a result of the fast molecular motions in gas or fast configuration rebuilding of the cluster, τ_f - characteristic time of the spin magnetization flip of the particle as a result of the interaction with nearest neighborhood spin (coincide with flip-flop transition time). As a result with accuracy ε cluster spin dynamics with spin ½ in nanocavities on time interval

$$\tau_m << \Delta t << \tau_f \tag{1}$$

is described by effective Hamiltonian *H* (see formula (2) of the first section) with space-independent effective spin-spin couplings. It is commonly known that main difficulty of the consecutive statistical calculation in big space-extended systems is the absence small adiabatic parameter. In such a case usually one have to use model Hamiltonians, the field of application of which is determined by comparison with results of sophisticated numerical calculations from first principles and also with results of the experiments. Contrary to that space-extended systems in which modeling linked with complicated accounting spatial-dependent interactions between spins at arbitrary values of coupling constants the spin dynamics and also thermodynamics with Hamiltonian (2) in limited nanocavities is actually precise and can be studied as much as possible in detail by analytic methods.

In papers [10, 11] with the help of the statistical Hamiltonian (2) the process of polarization transfer between nuclei in nanocavity is studied. The main result of this investigation was establishment of the fact that polarization transfer is nonergodic process. In paper [3] the method of the NMR line shape calculation of the gas of the spin bearing molecules in movable nanocontainers (described by Hamiltonian (2)) was developed. Taking into account fluctuation in time of the interdipolar bond constant the authors of this work for different time scales have obtained analytic expressions for line shape which differ from traditional Gauss or Lorentz dependencies. Particularly the line shape can have logarithmic singularity at $\omega \to 0$ and exponential decay on the tails. Singular behavior of the line shape can serve as recipe for finding the map of the angular distribution of the different ellipsoidal cavities.

Beginning with work [12] and then in works [13, 14] the authors offer to use model (2), which get the name of the model of the equal spin-spin interactions (ESSI), for description of the magnetoactive nanoclusters properties. For adequate description in the frame of the Hamiltonian (2) it is essential the presence in the system the small adiabatic parameter. Therefore it is necessary to consider clusters that are contained in containers (nanoclusters with matrix isolation) that can be presented by the pores with nanometer size. Under the influence of the container or due to any internal physicochemical features nanocluster can suffer fast configuration rebuilding (during time $\tau_m << \tau_f$). As an example one can give molecule bullvalene ($C_{10}H_{10}$) which (due to bond fluctuation) can suffer degenerate regrouping more than million times with the rate of the reorientation 10^{10} *Hz* ($\tau_m \simeq 10^{-10}$ sec) [15]. In paper [13] the thermodynamics of this model was studied in detail. Analysis of the thermodynamic properties of the model ESSI have revealed several specific features in them. Particularly it was shown that in finite spin system described by the model ESSI one can observe topological excitations (solitons) which firstly condition absence of the long-range order in the system

and secondly form anomalous behavior of the heat capacity at low temperatures (appearance of the additional low temperature peak). Anomalous behavior of the heat capacity of the model is connected with appearance of the spin gap in system considered. The presence of the spin gap in the spectrum of the magnetic excitations leads also to specific features in magnetic properties of the model [14], notably nonmonotonic behavior of the susceptibility and presence fractional plateau in field dependence of the magnetization.

In this work authors set the problem of the theory construction for NMR line inhomogeneous broadening of the isolated spin clusters in moving nanocontainers with self-similar correlation law. Description of the hierarchical (self-similar) structure of the medium and processes occurring in it is the crucial task at present [see, for example, 16-18 and their references]. Taking into account the self-similar character of the kinetic processes leads to fractional power behavior of the many time characteristics of the system. Particularly taking into account self-similarity in dielectric relaxation processes leads to non-exponential (fractional power) character of the time dependence for relaxation function of the macroscopic dipole moment of the system [19, 20], that agree with experimental data for frequency dielectric spectra.

2. NMR line shape of clusters in nanocontainers with time-dependent volume

Let us consider systems (clusters) of n spins ½, that are enclosed in moving nanocontainers in external magnetic field B. On time interval Δt (1) the effective spin dynamics is described by time-dependent averaged Hamiltonian

$$\bar{H}(t) = -\omega \cdot I^z - \frac{1}{2}\left(A_1(t) - A_2(t)\right)\left(I^z\right)^2 - \frac{A_2(t)}{2} I^2 + \frac{n}{8}(A_1(t) + 2A_2(t)), \tag{2}$$

where $\omega = \gamma B$ (γ - gyromagnetic ratio for protons), nuclear spins are given by spin operators I_f^α, $f = 1,...,n$, ($\alpha = x, y, z$), operators $I^\alpha = \sum_{f=1}^{n} I_f^\alpha$ determine projections of total spin operator on x, y, z-axes, $A_{1,2}(t)$ - time-dependent averaged constants of longitudinal and transversal spin-spin interaction. Time dependence of spin-spin interaction constants is determined by dynamics of nanoccontainer's geometrical parameters (volume, shape, orientation with respect to external field and others). The square of total nuclear spin operator has the form $I^2 = \left(I^+ I^- + I^- I^+\right)/2 + (I^z)^2$.

Line shape is determined as Fourier transform of free induction decay (FID), which in high-temperature limit has the form [21, 22]

$$G(t) = \frac{\mathrm{Sp}\left(I^+(t) I^-\right)}{\mathrm{Sp}\left(I^+ I^-\right)}. \tag{3}$$

Time dependence of operator $I^+(t) = e^{it\bar{H}} I^+ e^{-it\bar{H}}$ in Heisenberg representation is determined easily from motion equation

$$\frac{dI^+(t)}{dt} = i[\bar{H}, I^+] = -i(A_1(t) - A_2(t))(I^z - 1/2) I^+ \tag{4}$$

and has the appearance

$$I^+(t) = \exp\left(-i\varphi(t)\left(I^z - 1/2\right)\right) I^+(0), \tag{5}$$

where

$$\varphi(t) = \int_0^t (A_1(t') - A_2(t'))dt'. \tag{6}$$

For calculation of FID $G(t)$ let's represent it in the form $G(t)=R(t)/R(0)$, where $R(t)=\mathrm{Sp}\left(e^{-i\varphi(t)\left(I^z-1/2\right)}I^+I^-\right)$. So long as Hamiltonian (2) eigenvalues are known

$$E_{ms}(t)=-\frac{1}{2}\left(A_1(t)-A_2(t)\right)m^2-\frac{A_2(t)}{2}s(s+1)+\frac{n}{8}\left(A_1(t)+2A_2(t)\right), \tag{7}$$

where $s=s_{\min},...,n/2$ ($s_{\min}=1/2$ for odd particle quantity *n* and $s_{\min}=0$ for even particle quantity *n* in system), $m=-s,...,s$, the function $R(t)$ can be expressed in the form

$$R(t)=\sum_{s=s_{\min}}^{n/2}g(N,s)\sum_{m=-s}^{s}(s+m)(s-m+1)e^{i\varphi(t)(1/2-m)}, \tag{8}$$

where factor

$$g(n,s)=\frac{2s+1}{n+1}\cdot\binom{n+1}{n/2-s} \tag{9}$$

determines the number of grouping ways of *n* spins ½ into total spin *s*. Taking into account formulas

$$\sum_{m=-s}^{s}(s+m)(s-m+1)e^{i\cdot\varphi(t)(1/2-m)}=\frac{1}{2}\frac{(s+1)\sin s\varphi(t)-s\sin(s+1)\varphi(t)}{\sin^3\left(\varphi(t)/2\right)}, \tag{10}$$

$$\frac{1}{2}\sum_{s=s_{\min}}^{n/2}g(n,s)\frac{(s+1)\sin s\varphi(t)-s\sin(s+1)\varphi(t)}{\sin^3\left(\varphi(t)/2\right)}=n2^n\left(\cos\frac{\varphi(t)}{2}\right)^{n-1}, \tag{11}$$

let us represent $R(t)$ in the form

$$R(t)=n2^n\left(\cos\frac{\varphi(t)}{2}\right)^{n-1}. \tag{12}$$

As a result the expression for FID (3) is determined as

$$G(t)=\left(\cos\frac{\varphi(t)}{2}\right)^{n-1}. \tag{13}$$

On time scale of NMR observation $t\le t_{\mathrm{nmr}}\sim10^{-4}$ c we have $A_it\le10^{-2}$, then $\varphi(t)<<1$ and FID $G(t)$ for large numbers of spins *n* in nanocontainers transforms to the form

$$G(t)=e^{(n-1)\ln\cos(\varphi(t)/2)}\simeq e^{-n\varphi^2(t)/8}. \tag{14}$$

FID $G(t)$ (14) depends on constants $A_i(t)$ as internal parameters of function $\varphi(t)$ (6). Variation of the functions $A_i(t)$ leads to large variety of NMR line shape models, which mainly form two large groups: (a) homogeneous line broadening models and (b) inhomogeneous line broadening models [23, 24].

Nanosized containers are sensitive to the environment fluctuations, so constants $A_i(t)$ undergo fluctuations

$$A_i(t)=A_i+\delta A_i(t), \tag{15}$$

where fluctuation $\delta A_i(t)$ we will characterize by two moments

$$< \delta A_i(t) >= 0 \ , \ < \delta A_i(t_1)\delta A_j(t_2) >=< \delta A_i \delta A_j > K_{ij}(|t_1 - t_2|) \ , \tag{16}$$

$K_{ij}(t)$ designates correlation function, which, for example, can have appearance $K(t) = \exp(-t/\tau_c)$, τ_c - correlation time. Averaging the function $G(t)$ with respect to Gauss fluctuations $\delta A_i(t)$ leads to the next result [3]

$$\langle G \rangle(t) = \frac{\exp\left(-\frac{(A_1 - A_2)^2 nt^2}{8(1 + nC(t)/2)} \right)}{\sqrt{1 + nC(t)/2}} \ , \tag{17}$$

where

$$C(t) =< \delta\varphi(0)\delta\varphi(t) >=< \delta A_1^2 > M_{11}(t) + < \delta A_2^2 > M_{22}(t) - 2 < \delta A_1 \delta A_2 > M_{12}(t) \ , \tag{18}$$

$$M_{ij}(t) = \int_0^t (t - t') K_{ij}(t') dt' \ . \tag{19}$$

Introducing designations

$$\frac{A_1}{A_2} - 1 = \delta \ , \ \frac{< \delta A_i \delta A_j >}{A_i A_j} = \alpha_{ij} \ , \ \nu = \sqrt{\frac{n}{2}} A_2 \tag{20}$$

and taking into account (18), we transform expression for FID (17) to the form

$$\langle G \rangle(t) = \frac{\exp\left(-\frac{\delta^2 \gamma^2 t^2}{4(1 + \nu^2 \widetilde{C}(t))} \right)}{\sqrt{1 + \nu^2 \widetilde{C}(t)}} \ , \tag{21}$$

where

$$\widetilde{C}(t) = (1 + \delta)^2 \alpha_{11} M_{11}(t) + \alpha_{22} M_{22}(t) - 2(1 + \delta)\alpha_{12} M_{12}(t) \ . \tag{22}$$

In the case of fluctuation absence ($\alpha_{ij} = 0$) the line shape

$$J(\omega) = \frac{1}{\pi} \int_0^\infty G(t) \cos \omega t dt \ , \tag{23}$$

has Gauss form $J(\omega) = \exp(-\omega^2 / \delta^2 \nu^2) / \delta\nu\sqrt{\pi}$. Fluctuations of nanocavity lead to broadening of the line shape. For demonstration of the precise calculations of the line shape $J(\omega)$ (following the work [3]) let's choose correlation function in the form $K_{ii}(t) = \exp(-t/\tau_c)$ ($K_{12}(t) = 0$). This choice of correlation function form leads to the next expression for $M_{ii}(t)$

$$M_{ii}(t) = \tau_c^2 \left(\exp(-t/\tau_c) + t/\tau_c - 1 \right) \ . \tag{24}$$

Let's consider time fluctuations on two different time scales. When $\tau_c^2 < \delta A_i^2 ><< 1$ function $M_{ii}(t)$ has the appearance $M_{ii}(t) = \tau_c t$ for time $t >> \tau_c$, which leads equation (21) to the form

$$G(t) = \exp(-\delta^2 t / (4\gamma\tau_c)) / \sqrt{1 + \gamma\tau_c \nu^2 t} \ , \tag{25}$$

where $\gamma = (1+\delta)^2\alpha_{11} + \alpha_{22}$, and Fourier transformation of this expression gives next presentation for line shape [25]

$$J(\omega) = \frac{1}{\gamma\sqrt{\pi}\tau_c\nu^2}\mathrm{Re}\left(\frac{e^z}{\sqrt{z}}\mathrm{erfc}(\sqrt{z})\right), \quad z = (2\gamma\tau_c\nu)^{-2} + i\omega(\gamma\tau_c\nu^2)^{-1}. \tag{26}$$

Function $J(\omega)$ (26) has bell-shaped profile with intermediate Lorentz asymptotic behavior $J(\omega) = \Gamma/\pi(\Gamma^2+\omega^2)$, where $\Gamma = (4\gamma\tau_c)^{-1}$ (upon $\tau_c \to 0$). On high frequencies ($\omega \to \infty$) the line shape has next asymptotic behavior

$$J(\omega) \sim \frac{9\delta^2 n^2 A_2 \gamma}{16\pi\tau_c}\omega^{-4}. \tag{27}$$

In the case $\tau_c^2 < \delta A_i^2 >>> 1$ function $M_{ii}(t) = t^2/2$ for $0 \le t \le \tau_c \to \infty$. Therefore FID is represented in the form

$$G(t) = \exp(-\delta^2/2\gamma)/\sqrt{1+\gamma\nu^2 t^2/2}. \tag{28}$$

As a result for line shape we have next expression [3]

$$J(\omega) = \frac{\exp(-\delta^2/2\gamma)}{\pi\nu}\sqrt{\frac{2}{\gamma}}K_0\left(\frac{\omega\sqrt{2}}{\nu\sqrt{\gamma}}\right) = \begin{cases} \dfrac{\exp(-\delta^2/2\lambda)}{\pi\nu}\sqrt{\dfrac{2}{\gamma}}\left[-\ln\left(\dfrac{\omega\sqrt{2}}{\nu\sqrt{\gamma}}\right) + O(\omega)\right], & \omega \to 0, \\ \dfrac{\exp(-\delta^2/2\gamma)}{\sqrt{\pi\nu\sqrt{2\gamma}}}\dfrac{1}{\sqrt{\omega}}\exp\left(-\dfrac{\omega\sqrt{2}}{\nu\sqrt{\gamma}}\right), & \omega \to \infty. \end{cases} \tag{29}$$

In such a way this examples demonstratively proved wide applicability general formula (13), from which one can get different expressions for line shape under the assumption that random fluctuations have Gauss character.

3. The line shape of the clusters with self-similar correlation law of nanocontainers

In previous section we have shown calculation of the FID and line shape of spin clusters in fluctuating nanocavities with Gauss stochastic dynamics. Gauss ensemble of disordered containers is characterized by correlation time τ_c, changing of which leads to different line shapes.

According to recent ideas many experimental results can be described by entering conception about distribution of the correlation time. Taking into account this conception let us consider function of the correlation time distribution $g(\tau_c)$ and average function $M(t,\tau_c)$ (19) with this distribution. As a result we get average (effective) expression for this function

$$\overline{M}(t) = \int M(t,\tau_c)g(\tau_c)d\tau_c. \tag{30}$$

The simplest way to enter distribution function $g(\tau_c)$ is the next one. Let's divide set of nanocontainers (that form sample) on several groups, containing N_l nanocontainers with characteristic correlation time τ_{cl}. We assume that $M_{11}(t) = M_{22}(t) = M(t), \quad M_{12}(t) = 0$. The expression for $g(\tau_c)$ can be described by the formula

$$g(\tau_c) = \sum_l \frac{N_l}{N}\delta(\tau_c - \tau_{cl}), \tag{31}$$

where N – the number of pores in the sample. As a result the expression for averaged function $\overline{M}(t)$ of sample will accept the form

$$\overline{M}(t) = \sum_l \frac{N_l}{N} M(t, \tau_{cl}) . \tag{32}$$

In this work we propose self-similar character of container's dynamics. Therefore distributions of numbers N_l and set of correlation times τ_{cl} will obey self-similarity conditions [19, 20]

$$N_l = N_0 b^l , \quad \tau_{cl} = \tau_{c0} \xi^l \quad (-\infty < l \le L, b > 1, 0 < \xi < 1) . \tag{34}$$

From formula (24) one can see, that function $M(t, \tau_{cl})$ has structure $M(t, \tau_{cl}) = \tau_{cl}^2 f(t/\tau_{cl})$. As a result of the assumptions made the expression for effective memory function (32) will have the form

$$\overline{M}(\theta) = c\tau_{c0}^2 \sum_{l=-\infty}^{L} (b\xi^2)^l f(\theta \xi^{-l}) , \tag{36}$$

where $c = N_0 / N$, $\theta = t/\tau_{c0}$. For calculation of the sum (36) it is convenient to realize Mellin transform. Let's assume for definiteness that correlation function $K(t)$ has form $K(t) = \exp(-t/\tau_c)$, then $f(\theta) = e^{-\theta} + \theta - 1$. Mellin transform of the expression (36) leads to the next result

$$\mathfrak{M}(s) = c\tau_{c0}^2 \Gamma(s) \sum_{l=-\infty}^{L} \xi^{l(2-d+s)} = \frac{c\tau_{c0}^2 \Gamma(s) \xi^{(2-d+s)L}}{1 - \xi^{-(2-d+s)}} , \quad -2 < \mathrm{Re}\, s < -(2-d) . \tag{37}$$

Here $d = \ln b / \ln(1/\xi) > 0$, $\mathfrak{M}(s)$ – Mellin transform of the function $\overline{M}(\theta)$, $\Gamma(s)$ - gamma-function, and also we use formula $e^{-\theta} + \theta - 1 \overset{\text{MT}}{=} \Gamma(s), \quad -2 < \gamma = \mathrm{Re}\, s < -1$. Parameter d plays role of "dynamic" fractal dimension (i.e. dimension which connects geometrical b and dynamical ξ parameters of the system).

Making inverse Mellin transform in (37) we will get

$$\mathfrak{M}(s) \overset{\text{IMT}}{=} \overline{M}(\theta) = \frac{c\tau_{c0}^2}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \frac{\Gamma(s) \xi^{(s+2-d)L} \theta^{-s}}{1 - \xi^{-(s+2-d)}} ds . \tag{38}$$

For calculation of the Mellin-Barnes integral in the right part of (38) we enclose integration line on contour by right half of circle (contour $L_{i\infty}$) and by Cauchy theorem we find

$$\overline{M}(\theta) = -c\tau_{c0}^2 \sum_{s_k \in L_{i\infty}} \mathrm{Res}_{s_k} \left[\frac{\Gamma(s) \xi^{(s+2-d)L} \theta^{-s}}{1 - \xi^{-(s+2-d)}} \right], \tag{39}$$

where s_k – poles of function (37). Function $\mathfrak{M}(s)$ (37) has two groups of poles

$$s_k' = -(2-d) + i\Omega k, \quad \Omega = \frac{2\pi}{\ln(1/\xi)}, \quad k = 0, \pm 1, \pm 2, ... , \tag{40a}$$

$$s_k'' = -k, \quad k = 0, 1, 2, ... \tag{40б}$$

We take into account that inside of chosen contour there are all poles of the group (40a) and only poles $s_0'' = 0, s_1'' = -1$ of the group (40б) and $0 < d < 1$. As a result from (39) we will get

$$\overline{M}(\theta) = \frac{c\tau_{c0}^2 \theta^{2-d}}{\ln(1/\xi)} w_d \left(\frac{\ln \theta}{\ln(1/\xi)} \right) + c\tau_{c0}^2 \left(-\frac{\xi^{(2-d)L}}{1 - \xi^{-(2-d)}} + \frac{\xi^{(1-d)L} \theta}{1 - \xi^{-(1-d)}} \right), \tag{41}$$

where

$$w_d(z) = \sum_{k=-\infty}^{\infty} \Gamma(-(2-d)+i\Omega k)\exp\left[2\pi i k x\right], \tag{42}$$

- periodic function with period 1. In (41) we took into account, that $\operatorname{Res}_{-k}\Gamma(s) = (-1)^k / k!$. So long as we consider that $L \gg 1$ then expression in parentheses (41) is small and we neglect it. As a result expression for averaged function $\overline{M}(\theta)$ take the form

$$\overline{M}(\theta) = \frac{c\tau_{c0}^2 \theta^{2-d}}{\ln(1/\xi)} w_d\left(\frac{\ln\theta}{\ln(1/\xi)}\right). \tag{43}$$

So long as $\left|\Gamma(-(2-d)+i\Omega k)\right| \ll \Gamma(-(2-d))$ at $k \neq 0$ then in present work we neglect the presence of log-periodic oscillations. Investigation of the influence of the log-periodic oscillations on line shape will be the problem of the next work. Thus function $\overline{M}(\theta)$ will take next final form

$$\overline{M}(\theta) = \frac{c\tau_{c0}^2 \Gamma(d-2)\theta^{2-d}}{\ln(1/\xi)}. \tag{44}$$

As a result of substitution of the expression (45) in (21) we will get expression for FID with account of self-similar character of correlations in nanocavities motion

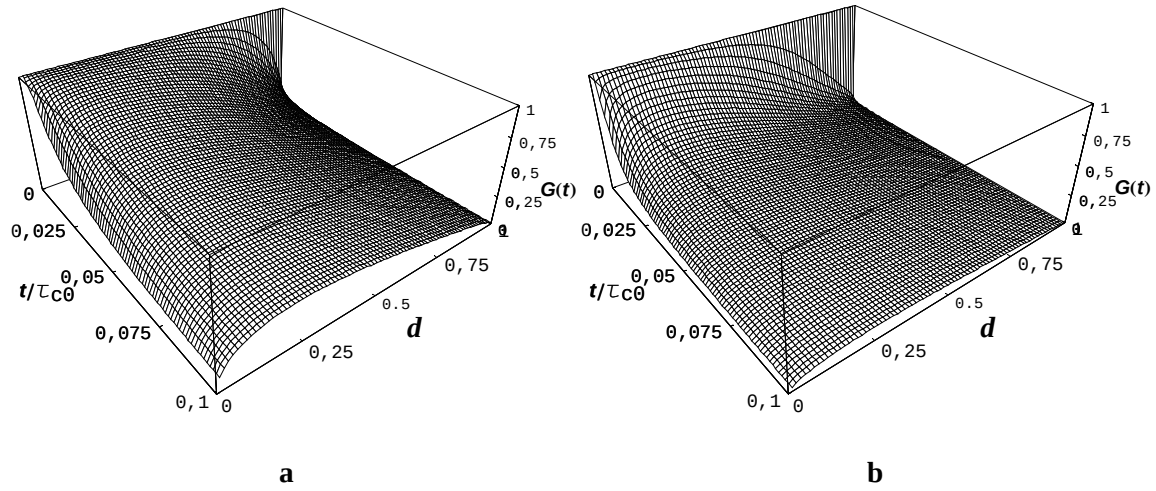
$$\widetilde{\langle G\rangle}(t) = \frac{\exp\left(-\dfrac{\delta^2 \nu^2 t^2}{4(1+\nu^2\gamma a(d) t^{2-d})}\right)}{\sqrt{1+\nu^2\gamma a(d) t^{2-d}}}, \tag{45}$$

where $a(d) = c\tau_{c0}^d \Gamma(d-2)/\ln(1/\xi)$. In case when $a(d) < \delta A_i^2 >>> 1$ expression (45) will take the form

$$\widetilde{\langle G\rangle}(t) \simeq \frac{\exp\left(-\dfrac{\delta^2 t^d}{4\gamma a(d)}\right)}{\sqrt{1+\nu^2\gamma a(d) t^{2-d}}}. \tag{46}$$

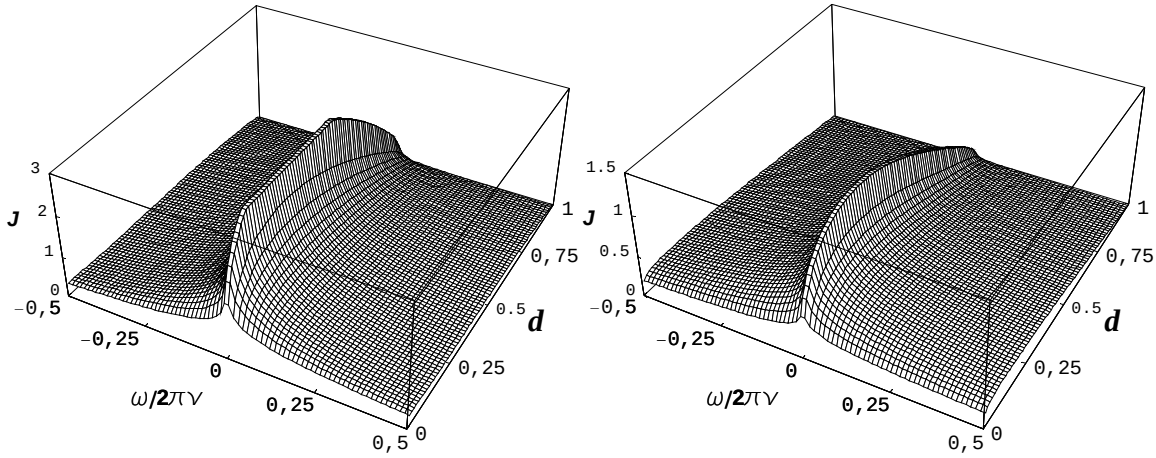
On figure 1 there are time dependences of the FID for different values of fractal dimension *d* at next values of parameters: $\tau_{c0} = 0,004$ c, $\alpha = 100$, $\gamma\tau_{c0} = 10$, $\delta = 0,5$, $c = 0,01$, $\xi = 0,1$ (fig. 1a) and $\xi = 0,8$ (fig. 1b). From this figure one can see that time dependence of the FID considerably depends on self-similarity parameters ξ and *d*, changing of which leads to change of the decay rate.

On figure 2 there are plots of line shape (23) for different values of fractal dimension *d* (parameter values corresponds to figure 1). From this figure one can see that line shape considerably changes at the edges of possible values interval of fractal dimension *d*.



a **b**

Figure 1. The free induction decay at different values of the fractal dimension *d*. The 2D plots are constructed at the following values of the parameters: $\tau_{c0} = 0,004$ c, α =100, $\gamma\tau_{c0} = 10$, $\delta = 0,5$, $c = 0,01$, $\xi = 0,1$ (a) and $\xi = 0,8$ (b).



a **b**

Figure 2. The line shape at different values of the fractal dimension *d*. The plot is constructed at the following values of the parameters: $\tau_{c0} = 0,004$ c, α =100, $\gamma\tau_{c0} = 10$, $\delta = 0,5$, $c = 0,01$, $\xi = 0,1$ (a) and $\xi = 0,8$ (b).

4. Conclusion

The aim of the present work was development of the theory of NMR line shape of isolated in fluctuating nanopores magnetoactive clusters with self-similar Gauss stochastic dynamics. The possibility of precise analytic description of the NMR line shape of isolated nanoclusters with fast configuration rebuilding opens the way for subsequent development of the theory to bring it closer to

real description of the physical systems, notably to take into account the self-similar character of pores dynamics.

In the frame of the model suggested and related to the self-similar hierarchy of the correlation times of fluctuations in nanocontainers it is shown how to take into account the scaling effects associated with collective dynamics of pores. The self-similar character of movement of nanocontainers leads to new analytical description of the NMR line shapes that are differed from the conventional Gaussian and Lorentz forms.The free decay and the corresponding line shape depends on the fractal dimension of the space-time self-similar ensemble and this important characteristic can serve as a convenient and clear understandable fitting parameter in interpretation of experimental data associated with NMR phenomena in disordered media.

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