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The generating functions formalism for the analysis of spin response to the periodic trains of RF pulses. Echo sequences with arbitrary refocusing angles and resonance offsets

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ABSTRACT

The generating functions (GF) formalism was applied for calculation of spin density matrix evolution under the influence of periodic trains of RF pulses. It was shown that in a general case, closed expression for the generating function can be found that allows in many cases to derive analytical expressions for the generating function of spin density matrix (magnetization, coherences). This approach was shown to be particularly efficient for the analysis of multi-echo sequences, where one has to average over various frequency isochromats. The explicit analytical expressions for the generating function for echo amplitudes in a Carr–Purcell–Meiboom–Gill (CPMG) echo sequence, a multiecho sequence with incremental phase of refocusing pulse, a gradient echo sequence including transient period were obtained for an arbitrary flip angle and an arbitrary resonance offset. Comparison of the theory and the spin-echo experiments was done, demonstrating a good agreement.

1. Introduction

Long periodic trains of RF pulses represent an integral part of MRI methods. The extensively used multiple spin echoes can serve as an example of such kind. However, these echo sequences are just a special case of magnetization evolution in a time-periodic Hamiltonian. The calculation of density matrix evolution in a periodic spin Hamiltonian is a complicated problem. There are only a few approaches to consider the problem [1]. Here, we suggest an approach based on the so-called generating functions (GF) formalism. This formalism is one of the powerful methods of discrete mathematics. The generating function for a series (infinite in general case) of numbers $M_1, \ldots M_n$ or matrices is defined as a function of the complex variable z in the following way:

$$f(z) = M_0 + M_1 z + \ldots + M_n z^n + \ldots = \sum_{n=0}^{\infty} M_n z^n, \quad (1)$$

where $|z| < 1$, which usually ensures the convergence of the series. For instance, one can consider echo amplitudes in the CPMG sequence with an arbitrary flip angle as the values M_n. It is often that GF for a number series varying according to a certain law has a simple analytical form, whereas the expression for the nth element of the sequence cannot be obtained analytically or is very cumbersome.

The specific property of GF is that it comprises complete information about all M_n values at once. The element M_n can be found by expanding GF in powers of z analytically or numerically. Also conventional Fourier algorithm can be used for determining M_n numbers from GF. Here we generalize the GF approach employed in our previous paper [2] for echo amplitudes for the calculation of spin density matrix evolution under the influence of arbitrary periodic trains of RF pulses. The efficiency of the method is demonstrated by calculating GF for the echo amplitudes in the CPMG echo sequence with an arbitrary refocusing flip angle and an arbitrary resonance offset, a multiecho sequence with incremental phase of refocusing pulse, a gradient echo sequence including transient period. Besides in this paper we present comparison between our theory and experiment for CPMG sequence with $\pi/4$ and $\pi/2$ flip angles of refocusing pulse.

2. General case of a periodic spin Hamiltonian

Let us consider density matrix evolution in Liouville space, where density matrix represents a vector containing density matrix elements. Let us denote the density matrix after the nth period of Hamiltonian as $\vec{\rho}_n$. To obtain GF it is necessary to know the evolution of spin density matrix during one period of the spin Hamiltonian. In other words, one needs the matrix $\mathbf{A}$ and the vector $\vec{B}$ relating $\vec{\rho}_{n+1}$ with $\vec{\rho}_n$ in the following way:

$$\vec{\rho}_{n+1} = \mathbf{A}\vec{\rho}_n + \vec{B}. \quad (2)$$

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If $\mathbf{A}$ and $\vec{B}$ are known and do not depend on n, it is easy to obtain an analytical expression for GF. To calculate GF let us multiply both sides of Eq. (2) by z^n and take a sum from $n = 0$ to infinity. The left-hand side of this summation is

$$\frac{1}{z}(\vec{\rho}_1 z + \vec{\rho}_2 z^2 + \vec{\rho}_3 z^3 + \ldots) = \frac{1}{z}(\vec{f}(z) - \vec{\rho}_0), \tag{3}$$

where $\vec{f}(z)$ is the GF:

$$\vec{f}(z) = \vec{\rho}_0 + \vec{\rho}_1 z + \ldots + \vec{\rho}_n z^n + \ldots = \sum_{n=0}^{\infty} \vec{\rho}_n z^n, \tag{4}$$

while the right-hand side summation gives

$$\mathbf{A}(\vec{\rho}_0 + \vec{\rho}_1 z + \vec{\rho}_2 z^2 + \ldots) + \vec{B}(1 + z + z^2 + \ldots)$$
$$= \mathbf{A}\vec{f}(z) + \frac{1}{1-z}\vec{B}. \tag{5}$$

Solving the resulting equation for GF $\vec{f}(z)$ one obtains

$$\vec{f}(z) = (\mathbf{I} - z\mathbf{A})^{-1}\left(\vec{\rho}_0 + \frac{z}{1-z}\vec{B}\right). \tag{6}$$

It is seen that according to (6), calculation of GF needs only matrix inversion and therefore in many cases an analytical expression for GF can be found. Generating functions for various periodic pulse sequences can then be tabulated as it is done for Laplace or Fourier transformations of various functions. This analogy is particularly relevant since as it is shown below GF is in fact a discrete Fourier (Laplace) transform.

Then, any density matrix element can be easily calculated analytically or numerically using, for instance, a software package where the expansion in power series is implemented as a couple of standard instructions.

Taking $z = e^{i\theta}$ $(0 \leqslant \theta < 2\pi)$ one can see that GF represents a discrete Fourier series:

$$\vec{f}(e^{i\theta}) = \vec{\rho}_0 + \vec{\rho}_1 e^{i\theta} + \vec{\rho}_2 e^{i2\theta} + \ldots + \vec{\rho}_n e^{in\theta} + \ldots \tag{7}$$

Therefore, the density matrix $\vec{\rho}_n$ can be calculated using Fourier transformation. One can also construct an experimental GF according to Eq. (1), taking the experimentally determined data as M_n. From comparison of the experimental GF with the theoretical GF one can obtain parameters of the spin system. In addition, the stationary density matrix $(n \to \infty)$ can be readily calculated from GF as follows:

$$\vec{\rho}_{st} = \lim_{n\to\infty} \vec{\rho}_n = \lim_{z\to 1}((1-z)\vec{f}(z)). \tag{8}$$

3. CPMG sequence with arbitrary resonance offset and flip angle

Application of multiple spin echoes is a topical question in MR imaging since these are very important techniques for measuring proton density, relaxation times T_1 and T_2, diffusion coefficients, etc. The properties of spin echo sequences with the arbitrary refocusing angles were addressed in a number of papers [3–14].

In the conventional CPMG sequence, the refocusing angle is equal to π. However, this demands a preliminary calibration of the RF probe that can be time-consuming. It is also known that any refocusing flip angle is able to produce spin echoes. Moreover, smaller flip angles appear to be more preferable as they permit one to decrease the RF load. Besides, the pulses usually have complex excitation frequency spectra, so the flip angle cannot be described by a single value of the refocusing angle. The approach proposed in this work appears to be a powerful tool for the analysis of multi-echo sequences since averaging over frequency isochromats can be performed in GF yielding GF directly for echo amplitudes. In the earlier paper [2], we obtained analytical expressions for GF for echo amplitudes in the CPMG pulse sequence with an arbitrary refocusing angle. In the present work, we generalized this GF approach for calculation of echo amplitudes for the CPMG sequence for an arbitrary resonance offset and an arbitrary RF magnetic field magnitude.

Consider now the pulse train $(\pi/2)_{-y} - TE/2 - \alpha_x - TE - \alpha_x - TE - \alpha_x - \ldots$. Let us assume that the $(\pi/2)_{-y}$-pulse is applied on resonance while the α_x-pulses are non-resonant with the frequency offset equal to $\Delta\omega$. Then the spin system evolution over one period is subdivided into two evolution steps: the rotation under the RF pulse and the precession period, accompanied also by spin relaxation. A relation between $\vec{M}_n$ and $\vec{M}_{n+1}$ is as follows:

$$\vec{M}_{n+1} = \mathbf{QPQ}\vec{M}_n + (\mathbf{QP} + \mathbf{I})\vec{S}_{eq}, \tag{9}$$

where

$$\vec{M}_n = (M_n^+, M_n^-, M_{zn})^{\mathbf{T}},$$
$$M_n^+ = M_n^{-*} = M_{xn} + iM_{yn},$$

superscript $\mathbf{T}$ stands for transposition; M_{xn},M_{yn} and M_{zn} are the x-, y- and z-components of the magnetization vector at the instant of nth echo, respectively, $\mathbf{P}$ is the RF pulse rotation matrix, $\mathbf{Q}$ is the matrix describing the spin relaxation and Larmor precession during one half of the inter-echo period ($TE/2$), the vector $\vec{S}_{eq}$ is

$$\vec{S}_{eq} = M_{eq}\left(0, \quad 0, \quad 1 - e^{-\frac{TE}{2T_1}}\right)^{\mathbf{T}},$$

where M_{eq} is the thermal equilibrium spin magnetization, TE is the echo time, T_1 is the longitudinal spin relaxation time, and $\mathbf{I}$ is unity matrix.

In the reference frame rotating with the frequency of RF field, the following expressions for matrices $\mathbf{Q}$ and $\mathbf{P}$ can be obtained:

$$\mathbf{Q} = \begin{pmatrix} \sqrt{\xi_2}U & 0 & 0 \\ 0 & \sqrt{\xi_2}U^{-1} & 0 \\ 0 & 0 & \sqrt{\xi_1} \end{pmatrix}, \tag{10}$$

$$\mathbf{P} = \begin{pmatrix} \lambda & \mu & \upsilon \\ \mu & \lambda^* & \upsilon^* \\ \frac{\upsilon}{2} & \frac{\upsilon^*}{2} & \zeta \end{pmatrix}, \tag{11}$$

where

$$\lambda = \left(\cos\frac{\alpha}{2} - i\sin\varphi\sin\frac{\alpha}{2}\right)^2, \tag{12}$$

$$\mu = \cos^2\varphi\sin^2\frac{\alpha}{2}, \tag{13}$$

$$\upsilon = 2i\cos\varphi\sin\frac{\alpha}{2}\left(\cos\frac{\alpha}{2} - i\sin\varphi\sin\frac{\alpha}{2}\right), \tag{14}$$

$$\zeta = \cos\alpha\cos^2\varphi + \sin^2\varphi, \tag{15}$$

$$\alpha = \sqrt{\Delta\omega^2 + \omega_1^2}\,\tau, \tag{16}$$

$$\varphi = \arctan\frac{\Delta\omega}{\omega_1}, \tag{17}$$

$$\xi_{1,2} = e^{-\frac{TE}{T_{1,2}}}, \tag{18}$$

$$U = e^{-i\psi} \tag{19}$$

and $\omega_1 = \gamma B_1$, B_1 is the RF magnetic field amplitude, ψ is the phase accumulated during one half of the inter-echo period ($TE/2$) for a definite isochromat, T_2 is the transverse spin relaxation time, τ is the pulse duration, γ is the nucleus magnetogyric ratio. Then one can write:

$$\vec{M}_{n+1} = \mathbf{A}\vec{M}_n + \vec{B} \tag{20}$$

where $\mathbf{A} = \mathbf{QPQ}$ and $\vec{B} = (\mathbf{QP} + \mathbf{I})\vec{S}_{eq}$. Using Eq. (6) one can obtain the following expression for GF of transverse magnetization M_n^+:

$$f_+(z,U) = \sum_{n=0}^{\infty} M_n^+ z^n = M_{eq} \frac{C_3U^3 + C_2U^2 + C_1U + C_0}{D_0 + D_1U^2 + D_2U^4}, \tag{21}$$

where

$$\begin{aligned}
C_0 &= z\xi_2(1-z\xi_1)\left(\sin\varphi\sin\frac{\alpha}{2} - i\cos\frac{\alpha}{2}\right)^2,\\
C_1 &= \frac{2z^2\xi_2^{3/2}(1-\sqrt{\xi_1})(1+z\sqrt{\xi_1})\sin\frac{\alpha}{2}\cos\varphi(\sin\varphi\sin\frac{\alpha}{2} - i\cos\frac{\alpha}{2})}{1-z},\\
C_2 &= 1 - z\xi_1\sin^2\varphi + z\cos^2\varphi\left(\xi_2(1+z\xi_1)\sin^2\frac{\alpha}{2} - \xi_1\cos\alpha\right),\\
C_3 &= \frac{2z\sqrt{\xi_2}(1-\sqrt{\xi_1})(1+z\sqrt{\xi_1})\sin\frac{\alpha}{2}\cos\varphi(\sin\varphi\sin\frac{\alpha}{2} + i\cos\frac{\alpha}{2})}{1-z},\\
D_0 &= C_0,\\
D_1 &= -\xi_1\xi_2^2z^3 + \xi_2^2z^2\left(\cos^2\frac{\alpha}{2} - \cos 2\varphi\sin^2\frac{\alpha}{2}\right) - \xi_1 z(\cos^2\varphi\cos\alpha + \sin^2\varphi) + 1,\\
D_2 &= z\xi_2(1-z\xi_1)\left(\sin\varphi\sin\frac{\alpha}{2} + i\cos\frac{\alpha}{2}\right)^2.
\end{aligned} \tag{22}$$

It is seen that quantities C_0, C_1, C_2, C_3 as well as D_0, D_1, D_2 (given by Eqs. (22)) are functions of the variable z only and parameterically depend on α, φ, ξ_1 and ξ_2.

The expression (21) gives the GF for one definite isochromat. Note that steady state magnetization can be easily found for a separate isochromat, thus from Eqs. (8), (21) and (22) it follows:

$$M_{st}^+ = \frac{\sin\alpha\cos\varphi(1-\xi_1)\sqrt{\xi_2}}{\left(\frac{D_0}{U^2} + D_1 + D^2U^2\right)\big|_{z=1}U}\left(i(U^2-\xi_2) + (U^2+\xi_2)\tan\frac{\alpha}{2}\sin\varphi\right). \tag{23}$$

In the absence of spin relaxation, the steady state magnetization is

$$M_{st}^+ = \frac{2\tan\frac{\alpha}{2}\cos\varphi}{(U^2-1)^2 + (U^2+1)^2\tan^2\frac{\alpha}{2}\sin^2\varphi}\left((U^2+1)\tan\frac{\alpha}{2}\sin\varphi - i(U^2-1)\right). \tag{24}$$

At the first glance, the use of recurrent Eq. (20) is preferred for the calculation of magnetization since expression for the GF is rather cumbersome. But calculations according to Eq. (20) can be done only numerically, and from our point of view it is always preferable to have an analytical expression in hands, even if a cumbersome one. Moreover, this expression is for one isohromat only. To obtain the echo amplitudes, one should make an averaging over isohromats. It is clear that this procedure can be rather inconvenient if one has to use Eq. (20). Alternatively, averaging of GF over isohromats as we will show below yields a very compact expression for the GF of echo amplitudes.

To obtain the echo amplitudes, we have to average over all isochromats. It is obvious that magnetization of each M_n isochromat can be represented as

$$M_n^+ = \sum_{k=-2n}^{2n} K_{nk}U^k \tag{25}$$

This expression is used in the so-called Configurations approach [15] and directly follows from Eqs. (9)–(11). U is different for different isochromats, and it is clear that all U^n for $n \neq 0$ average to zero. Therefore, the null-configuration K_{n0} is the only term that makes a contribution to the echo signal (all other configurations give zero when averaged over isochromats).

Similarly to Eq. (25), GF can be represented as

$$f_+(z,U) = \sum_{k=-\infty}^{+\infty} F_k(z)U^k, \tag{26}$$

which is the GF representation in the form of Laurent series in U.

To find the echo amplitudes GF, one has to omit the terms $F_k(z)U^k$ with $k \neq 0$ and to keep only the term $F_0(z)$. It is possible to do this by integration of $\frac{f(z)}{U}$ over variable U along the unity circle contour in the complex plane, and we obtain for $F_0(z)$:

$$F_0(z) = \frac{1}{2\pi i}\oint_{|U|=1}\frac{f_+(z,U)}{U}dU. \tag{27}$$

This integral can be found by calculating residues inside the unity circle according to the theory of complex variable [16]. Finally, for the echo amplitude generating function $F_0(z)$ we obtain the following expression:

$$F_0(z) = \frac{M_{eq}}{2}\left[1 + \sqrt{\frac{X}{Y}}\right], \tag{28}$$

where

$$\begin{aligned}
X &= (1+z\xi_2)(1 - z(\cos\alpha\cos^2\varphi + \sin^2\varphi)(\xi_1+\xi_2) + z^2\xi_1\xi_2),\\
Y &= (1-z\xi_2)(1 - z(\cos\alpha\cos^2\varphi + \sin^2\varphi)(\xi_1-\xi_2) - z^2\xi_1\xi_2).
\end{aligned} \tag{29}$$

In resonance, the offset $\Delta\omega = 0$ and the angle $\varphi = 0$, so the expression for F_0 coincides with the result obtained in [2]. Furthermore, defining angle α_e as

$$\cos\alpha_e = \cos\alpha\cos^2\varphi + \sin^2\varphi \tag{30}$$

one can rewrite (28) and (29) as

$$\begin{aligned}
F_0(z) &= \frac{M_{eq}}{2}\left[1 + \sqrt{\frac{X_e}{Y_e}}\right],\\
X_e &= (1+z\xi_2)(1 - z\cos\alpha_e(\xi_1+\xi_2) + z^2\xi_1\xi_2),\\
Y_e &= (1-z\xi_2)(1 - z\cos\alpha_e(\xi_1-\xi_2) - z^2\xi_1\xi_2).
\end{aligned} \tag{31}$$

One can see that this expression coincides with the one for the resonant case, $\Delta\omega = 0$ [2], if one redefines α as α_e.

If M_{x0} and M_{y0} are the initial transverse magnetization components, the GF for echo amplitudes takes the following form:

$$F_0(z) = \frac{M_{x0}}{2}\left[1 + \sqrt{\frac{X}{Y}}\right] + i\frac{M_{y0}}{2}\left[1 + \sqrt{\frac{Y}{X}}\right]. \tag{32}$$

In a particular case, let us consider the excitation pulse which is non-resonant with the same offset $\Delta\omega$ and $\alpha_1 = \sqrt{\omega_1^2 + \Delta\omega^2}\tau_1$ ($\varphi_1 = \arctan\frac{\Delta\omega}{\omega_1}, \tau_1$ is the excitation pulse duration), then the expressions for M_{x0} and M_{y0} are as follows:

$$\begin{aligned}
M_{x0} &= M_{eq}\sin\alpha_1\cos\varphi_1,\\
M_{y0} &= -M_{eq}\sin^2\frac{\alpha_1}{2}\sin 2\varphi_1.
\end{aligned} \tag{33}$$

The expression for the steady state obtained from null configuration of GF appears to be considerably more simple than (23) and (24): if the relaxation is neglected, then from Eqs. (8), (29) and (32) one can obtain:

$$M_{st}^+ = \frac{M_{x0}\omega_1}{\sqrt{\omega_1^2 + \Delta\omega^2}}\left|\sin\frac{\sqrt{\omega_1^2 + \Delta\omega^2}t}{2}\right|, \tag{34}$$

whereas in the presence of relaxation $M_{st}^+ = 0$.

If $T_1 = T_2(\xi_1 = \xi_2 = \xi)$, the magnetization amplitudes can be represented as the sum of Legendre polynomials:

$$M_n^+ = \frac{\xi^n M_{x0}}{2}\left[\sum_{k=0}^{n}P_k(\cos\alpha_e) - 2\cos\alpha_e\sum_{k=0}^{n-1}P_k(\cos\alpha_e) + \sum_{k=0}^{n-2}P_k(\cos\alpha_e)\right] + i\frac{\xi^n M_{y0}}{2}[P_n(\cos\alpha_e) - P_{n-1}(\cos\alpha_e)]. \tag{35}$$

Having used this expansion and an integral representation of Legendre polynomial $P_n(\cos\alpha_e)$ [17]

$$P_n(\cos\alpha_e) = \frac{1}{\pi\sqrt{2}} \int_{-\alpha_e}^{\alpha_e} \frac{e^{i\left(n+\frac{1}{2}\right)\theta}}{\sqrt{\cos\theta - \cos\alpha_e}} d\theta$$

one can obtain an asymptotic behavior of echo amplitudes ($n \to \infty$) for α_e in the range $(0, \pi)$:

$$M_n^+ = \xi^n M_{x0}\left[\sin\frac{\alpha_e}{2} - \frac{1}{2\sqrt{\pi\tan\frac{\alpha_e}{2}}}\frac{\cos\left(n\alpha_e - \frac{\pi}{4}\right)}{n^{3/2}}\right] + i\xi^n M_{y0} \times \sqrt{\frac{\tan\frac{\alpha_e}{2}}{\pi n}}\cos n\alpha_e. \quad (36)$$

This asymptotic limit becomes valid for $n\sin\alpha_e \gg 1$.

Furthermore, the GF formalism can be extended to the echo-sequence with phase cycling of refocusing pulse. It may be shown that the generating function $F_0^c(z)$ for such sequence has the following form:

$$F_0^c(z) = \sum_{n=0}^{\infty} M_n^+ z^n = e^{i\phi/2} F_0(z e^{-i\phi}), \quad (37)$$

where ϕ stands for the phase increment and $F_0(z)$ is defined in Eq. (32). The derivation of the result is given in Appendix A.

4. Gradient echo sequences with arbitrary resonance offset and flip angle

Consider the pulse train of gradient echo method $\alpha_x - TR - \alpha_x - TR - \alpha_x - TR - \ldots$, where α_x is the flip angle of excitation pulses, between the pulses magnetic field gradient $G(t)$ is applied. We consider separately two cases. The first one is when the gradient area $\mathbb{S}$ defined as

$$\mathbb{S} = \int_0^{TR} G(t)dt \quad (38)$$

is nonzero, i.e. the gradient is not compensated. The second case is when the gradient is compensated, i.e. $\mathbb{S} = 0$.

4.1. Uncompensated gradient ($\mathbb{S} \neq 0$)

4.1.1. The generating function for FID

For magnetizations which are measured just after each α-pulse, i.e. FIDs, the following generating function can be obtained:

$$F_0(z) = \frac{M_{eq}\upsilon}{(1-z)(1+\cos\alpha_e)}\left[1 + \frac{(\cos\alpha_e - z\xi_1)(1 - z^2\xi_2^2)}{\sqrt{X_e Y_e}}\right] = \sum_{n=0}^{\infty} M_n^+ z^n, \quad (39)$$

where X_e and Y_e are the same as in Eq. (31) and υ is defined in Eq. (14). In the derivation of the GF in Eq. (39), averaging over all uncompensated phases due to field gradient was performed. Note that the sum in Eq. (39) begins from $n = 0$, here n corresponds to the pulse number preceding the FID and $n = 0$ corresponds to the first pulse. The steady state magnetization can be easily obtained from (39) according to (8):

$$M_{st}^+ = \frac{M_{eq}\upsilon}{1+\cos\alpha_e}\left[1 + \frac{(\cos\alpha_e - \xi_1)\sqrt{1-\xi_2^2}}{\sqrt{(1-\xi_1\cos\alpha_e)^2 - \xi_2^2(\xi_1 - \cos\alpha_e)^2}}\right] \quad (40)$$

and coincides with the well known result [6]. If $T_1 = T_2$ ($\xi_1 = \xi_2 = \xi$) then the transverse magnetization M_n^+ can be expressed explicitly as the sum of Legendre polynomials:

$$M_n^+ = M_{eq}\frac{\upsilon}{1+\cos\alpha_e}\left(1 + \cos\alpha_e\sum_{k=0}^{n}\xi^k P_k(\cos\alpha_e) - \sum_{k=0}^{n-1}\xi^{k+1}P_k(\cos\alpha_e)\right) \quad (41)$$

and the asymptotic behavior at $n\sin\alpha_e \gg 1$ is as following ($0 < \alpha_e < \pi$):

$$M_n^+ - M_{st}^+ = \frac{M_{eq}\upsilon\xi^{n+2}\sqrt{2}}{\cos^2\frac{\alpha_e}{2}(1 - 2\xi\cos\alpha_e + \xi^2)\sqrt{\pi n\sin\alpha_e}} \times \left[\sin\left((n+1)\alpha_e + \frac{\pi}{4}\right) \times \left(\sin\frac{\alpha_e}{2}\sin\alpha_e - \frac{1-\xi}{2\xi}\cos\frac{3\alpha_e}{2}\right) + \frac{1-\xi}{2\xi}\sin\left(n\alpha_e + \frac{\pi}{4}\right) + \cos\frac{\alpha_e}{2}\right]. \quad (42)$$

4.1.2. The generating function for echo

For the magnetization measured before each α pulse, i.e. echo, the GF is as follows:

$$F_0(z) = \frac{M_{eq}\upsilon^*}{(1-z)(1+\cos\alpha_e)}\left[1 - \frac{(1 - z\xi_1\cos\alpha_e)(1 - z^2\xi_2^2)}{\sqrt{X_e Y_e}}\right] = \sum_{n=1}^{\infty} M_n^+ z^n, \quad (43)$$

where X_e and Y_e are defined in Eq. (31) and υ^* can be obtained from Eq. (14). Here M_n^+ corresponds to the echo signal before the nth pulse. Then the steady state magnetization is

$$M_{st}^+ = \frac{M_{eq}\upsilon^*}{1+\cos\alpha_e}\left[1 - \frac{(1 - \xi_1\cos\alpha_e)\sqrt{1-\xi_2^2}}{\sqrt{(1-\xi_1\cos\alpha_e)^2 - \xi_2^2(\xi_1 - \cos\alpha_e)^2}}\right], \quad (44)$$

that also coincides with the well known result [6]. Note that the first magnetization amplitude M_1^+ is equal to zero, while the second one is not:

$$M_2^+ = 2M_{eq}\xi_2^2\sin^3\frac{\alpha}{2}\cos^3\varphi\left(\sin\frac{\alpha}{2}\sin\varphi - i\cos\frac{\alpha}{2}\right). \quad (45)$$

Again, if $T_1 = T_2 (\xi_1 = \xi_2 = \xi)$ the transverse magnetization can be represented in explicit form by the sum of Legendre polynomials:

$$M_n^+ = M_{eq}\frac{\upsilon^*}{1+\cos\alpha_e}\left(\cos\alpha_e\sum_{k=0}^{n-1}\xi^{k+1}P_k(\cos\alpha_e) - \sum_{k=0}^{n-1}\xi^{k+1}P_{k+1}(\cos\alpha_e)\right) \quad (46)$$

and for the asymptotic behavior $n\sin\alpha_e \gg 1$ we have ($0 < \alpha_e < \pi$):

$$M_n^+ - M_{st}^+ = -\frac{2M_{eq}\upsilon^*\xi^{n+2}\sqrt{\tan\frac{\alpha_e}{2}}}{\cos\frac{\alpha_e}{2}\sqrt{\pi n}(1 - 2\xi\cos\alpha_e + \xi^2)} \times \left[\sin\left(n\alpha_e + \frac{\pi}{4}\right)\sin\frac{\alpha_e}{2} - \frac{1-\xi}{2\xi}\cos\left(\left(n + \frac{1}{2}\right)\alpha_e + \frac{\pi}{4}\right)\right]. \quad (47)$$

4.2. Compensated gradient ($\mathbb{S} = 0$)

If the gradient is compensated during inter-pulse period ($\mathbb{S} = 0$) there is no need for averaging of GF over isochromats. Let us suppose that not only the total gradient area between pulses is zero, but also $\int_0^{TR/2} G(t)dt = 0$, i.e. the signal appears in the center of the inter-pulse period. Then for the generating function one can obtain the following expression:

$$F(z) = \frac{M_{eq}\sqrt{\xi_2}(1 - z\xi_1)(U_0^{1/2}\upsilon + z\xi_2 U_0^{-1/2}\upsilon^*)}{(1-z)\left[1 - z^3\xi_1\xi_2^2 + z\cos\alpha_e(z\xi_2^2 - \xi_1) - z\xi_2(1 - z\xi_1)(\lambda^* U_0^{-1} + \lambda U_0)\right]} = \sum_{n=0}^{\infty} M_n^+ z^n \quad (48)$$

the magnetization number corresponds to the inter-pulse period number, the null-number being assigned to the first period, the quantity $U_0 = e^{-i\Delta\omega TR}$ accounts for phase increment due to the resonance offset, υ and λ are defined in Eqs. (12) and (14) respectively.

The stationary magnetization can be easily obtained with the use of Eqs. (8) and (48):

$$M_{st}^{+} = \frac{M_{eq}\sqrt{\xi_2}(1-\xi_1)(U_0^{1/2}\upsilon + \xi_2 U_0^{-1/2}\upsilon^*)}{1-\xi_1\xi_2^2+\cos\alpha_e(\xi_2^2-\xi_1)-\xi_2(1-\xi_1)(\lambda^* U_0^{-1}+\lambda U_0)}. \quad (49)$$

An explicit analytical expression for M_n^+ can be found from the GF in two particular cases. The first one is when $T_1 = T_2$ ($\xi_1 = \xi_2 = \xi$) and the expression for magnetization is as follows:

$$M_n^{+} = \frac{M_{eq}}{\xi^{3/2}}\left[\frac{\xi^2\left(U_0^{1/2}\upsilon + \xi U_0^{-1/2}\upsilon^*\right)}{1+2\xi\left(\sin^2\frac{\alpha_e}{2} - \frac{\lambda^* U_0^{-1}+\lambda U_0}{2}\right)+\xi^2} - \frac{U_0^{1/2}\upsilon + z_1\xi U_0^{-1/2}\upsilon^*}{z_1^{n+1}(1-z_1)(z_1-z_2)} + \frac{U_0^{1/2}\upsilon + z_2\xi U_0^{-1/2}\upsilon^*}{z_2^{n+1}(1-z_2)(z_1-z_2)}\right], \quad (50)$$

where $z_{1,2}$ are the roots of the quadratic equation

$$1+2z\xi\left(\sin^2\frac{\alpha_e}{2} - \frac{\lambda^* U_0^{-1}+\lambda U_0}{2}\right)+z^2\xi^2 = 0.$$

The second case is when $\Delta\omega = 0$ (i.e. resonance), then $U_0 = 1$, $\alpha_e = \alpha$ and the nth magnetization amplitude M_n^+ is given by

$$M_n^{+} = M_{eq}\frac{i\sin\alpha}{\xi_1\xi_2^{1/2}}\left[\frac{\xi_1\xi_2(1-\xi_1)}{1-(\xi_1+\xi_2)\cos\alpha+\xi_1\xi_2} - \frac{1-Z_1\xi_1}{Z_1^{n+1}(1-Z_1)(Z_1-Z_2)} + \frac{1-Z_2\xi_1}{Z_2^{n+1}(1-Z_2)(Z_1-Z_2)}\right], \quad (51)$$

where $Z_{1,2}$ are the roots of the following quadratic equation

$$1 - z(\xi_1+\xi_2)\cos\alpha + z^2\xi_1\xi_2 = 0.$$

5. Comparison of theory and experiment

To illustrate the use of our method, we carried out two experiments. The first spin-echo experiment was conducted on a Bruker Tomikon S50 tomography system (0.5 T). Spin echo measurements were carried out with a phantom prepared as an aqueous solution of copper sulfate. For all images, the parameters were as follows: non-selective rectangular-shaped RF pulses with $\omega_1 = 3140$ rad/s and flip angle $\omega_1\tau = \frac{\pi}{2}$, echo time $TE = 15$ ms. In this experiment, eight refocusing $\frac{\pi}{2}$-pulses were applied and eight echo signals were collected, the excitation pulse flip angle was equal to $\frac{\pi}{2}$. The resonance offset was set to $\Delta\omega = 0$ rad/s. Fitting the experimental echoes under the assumption that $T_1 = T_2$, we found the best fit for $T_1 = T_2 = 268$ ms. These values agree with the ones measured with conventional CPMG sequence and inversion-recovery methods. As it is seen in Fig. 1, there is a good agreement between the experimental echo amplitudes and the values calculated from Eq. (32).

The second spin-echo experiment was done at 300 MHz on a Bruker DRX-300 NMR spectrometer equipped with the microimaging accessory. The refocusing flip angle in this experiment was equal to $\pi/4$, and tap water was used to prepare the sample. RF magnetic field magnitude was equal to 22,430 rad/s, $TE = 780$ µs, 32 echoes were collected. There were two measurements, one with the pulses applied on resonance, another one with the resonance offset $\Delta\omega = 37{,}700$ rad/s. Since $T_1 \sim T_2 \sim 3s \gg TE = 780$ µs, one can neglect spin relaxation for all 32 echoes and Eqs. (35) and (36) can be employed. The results of comparison of the calculated and the experimental echo amplitudes are depicted in Figs. 2 and 3. They show a good though not a perfect fit of the experimental data (open circles) with the calculated (solid circles connected with a dotted line) echo amplitudes even for large resonance offsets comparable to the RF pulse amplitude. The small deviations of theoretical echo amplitudes from experimental ones we attribute to the nonhomogeneity of RF field within the sample.

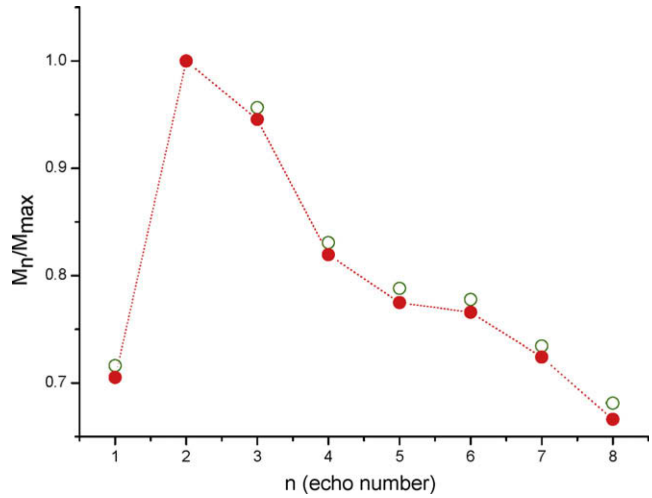

Fig. 1. Experimental (open circles) and calculated (solid circles connected with dotted line) amplitudes of eight successive echoes. Resonance excitation and refocusing ($\Delta\omega = 0$ rad/s), RF field amplitude is equal to $\omega_1 = 3140$ rad/s, RF-pulse flip angle is $\pi/2$. $T_1^{conv} = 273$ ms, $T_1^{GF} = 268$ ms (subscripts "conv" and "GF" denote "conventional method" and "generating function", respectively).

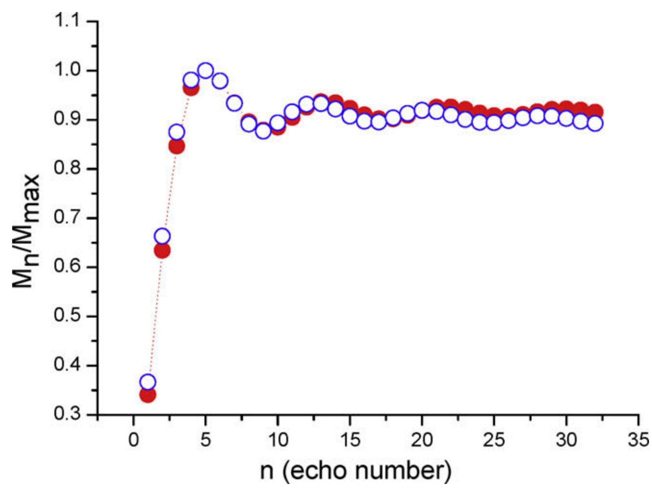

Fig. 2. Experimental (open circles) and calculated (solid circles connected with dotted line) amplitudes of 32 successive echoes. Resonance excitation and refocusing ($\Delta\omega = 0$ rad/s), RF field amplitude is equal to $\omega_1 = 22{,}430$ rad/s, RF-pulse flip angle is $\pi/4$.

6. Conclusions

A new approach for analyzing the behavior of a spin system in a periodic spin Hamiltonian was suggested. The approach is based on the so-called generating function formalism and simplifies the analysis of the spin system behavior under the influence of periodic trains of RF pulses since this function comprises complete information about all density matrices at once. General expression for GF was found that allows one to derive analytical expressions for GF of spin density matrix (magnetization, coherences) in each particular case.

The approach is especially efficient for the analysis of multiecho sequences, when to find the echo amplitude one has to average over different isochromats. Furthermore the generating function formalism allows one to extract easily the spin system parameters from experimental data either by constructing the "experimental" GF [2] and fitting it by the theoretical one or by direct fitting of

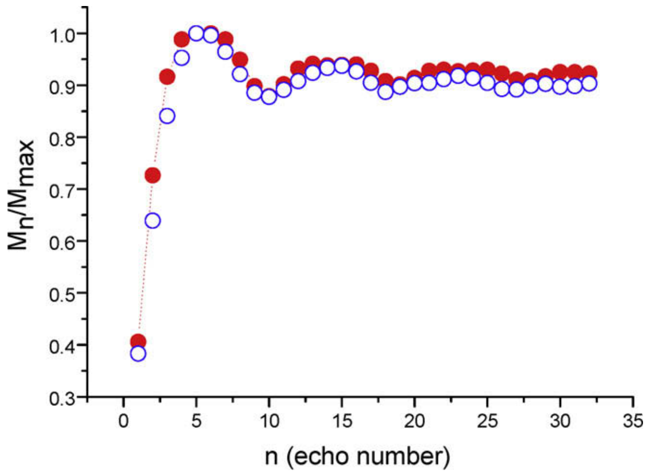

Fig. 3. Experimental (open circles) and calculated (solid circles connected with dotted line) amplitudes of 32 successive echoes. Resonance offset for refocusing pulses is $\Delta\omega$ = 37,700 rad/s, RF field amplitude is equal to ω_1 = 22,430 rad/s, RF-pulse is $\pi/4$.

experimental and theoretical (obtained from the GF) magnetizations. The latter can be easily done by using the Fourier transform.

Two spin-echo experiments were performed with flip angles of refocusing pulses equal to $\pi/2$ or $\pi/4$. In the latter experiment, two measurements with the same sample were performed, with the on resonance and out of resonance excitation and refocusing pulses. It was shown that echo amplitudes calculated using the generating function formalism nicely fit the experimental echo amplitudes.

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Appendix A. Derivation of Eq. (37)

Let us consider the recursion Eq. (20) for the case of phase cycling of refocusing pulse. The nth refocusing pulse then has the phase $(n-1)\phi$, where ϕ is the phase increment. The rotation matrix P_n of the pulse can be represented as:

$$\mathbf{P}_n = \mathbf{\Lambda}^{-(n-1)}\mathbf{P}\mathbf{\Lambda}^{n-1}, \tag{A.1}$$

where

$$\mathbf{\Lambda} = \begin{pmatrix} e^{i\phi} & 0 & 0 \\ 0 & e^{-i\phi} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{A.2}$$

and $\mathbf{P}$ is the same as in Eq. (11), i.e. the rotation matrix of RF pulse with zero phase. Then the magnetization at the instant of the $(n+1)$th echo $\vec{M}_{n+1}$ is related with $\vec{M}_n$ in the following way:

$$\begin{aligned}\vec{M}_{n+1} &= \mathbf{Q}\mathbf{P}_{n+1}\mathbf{Q}\vec{M}_n + (\mathbf{Q}\mathbf{P}_{n+1} + \mathbf{I})\vec{S}_{eq} \\ &= \mathbf{Q}\mathbf{\Lambda}^{-n}\mathbf{P}\mathbf{\Lambda}^{n}\mathbf{Q}\vec{M}_n + (\mathbf{Q}\mathbf{\Lambda}^{-n}\mathbf{P}\mathbf{\Lambda}^{n} + \mathbf{I})\vec{S}_{eq}.\end{aligned} \tag{A.3}$$

Taking into account that matrices $\mathbf{Q}$ and $\mathbf{P}$ commute with each other we can recast Eq. (A.3) as:

$$\vec{M}_{n+1} = \mathbf{\Lambda}^{-n}\mathbf{QPQ}\mathbf{\Lambda}^{n}\vec{M}_n + (\mathbf{\Lambda}^{-n}\mathbf{QP}\mathbf{\Lambda}^{n} + \mathbf{I})\vec{S}_{eq}. \tag{A.4}$$

Introducing $\vec{\tilde{M}}_n$:

$$\vec{\tilde{M}}_n = \mathbf{\Lambda}^{n-1/2}\vec{M}_n = (e^{i(n-1/2)\phi}M_n^+, e^{-i(n-1/2)\phi}M_n^-, M_{zn})^{\mathbf{T}} \tag{A.5}$$

one can obtain the following recursion:

$$\vec{\tilde{M}}_{n+1} = \tilde{\mathbf{Q}}\mathbf{P}\tilde{\mathbf{Q}}\vec{\tilde{M}}_n + (\tilde{\mathbf{Q}}\mathbf{P} + \mathbf{\Lambda}^{1/2})\mathbf{\Lambda}^{n}\vec{S}, \tag{A.6}$$

where

$$\tilde{\mathbf{Q}} = \mathbf{Q}\mathbf{\Lambda}^{1/2} = \begin{pmatrix} \sqrt{\xi_2}Ue^{i\phi/2} & 0 & 0 \\ 0 & \sqrt{\xi_2}U^{-1}e^{-i\phi/2} & 0 \\ 0 & 0 & \sqrt{\xi_1} \end{pmatrix}. \tag{A.7}$$

Then the GF for $\vec{\tilde{M}}_n$ can be found with use of Eq. (6):

$$\vec{\tilde{f}}(z,U) = (\mathbf{I} - z\tilde{\mathbf{Q}}\mathbf{P}\tilde{\mathbf{Q}})^{-1}\left[\vec{\tilde{M}}_0 + \frac{z}{1-z}(\tilde{\mathbf{Q}}\mathbf{P} + \mathbf{I})\vec{S}_{eq}\right], \tag{A.8}$$

taking into account that

$$z(1 - z\mathbf{\Lambda})^{-1}\vec{S}_{eq} = \frac{z}{1-z}\vec{S}_{eq} \quad \text{and} \quad \mathbf{\Lambda}^{1/2}\vec{S}_{eq} = \vec{S}_{eq}.$$

It is easy to see that $\tilde{\mathbf{Q}}$ can be obtained from $\mathbf{Q}$ given by (10) just by substitution $U \to Ue^{i\phi/2}$. This makes obvious that averaging $\vec{\tilde{f}}(z,U)$ over U within unity circle (see. Eq. (27)) yields for averaged $\tilde{F}_0(z)$ exactly the same function as given by Eq. (32). Therefore one can write down that

$$\sum_{n=0}^{\infty}\tilde{M}_n^+ z^n = e^{-i\phi/2}\sum_{n=0}^{\infty}M_n^+ z^n e^{in\phi} = F_0(z), \tag{A.9}$$

where $F_0(z)$ is the same as in Eq. (32). From this equation one obtains the following expression for M_n^+ generating function:

$$\sum_{n=0}^{\infty}M_n^+ z^n = e^{i\phi/2}F_0(ze^{-i\phi}). \tag{A.10}$$

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