

Analytical derivation of multiple spin echo amplitudes with arbitrary refocusing angle

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Abstract

Explicit non-recursive expressions for spin echo amplitudes have been derived for CPMG sequences with arbitrary refocusing flip angle.

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1. Introduction

Spin echos are widely used in many areas of magnetic resonance for more than 50 years. Multiple spin echo sequence forms the base for one of the most important method of MR imaging, known as Fast (Turbo) Spin Echo (FSE, TSE). In most cases, the spin echos are generated by classic Carr-Purcell-Meiboom-Gill pulse sequence, where the excitation phase differs from the refocusing phases by 90°, which allows to obtain high signal amplitudes in inhomogeneous fields.

$$\pi/2_y - \tau/2 - \pi_x - \tau - \pi_x - \tau - \pi_x \dots$$

Usage of π refocusing pulses is also a common practice, because they provide highest possible echo amplitudes. Nevertheless, it is known that any refocusing flip angle is able to produce spin echos and in some specific cases it is preferable to use smaller angles e.g. on high-field imaging systems which may impose unacceptable RF power load on a patient by long trains of π radiofrequency pulses.

Also, selective pulses used in MR imaging usually have complex spectra and cannot be described by a single value of refocusing angle. Finally, RF field inhomogeneities make technically impossible creation of exact π pulses. Properties of spin echo sequences with arbitrary refocusing angles were addressed in a number of papers [1–12]. The general response of a nuclear spin system to CPMG-like pulse sequence with arbitrary phases and flip angles was investigated there. The different magnetization pathways generated by a pulse train have been considered in details. The most advanced and complete methods of echo amplitudes calculation were elaborated in [10] and [11]. In [10] it was shown that treatment of the problem in Fourier space (conjugated to space coordinate) leads to rather simple recursive procedure of analytical as well as exact numerical calculation of echo amplitudes. The key point of the work is that the magnetization vector in Fourier space is a sum of finite number of delta functions and such the form keeps on each next step. Isotropic diffusion, transverse and longitudinal relaxation as well as the global transport were taken into account. The similar approach has been developed in [11]. There evolution of the magnetization has been considered in direct space that required numerical integration over the space coordinate. Nevertheless, even these advanced approaches are recursive in origin and do not allow to obtain explicit analytical expressions

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for echo amplitudes. Besides, programming of these algorithms are not so straightforward. To our knowledge the theory still lacks a closed form expression for echo amplitudes. In the present work, we fill partially this gap. Though we did not succeed to take into account self-diffusion we managed to obtain explicit analytical expression for the echo amplitudes in neglect of spin relaxation. In presence of the spin relaxation so-called generating function for echo amplitudes has been obtained. It makes possible to calculate analytically as well as numerically any given number of echo amplitudes all at once using, for instance, Taylor series expansion procedures in Matlab, Mathematica, Maple. The amplitudes can be also calculated numerically employing conventional Fourier transform algorithm.

2. Expansion of the magnetization into configurations

Our treatment of the spin echo evolution is based on the theory of configurations, outlined in [4, chapter 8], with some modifications for the spin echo case.

The formalism is based on the representation of the magnetization of an isochromate after a number of pulses and precession periods as a finite Fourier series. The basic frequency of this series is equal to the phase increment acquired by the transverse magnetization during the inter-echo period (or during half of it). Each term of the Fourier series corresponds to a definite “configuration” that includes all the phase pathways with the same difference of the net number of dephasing and the net number of rephasing periods.

Let θ represent the phase increment which a spin system acquires during half of the inter-echo period due to field inhomogeneities and applied gradients. θ is assumed to be constant for a given voxel position. At the echo time after n th refocusing pulse, in the middle of inter-pulse interval, the transverse magnetization $M_+ = M_x + iM_y$ and the longitudinal magnetization M_z have experienced a whole number of half-periods of evolution. Both may be expressed as discrete sums

$$\begin{aligned} M_+(n, \theta) &= \sum_{k=-2n}^{2n} F_k e^{ik\theta} \\ M_-(n, \theta) &= \sum_{k=-2n}^{2n} F_k^* e^{-ik\theta} = \sum_{k=-2n}^{2n} F_{-k}^* e^{ik\theta} \\ M_z(n, \theta) &= \sum_{k=-2n}^{2n} Z_k e^{ik\theta} \end{aligned} \quad (1)$$

where k is the difference between the number of dephasing and rephasing half-periods.

Consider now how the magnetization and configuration amplitudes F_k, F_{-k}, Z_k evolve from one middle of an inter-pulse interval to the middle of the next one. To this end the rotation of the magnetization vector $\vec{M} = (M_+, M_-, M_z)$ due to refocusing pulse with angle α has to be taken into account. It is given by the following expression:

$$\vec{M}^{(0+)} = \begin{pmatrix} \frac{1 + \cos \alpha}{2} & \frac{1 - \cos \alpha}{2} & -i \sin \alpha \\ \frac{1 - \cos \alpha}{2} & \frac{1 + \cos \alpha}{2} & i \sin \alpha \\ -i \sin \alpha & i \sin \alpha & \cos \alpha \end{pmatrix} \vec{M}^{(0-)} = \mathbf{P} \vec{M}^{(0-)} \quad (2)$$

where the superscripts “(0–)” and “(0+)” stand for the states before and after the pulse, respectively.

Now, combining (1) and (2) we see that

$$\begin{pmatrix} \sum_k F_k e^{ik\theta} \\ \sum_k F_k^* e^{-ik\theta} \\ \sum_k Z_k e^{ik\theta} \end{pmatrix}^{(0+)} = \mathbf{P} \begin{pmatrix} \sum_k F_k e^{ik\theta} \\ \sum_k F_k^* e^{-ik\theta} \\ \sum_k Z_k e^{ik\theta} \end{pmatrix}^{(0-)} \quad (3)$$

which reduces to

$$\begin{pmatrix} F_k \\ F_{-k} \\ Z_k \end{pmatrix}^{(0+)} = \mathbf{P} \begin{pmatrix} F_k \\ F_{-k} \\ Z_k \end{pmatrix}^{(0-)} \quad (4)$$

Therefore, we observe the following behavior of the spin system in a multi-echo experiment: after the excitation 90_y° pulse the transverse magnetization is aligned to x' axis, so that $M_+ = F_0 = M_0$, all other configurations are void. Then the magnetization evolves during $\tau/2$ period, all indices of the transverse components are incremented by one. Z states do not change. Next, the refocusing pulse α_x mixes F, F^*, Z configurations of the same order according to Eq. (4). Another half-period of evolution increments all transverse configuration indices, F_{-1}^* becomes $F_0^* = F_0$ and forms the echo. Its amplitude is what we seek. The cycle continues.

3. Derivation of n th echo amplitude

Let us denote the values F_k, F_{-k}, Z_k at the instant of n th echo detection as $F_k(n), F_{-k}^*(n), Z_k(n)$, respectively. Assume that $F_0(0) = F_0^*(0) = M_0$ and $F_k(0) = F_{-k}^*(0) = 0$ for $k > 0$ where M_0 is the value of transverse magnetization just after the initial excitation pulse, $Z_k(0) = 0$ for all k . Now we define functions of complex variable u : $S_n(u), \tilde{S}_n(u), \Omega_n(u)$ in the following way:

$$\begin{aligned} S_n(u) &= \sum_{k=-\infty}^{k=\infty} F_k(n) u^k \\ \tilde{S}_n(u) &= \sum_{k=-\infty}^{k=\infty} F_{-k}^*(n) u^k \\ \Omega_n(u) &= \sum_{k=-\infty}^{k=\infty} Z_k(n) u^k \end{aligned} \quad (5)$$

Actually these functions are Laurent series with quantities $F_k(n), F_{-k}^*(n), Z_k(n)$ as their coefficients. Setting $u = e^{i\theta}$ one obtains the magnetization components defined by Eq.

(1). Let us now find relation between these functions for index n and $n + 1$. One has to consider evolution of this quantity during half of an inter-echo period, then action of α angle pulse and again evolution during next half of the inter-echo period. Quantities $F_k(n), F_{-k}^*(n), Z_k(n)$ transform themselves during half inter-echo period in the following way:

$$\begin{aligned} F_k(n) &\rightarrow F_{k+1}(n) \\ F_{-k}^*(n) &\rightarrow F_{-(k-1)}^*(n) \\ Z_k(n) &\rightarrow Z_k(n) \end{aligned} \tag{6}$$

It is easy then to derive that functions $S_n(u), \tilde{S}_n(u), \Omega_n(u)$ are changed after half of inter-echo period by the simple law:

$$\begin{aligned} S_n(u) &\rightarrow uS_n(u) \\ \tilde{S}_n(u) &\rightarrow \frac{1}{u}\tilde{S}_n(u) \\ \Omega_n(u) &\rightarrow \Omega_n(u) \end{aligned} \tag{7}$$

Taking into account the effect of α pulse given by Eq. (2) and evolution during the second half of inter-echo period we arrive at the following relations between these functions on n and $n + 1$ step:

$$\begin{pmatrix} S_{n+1}(u) \\ \tilde{S}_{n+1}(u) \\ \Omega_{n+1}(u) \end{pmatrix} = \Lambda \mathbf{P} \Lambda \begin{pmatrix} S_n(u) \\ \tilde{S}_n(u) \\ \Omega_n(u) \end{pmatrix}, \quad \Lambda = \begin{pmatrix} u & 0 & 0 \\ 0 & 1/u & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{8}$$

or explicitly

$$\begin{pmatrix} S_{n+1}(u) \\ \tilde{S}_{n+1}(u) \\ \Omega_{n+1}(u) \end{pmatrix} = \begin{pmatrix} \frac{u^2}{2}(1 + \cos \alpha) & \frac{1 - \cos \alpha}{2} & -iu \sin \alpha \\ \frac{1 - \cos \alpha}{2} & \frac{1}{2u^2}(1 + \cos \alpha) & \frac{i \sin \alpha}{u} \\ \frac{-iu \sin \alpha}{2} & \frac{i \sin \alpha}{2u} & \cos \alpha \end{pmatrix} \times \begin{pmatrix} S_n(u) \\ \tilde{S}_n(u) \\ \Omega_n(u) \end{pmatrix} \tag{9}$$

Let us now introduce complex functions of two variables u and z :

$$\begin{aligned} S(u, z) &= \sum_{n=0}^{\infty} S_n(u) z^n = \sum_{k=-\infty}^{+\infty} \sum_{n=0}^{\infty} F_k(n) u^k z^n \\ &= \sum_{k=-\infty}^{\infty} u^k \left(\sum_{n=0}^{\infty} F_k(n) z^n \right) \end{aligned}$$

$$\begin{aligned} \tilde{S}(u, z) &= \sum_{n=0}^{\infty} \tilde{S}_n(u) z^n = \sum_{k=-\infty}^{+\infty} \sum_{n=0}^{\infty} F_{-k}^*(n) u^k z^n \\ &= \sum_{k=-\infty}^{\infty} u^k \left(\sum_{n=0}^{\infty} F_{-k}^*(n) z^n \right) \\ \Omega(u, z) &= \sum_{n=0}^{\infty} \Omega_n(u) z^n = \sum_{k=-\infty}^{+\infty} \sum_{n=0}^{\infty} Z_k(n) u^k z^n \\ &= \sum_{k=-\infty}^{\infty} u^k \left(\sum_{n=0}^{\infty} Z_k(n) z^n \right) \end{aligned} \tag{10}$$

Taking into account Eq. (9) one can easily obtain the following system of linear equations with respect to functions $S(u, z), \tilde{S}(u, z)$ and $\Omega(u, z)$:

$$\begin{pmatrix} S(u, z) - S_0 \\ \tilde{S}(u, z) - \tilde{S}_0 \\ \Omega(u, z) - \Omega_0 \end{pmatrix} = \begin{pmatrix} \frac{zu^2}{2}(1 + \cos \alpha) & \frac{z}{2}(1 - \cos \alpha) & -izu \sin \alpha \\ \frac{(1 - \cos \alpha)z}{2} & \frac{z}{u^2} \frac{(1 + \cos \alpha)}{2} & \frac{iz \sin \alpha}{u} \\ \frac{-i \sin \alpha}{2} zu & \frac{iz \sin \alpha}{2u} & z \cos \alpha \end{pmatrix} \times \begin{pmatrix} S(u, z) \\ \tilde{S}(u, z) \\ \Omega(u, z) \end{pmatrix} \tag{11}$$

where $S_0 = \tilde{S}_0 = M_0, \Omega_0 = 0$. This system can be rewritten as

$$\begin{pmatrix} 1 - \frac{zu^2}{2}(1 + \cos \alpha) & -\frac{z}{2}(1 - \cos \alpha) & izu \sin \alpha \\ -\frac{(1 - \cos \alpha)z}{2} & 1 - \frac{z}{u^2} \frac{(1 + \cos \alpha)}{2} & -\frac{iz \sin \alpha}{u} \\ \frac{i \sin \alpha}{2} zu & -\frac{iz \sin \alpha}{2u} & 1 - z \cos \alpha \end{pmatrix} \times \begin{pmatrix} S(u, z) \\ \tilde{S}(u, z) \\ \Omega(u, z) \end{pmatrix} = \begin{pmatrix} M_0 \\ M_0 \\ 0 \end{pmatrix} \tag{12}$$

Resolving this system one obtains the following expression for $S(u, z)$:

$$\begin{aligned} S(u, z) &= \frac{z - z^2 - u^2(2 + z + z^2) + z(1 - z + u^2(3 + z)) \cos \alpha}{(-1 + z)[z + u^4z - 2u^2(1 + z + z^2) + (1 + u^2)^2z \cos \alpha]} M_0 \end{aligned} \tag{13}$$

It depends only on z and $q = u^2$ and can be recast as

$$\begin{aligned} S(q, z) &= \frac{z - z^2 - q(2 + z + z^2) + z(1 - z + q(3 + z)) \cos \alpha}{[(-1 + z)z + (-1 + z)z \cos \alpha](q - q_1)(q - q_2)} M_0 \end{aligned} \tag{14}$$

where

$$q_1 = \frac{2 + 2z + 2z^2 - 2z \cos \alpha - 2(1+z)\sqrt{1+z^2-2z \cos \alpha}}{2(z+z \cos \alpha)}$$

$$q_2 = \frac{2 + 2z + 2z^2 - 2z \cos \alpha + 2(1+z)\sqrt{1+z^2-2z \cos \alpha}}{2(z+z \cos \alpha)} \quad (15)$$

Now let us find the amplitude of n th echo that is quantity $F_0(n)$. As the first step we obtain the value of coefficient preceding u^0 in function $S(u, z)$ Laurent expansion or, what is the same, coefficient preceding q^0 . This coefficient is actually a function of variable z . Let us denote it as $\mathcal{F}(z)$. It is obvious from Eq. (10) that

$$\mathcal{F}(z) = \sum_{n=0}^{\infty} F_0(n) z^n \quad (16)$$

That is n th coefficient of Taylor expansion of $\mathcal{F}(z)$ with respect to z gives amplitude $F_0(n)$ of n th echo signal. One can say that $\mathcal{F}(z)$ is a generating function for echo amplitudes. It is known from the theory of functions of complex variables [13] that “coefficient” $\mathcal{F}(z)$ at zero degree of u or that is the same at zero degree of $q = u^2$ in Laurent expansion of function $S(u, z)$ can be found as integral along the unity circle contour in the complex plane, i.e.

$$\mathcal{F}(z) = \frac{1}{2\pi i} \oint_{|q|=1} \frac{S(q, z)}{q} dq \quad (17)$$

We can represent the function $S(u, z)$ as

$$S(q, z) = \frac{\varphi(q, z)}{(q - q_1)(q - q_2)} \quad (18)$$

where

$$\varphi(q, z) = -\frac{z - z^2 - q(2 + z + z^2) + z(1 - z + q(3 + z)) \cos \alpha}{(-1 + z)z + (-1 + z)z \cos \alpha} M_0 \quad (19)$$

For roots q_1, q_2 occurs $q_1 q_2 = 1$. This means that one root lies inside the unity circle, whereas the another one outside it. Namely q_1 lies inside the unity circle and q_2 outside it for $|z| < 1$. Then for evaluating of the integral (17) one needs to calculate residues of the function $S(q, z)$ with respect to variable q inside the unity circle. There are two poles inside the circle: $q = q_1$ and $q = 0$. Thus, the integral (17) is equal to

$$\mathcal{F}(z) = \text{res}_{q=0} S(q, z) + \text{res}_{q=q_1} S(q, z)$$

$$= \varphi(0, z) + \frac{\varphi(q_1, z)}{q_1(q_1 - q_2)} \quad (20)$$

For calculation of the residue at $q = 0$ we took into account that $q_1 q_2 = 1$. Performing calculation of $\mathcal{F}(z)$ according to Eq. (20) we arrive at the following result:

$$\mathcal{F}(z) = M_0 \left(\frac{1}{2} + \frac{1}{2} \frac{\sqrt{1+z^2-2z \cos \alpha}}{1-z} \right) \quad (21)$$

The coefficient at z^n degree in Taylor expansion of the function $\mathcal{F}(z)$ gives quantity $F_0(n)$ —magnitude of n th echo. Using the well-known expansion

$$\frac{1}{\sqrt{1+z^2-2z \cos \alpha}} = \sum_{n=0}^{\infty} z^n P_n(\cos \alpha) \quad (22)$$

where $P_n(\cos \alpha)$ are Legendre polynomials and representing $\mathcal{F}(z)$ in equivalent form

$$\mathcal{F}(z) = \frac{M_0}{2} \left(1 + \frac{1+z^2-2z \cos \alpha}{(1-z)\sqrt{1+z^2-2z \cos \alpha}} \right) \quad (23)$$

one obtains for the amplitude of n th echo $F_0(n)$

$$F_0(n) = \frac{M_0}{2} \left(\sum_{k=0}^n P_k(\cos \alpha) - 2 \cos \alpha \sum_{k=0}^{n-1} P_k(\cos \alpha) + \sum_{k=0}^{n-2} P_k(\cos \alpha) \right) \quad (24)$$

It is interesting to note that there is an efficient way to compute the sums of Legendre polynomials using Clenshaw method [14]. The algorithm may be summarized as

$$\sum_{k=0}^n P_k(x) = b_0(x)$$

$$b_j(x) = x \frac{2j+1}{j+1} b_{j+1}(x) - \frac{j+1}{j+2} b_{j+2}(x) + 1 \quad (25)$$

$$b_{n+1} = b_{n+2} = 0$$

One can find asymptotic of the expression when $n \rightarrow \infty$ employing an integral representation of Legendre polynomial $P_n(\cos \alpha)$

$$P_n(\cos \alpha) = \frac{1}{\pi \sqrt{2}} \int_{-\alpha}^{\alpha} \frac{e^{i(n+\frac{1}{2})\vartheta} d\vartheta}{\sqrt{\cos \vartheta - \cos \alpha}} \quad (26)$$

Asymptotic of $F_0(n)$ is then

$$F_0(n \rightarrow \infty) = M_0 \left(\sin \frac{\alpha}{2} - \frac{1}{2\sqrt{2\pi}} \frac{\sqrt{\sin \alpha} \cos(n\alpha - \pi/4)}{\sin \frac{\alpha}{2} n^{3/2}} \right) \quad (27)$$

Notice that to exploit this asymptotic for an arbitrary value of angle α one has to substitute α with angle α_0 , $0 \leq \alpha_0 \leq \pi$ i.e. lies in range $(0, \pi)$ and so that $\cos \alpha_0 = \cos \alpha$.

Expression (27) confirms the long known fact [2] that spin echo amplitudes converge to $M_0 \sin(\alpha/2)$ oscillating with the period $2\pi/\alpha$.

4. Echo trains in presence of spin relaxation

Hitherto we neglected spin relaxation effects. Carrying out similar treatment as on derivation of Eq. (9) and taking into account effects of relaxation between RF pulses only

(neglecting relaxation during RF pulse) one easily arrives at the following equations

$$\begin{pmatrix} S_{n+1}(u) \\ \tilde{S}_{n+1}(u) \\ \Omega_{n+1}(u) \end{pmatrix} = \begin{pmatrix} \frac{u^2}{2}(1 + \cos \alpha)\kappa_2 & \frac{1 - \cos \alpha}{2}\kappa_2 & -iu\sqrt{\kappa_1\kappa_2} \sin \alpha \\ \frac{1 - \cos \alpha}{2}\kappa_2 & \frac{(1 + \cos \alpha)}{2u^2}\kappa_2 & \frac{i \sin \alpha}{u}\sqrt{\kappa_1\kappa_2} \\ \frac{-iu \sin \alpha}{2}\sqrt{\kappa_1\kappa_2} & \frac{i \sin \alpha}{2u}\sqrt{\kappa_1\kappa_2} & \kappa_1^2 \cos \alpha \end{pmatrix} \times \begin{pmatrix} S_n(u) \\ \tilde{S}_n(u) \\ \Omega_n(u) \end{pmatrix} \quad (28)$$

where $\kappa_1 = e^{-\tau/T_1}$ and $\kappa_2 = e^{-\tau/T_2}$. Proceeding further in a similar way as on derivation of Eq. (21) one obtains

$$\mathcal{F}(z) = \frac{M_0}{2} \left(1 + \sqrt{\frac{(1 + z\kappa_2)[1 - z \cos \alpha(\kappa_1 + \kappa_2) + z^2\kappa_1\kappa_2]}{(-1 + z\kappa_2)[-1 + z \cos \alpha(\kappa_1 - \kappa_2) + z^2\kappa_1\kappa_2]}} \right) \quad (29)$$

It is easy to see that in absence of relaxation i.e. for $\kappa_1 = \kappa_2 = 1$ this expression reduces to Eq. (21). For particular angle $\alpha = \pi$ one has for any κ_1

$$\mathcal{F}(z) = \frac{M_0}{1 - \kappa_2 z} = M_0(1 + \kappa_2 z + \kappa_2^2 z^2 + \dots + \kappa_2^n z^n + \dots) \quad (30)$$

Thus, the coefficient at n th degree of z that gives the amplitude of n th echo is equal to $M_0\kappa_2^n = M_0e^{-n\tau/T_2}$, which is the well-known result for CPMG sequence. In practically important “extreme narrowing” conditions, when $\kappa_1 = \kappa_2$ we observe the signal according to Eq. (24) damped by monoexponential relaxation decay for any flip angle α because the spin-lattice interaction equally effective destroys S, \tilde{S} and Ω components of the magnetization.

The coefficients in Taylor expansion of Eq. (29) can be easily found by numerical calculations. It is obvious that for $\kappa_{1,2} < 1$, i.e. in presence of spin relaxation the series converges for $z = e^{i\theta}$, $|z| = 1$. Then one has

$$\mathcal{F}(z = e^{i\theta}) = F_0(0) + F_0(1)e^{i\theta} + F_0(2)e^{2i\theta} + \dots + F_0(n)e^{in\theta} + \dots \quad (31)$$

which clearly indicates that all F_0 values may be instantly calculated by discrete Fourier transform of a sampled variant of $\mathcal{F}(z)$

$$F_0(0 \dots n) = \text{FT} \left(\mathcal{F}(e^{i\theta}) \sum_{j=1}^m \delta \left(\theta - \frac{2\pi j}{m} \right) \right) \quad (32)$$

The number of samples m should be selected large enough to ensure $F_0(n) \gg F_0(n + m)$.

In case of reverse task when it is necessary to find relaxation times and angle α from experimentally measured echo amplitudes one can calculate “experimental” generating function according to (16) and then find T_1, T_2, α from best fit of it by analytical expression (29) for set of parameters $|z| \leq 1$, for instance taken on the unity circle $|z| = 1$. In the case when amplitude of experimental highest echo is not vanishingly small one should use an apodization procedure to make amplitude of highest echo negligible. This apodization provides accurate comparison of experimental and analytical generating function since allows one to cut off infinite series (16) while calculating “experimental” function $\mathcal{F}(z)$. This apodization procedure can be done by entering of an exponential decay for echoes that is equivalent to redefinition of relaxation times in a following way: $1/\tilde{T}_i = 1/T_i + 1/\tau_a$. Here, \tilde{T}_i is redefined relaxation time ($i = 1, 2$) and τ_a is the apodization decay time.

5. Conclusions

Closed analytical expressions for echo amplitudes in multiple spin echo sequences have been obtained for arbitrary refocusing pulse angle. In neglectation of spin relaxation these amplitudes were represented in terms of sums of Legendre polynomials. Analytical expression for so-called generating function whose Taylor series coefficients are equal to the echo amplitudes was derived for a general case including relaxation. The latter allows efficient numerical calculation of the amplitudes using fast Fourier transform algorithm.

Asymptotic behavior of the spin echo amplitudes has been shown to confirm with earlier numerical evaluations.

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