Effects of Restricted Diffusion on FID Signal Formation

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Abstract: BOLD imaging has boosted interest in the theory of free induction decay (FID) signal formation. Known theoretical approaches describe FID signal in two opposite regimes: static dephasing regime (1-3), when characteristic dephasing time t_c is much shorter than diffusion time t_D, and motional narrowing regime (t_c>> t_D) (4). Herein we describe an exact solution to the problem of FID signal formation in 1D, 2D, and 3D models of restricted diffusion and demonstrate how signal shape in the static dephasing regime transforms with increasing diffusion coefficient to Lorentzian shape in the motional narrowing regime. The theory also gives new insights into lung MRI with hyperpolarized gases.

Methods: The presence of inhomogeneous magnetic field $\mathbf{H}(\mathbf{r})$ modifies FID signal by a factor

$$S(t) = \langle \exp[i\varphi(t)] \rangle , \qquad [1]$$

where $\varphi(t)$ is the phase accumulated by a single spin by time t after RF pulse , and <...> means averaging over all possible spin's initial positions and trajectories. The phase of the spin moving along a given trajectory $\mathbf{r}=\mathbf{r}(t)$ is

$$\varphi(t) = \int_0^t dt' \omega(\mathbf{r}(t'), t') \qquad [2]$$

where $\omega = \gamma$H is the Larmor frequency, γ is the gyromagnetic ratio. Using the trapezoidal approximation for numerical calculation of integrals, we divide the spin's trajectory into N small intervals, Δt, $t=N\cdot\Delta t$. In the case of a constant field gradient $\mathbf{G}$, the phase takes the form

$$\varphi(t) \simeq \mathbf{q} \cdot \left(\frac{\mathbf{r}_0 + \mathbf{r}_N}{2} + \sum_{n=1}^{N-1} \mathbf{r}_n \right) \qquad [3]$$

where $\mathbf{r}_n$ is a spin position at an instant ($n\cdot\Delta t$) and $\mathbf{q}=\gamma\mathbf{G}\,\Delta t$.

The phase [3] corresponds to the specific spin's trajectory; we should further average it over all possible trajectories, introducing the probability that the spin, starting at the point $\mathbf{r}_0$, successively passes the points $\mathbf{r}_1$, $\mathbf{r}_2$, ···, $\mathbf{r}_N$. This probability is a product $\rho(\mathbf{r}_0) \cdot P(\mathbf{r}_1, \mathbf{r}_0, \Delta t) \cdot .. \cdot P(\mathbf{r}_N, \mathbf{r}_{N-1}, \Delta t)$, where $\rho(\mathbf{r}_0)$ is the initial spin distribution (for the homogeneous distribution, $\rho(x_0)=1/V$, V is the system volume). $P(\mathbf{r}, \mathbf{r}', \Delta t)$ is the propagator determining the probability that a particle starting at the point $\mathbf{r}'$ moves to the point $\mathbf{r}$ during the time interval Δt, satisfying the diffusion equation. It allows the expansion in terms of the orthonormal set of eigenfunctions $\{u_k(\mathbf{r})\}$ of the Sturm-Liouville problem:

$$P(\mathbf{r}, \mathbf{r}', t) = \sum_{k=0}^{\infty} u_k(\mathbf{r}) u_k^*(\mathbf{r}') \exp(-\lambda_k t) , \qquad [4]$$

where λ_k are the corresponding eigenvalues.

Making use of Eqs.[1]-[4], the signal can be written in the form of a matrix product

$$S(t) = \mathbf{F}(\mathbf{q}/2) \cdot \hat{\mathbf{\Lambda}}(\Delta t) \cdot \left[\hat{\mathbf{U}}(\mathbf{q}) \cdot \hat{\mathbf{\Lambda}}(\Delta t) \right]^{N-1} \cdot \mathbf{F}^{\dagger}(-\mathbf{q}/2) , \qquad [5]$$

where $F_k(\mathbf{q}) = V^{-1/2} \int_V d\mathbf{r}\, u_k(\mathbf{r}) \exp(-i\mathbf{q}\mathbf{r})$,

$$U_{kk'}(\mathbf{q}) = \int_V d\mathbf{r}\, u_k^*(\mathbf{r}) u_{k'}(\mathbf{r}) \exp(-i\mathbf{q}\mathbf{r}), \quad \Lambda_{kk} = \exp(-\lambda_k \Delta t)$$

The expression [5] is similar to that obtained in Ref.(5) (as a particular case $\mathbf{G}(t)$=const) in the framework of the multipulse approach first proposed in Ref.(6). The minor difference is in the argument in the elements of $\mathbf{F}$. For numerical calculations we should choose an appropriate time step Δt and a number M of eigenfunctions involved in the expansion [4]. The value of Δt should be much less than both characteristic times, Δt<<t_D, t_c. The exponential decrease of the elements of the diagonal matrix $\hat{\mathbf{\Lambda}}$ makes it possible to restrict to M<10 for most cases of interest.

Results: Making use of the known solutions of the diffusion equation in 1D, 2D, and 3D models with reflecting boundaries (within segment, circle and sphere, respectively), we calculate the elements of $\mathbf{F}$, $\hat{\mathbf{U}}$ and $\hat{\mathbf{\Lambda}}$ and the FID signal $S(t)$. The behavior of the latter is determined by the characteristic dephasing time $t_c = 2\pi/(\gamma G a)$ and the diffusion time $t_D=a^2/D$, where a is a size of the system (segment length, circle or sphere diameter) and D- is the diffusion coefficient. In Fig.1 we plot the logarithm (base 10) of the modulus of the signal in 1D system as a function of dimensionless time $\tau = t/t_c$ for several values of the parameter $p = t_c/t_D = 2\pi D/(\gamma G a^3)$ (the general picture of the signal behavior is the same in 2D and 3D systems).

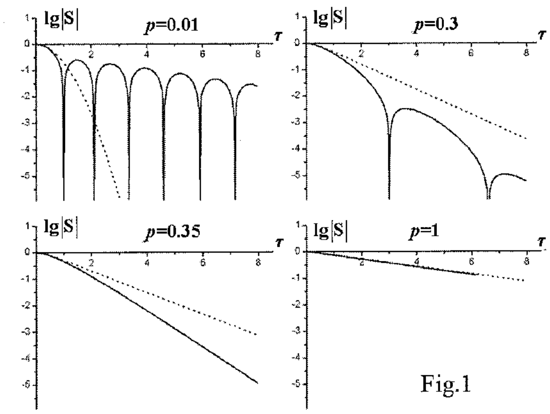

Fig.1

In the static dephasing regime (p=0), the FID signal is described by the *sinc*-function: $S=\sin(\pi\tau)/(\pi\tau)$. For small values of p the sign of the FID signal remains with time τ (in contrast to spin-echo signal, which always remains positive). The sharp minima in Fig.1 correspond to $S(\tau)$=0. As p increases, the "period" of the oscillations increases, the zeros of $S(\tau)$ shifting to larger values of τ. For $p\geq0.35$ the function $S(t)$ decreases monotonically (at least, there is no zero of $S(t)$ in the range τ<8); however, the question whether there are oscillations for large values of p or a "phase transition" to monotone behavior takes place for a certain $p=p^*$ remains open. As p further increases, the slope of the curves $\lg|S(\tau)|$ decreases, meaning decreased in the signal attenuation (motional narrowing).

The signal calculated in the framework of the Gaussian approximation is shown in Fig.1 by dashed lines. Comparison shows that this approximation is valid in two cases: 1) in the short-time interval, τ < 0.5 (i.e. t < 0.5 t_c) for any value of p, and 2) in motional narrowing regime (p > 1) for all τ.

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