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Parallel acquisition of q-space using second order magnetic fields for single-shot diffusion measurements

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ABSTRACT

A proof of concept is presented for the parallel acquisition of q-space under diffusion using a second order magnetic field. The second order field produces a gradient strength which varies in space, allowing a range of gradients to be applied in a single pulse, and q-space encoded into real space. With the use of a read gradient, the spatial information is regained from the NMR signal, and real space mapped onto q-space for a thin slice excitation volume. As the diffusion encoded image for a thin slice can be mapped onto q-space, and the average propagator is the inverse Fourier transform of the q-space data, it follows that the acquisition of the echo is a direct measurement of the average propagator. In the absence of a thin slice selection, the real space to q-space mapping is lost, but the ability to measure the diffusion coefficient retained with an increase in signal to noise.

1. Introduction

Measurement of the diffusive process using magnetic gradient fields was first described by Hahn [1], with implementation and further development using constant and pulsed gradient fields by others [2–5]. Of particular significance to this research is the method developed by Stejskal and Tanner [4], often referred to as pulsed gradient spin echo (PGSE) [6]. The measurement of diffusion has since developed into a powerful tool for probing a range of properties, including the pore space geometry of porous media [7–17], the average propagator for displacement [18,19], and for the characterisation of emulsions [20,21].

With the application of pulsed magnetic field gradients in PGSE, a wave vector $\mathbf{q} = \gamma\delta\mathbf{g}$ is used to encode for displacement $\mathbf{R}$ over a time Δ, where $\mathbf{g}$ is the magnetic gradient field and δ is the gradient pulse duration. As spins diffuse, and the diffusive process is random, they accumulate random phase shifts due to the pulsed gradients. These random phase shifts result in attenuation of the echo to a degree related to experimental parameters and the diffusion coefficient D. For diffusion in the Gaussian regime, the normalised signal amplitude as a function of $q = |\mathbf{q}|$ obeys the relation

$$E_N(q) = \exp\{-q^2 D\Delta\} \tag{1}$$

for $\delta \ll \Delta$. By collecting data points in q-space, this relation can be used to measure D.

Traditionally, pulses of a constant magnetic field gradient have been used to encode for q-space. For such a gradient field, the magnitude of the magnetic field component along the direction of B_0 exhibits a linear relationship with respect to position along an axis. The amplitude of these gradient pulses is varied from experiment to experiment, each one yielding a single data point in q-space. For the parallel acquisition of q-space and single-shot diffusion measurement presented here, a second order magnetic field coil is employed to produce a field strength which varies quadratically with respect to two axes, and a gradient strength which varies linearly in space. By encoding for displacement with such a field, a range of q-space is encoded into real space in a single experiment. With the use of a read image and slice selection, a real space image is acquired which can be mapped onto q-space, and a data set $E(\mathbf{q})$ acquired in parallel for a homogeneous sample. Here the homogeneity of the sample is of importance to this technique. As the diffusive attenuation is measured across the read image, the value of the diffusion coefficient and spin density must remain constant in order for the analysis presented in this paper to hold.

In the past, this second order magnetic field has sometimes been referred to as a parabolic field, which is misleading as a parabolic magnetic field is impossible to generate due to Maxwell's

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equations. These second order magnetic fields have been used for new imaging techniques such as *o*-space imaging [22], qualitative single-shot measurements of diffusion coefficients in DOSY spectra [23], and the effects on diffusion measurements thoroughly investigated [24,25], but have never before been used for the parallel acquisition of *q*-space.

Some single-shot diffusion measurements have been developed which rely on multiple excitations and multiple echoes [26,27], multiple observation times [28], and multiple gradient echoes [29]. With the measurement technique presented in this paper, the diffusion coefficient can be measured at a well defined observation time through the acquisition of a single echo, using a single excitation pulse.

In addition to providing a method for parallel acquisition of *q*-space, this method allows for the direct measurement of the average propagator $\overline{P}$. For diffusion within the Gaussian regime, the propagator obeys the relation

$$\overline{P}(\mathbf{R},\Delta) = (4\pi D\Delta)^{-n/2}\exp\left\{-\frac{\mathbf{R}\cdot\mathbf{R}}{4D\Delta}\right\} \quad (2)$$

where n is the number of dimensions in which diffusion is measured. Conventionally, the average propagator is imaged by collecting *q*-space data and exploiting the Fourier relationship

$$E(\mathbf{q},\Delta) = \int \overline{P}(\mathbf{R},\Delta)\exp\{-\mathrm{i}(\mathbf{q}\cdot\mathbf{R})\}d\mathbf{R}. \quad (3)$$

By taking the inverse Fourier transform of $E(\mathbf{q},\Delta)$, the average propagator is obtained. For this new experiment as shown in Fig. 4, real space can be mapped onto *q*-space since $\mathbf{q} \propto \mathbf{r}$. However, the inverse Fourier transform of the real space image is the echo. Therefore, there is no need to perform any Fourier transforms since the echo is the average propagator when normalised and plotted against displacement space.

2. Theory and experimental design

2.1. Maxwell's equations and concomittant fields

For a well defined mapping of a one dimensional read image onto *q*-space, the gradient strength for displacement encoding should vary from pixel to pixel in the read image. As each pixel is composed of signal from a slice of volume along the read direction, and the gradient strength should be constant across each entire slice, the ideal magnetic field for a *q*-space encoded read image is parabolic. This field would give a linear relationship between position along the read direction and *q*. Unfortunately, due to Maxwell's equations, this is impossible as concomitant fields will exist. For conventional gradient coils, the effects of the concomitant fields are sometimes encountered and their effect are well understood [30,31]. In many experiments they can be ignored as they lie perpendicular to the B_0 field, only slightly bending B_0, and do not significantly contribute to its magnitude [32].

At the site of the sample in an NMR system where the field is to be generated, it is safe to assume that in the absence of quickly changing fields, the displacement current will obey $\partial\mathbf{D}/\partial t = 0$, and the current density $\mathbf{J} = 0$ as no current carrying conductors will be present. This results in the magnetic field satisfying Laplace's equation

$$\nabla^2\mathbf{B} = 0 \quad (4)$$

Assuming the Halbach geometry for the NMR magnet to be used, where the static field lies perpendicular to the axis of the magnet bore such that $\mathbf{B}_0 = B_y$, the desired parabolic magnetic field obeys the relation $\partial^2 B_y/\partial y^2 = C$, where C is a constant describing the gradient per meter of the field. Substituting this into Eq. (4), it is found that the desired field cannot exist without $\partial^2 B_y/\partial x^2 + \partial^2 B_y/\partial z^2 = -C$. These are concomitant fields which, because they lie along the direction of B_0, cannot be ignored. To make this field dependent on as few dimensions as possible, the best attempt at creating a parabolic magnetic field is a second order magnetic field obeying $B_y = C(x^2 - y^2)/2$.

To alleviate the dependence of the magnetic field on the $\hat{x}$ direction, either a thin sample should be used, or a slice selection may be applied to excite only a thin slice about $x = 0$. By doing this, the excited volume of the sample will experience a field due to the second order coil which can be approximated by a parabolic field.

2.2. Hardware and coil characterisation

The gradient coils necessary for these experiments are a *y*-gradient to produce a read image, the second order coil to apply a gradient field whose strength is spatially dependent, and an *x*-gradient for slice selection. The NMR magnet used was a Magritek Ltd. 2 MHz Rock Core Analyser, and the gradients were driven by B-AFPA 40 amplifiers.

The conventional *x* and *y* gradient coils for Halbach geometry are known to have a $sin(2\theta)\hat{z}$ current distribution on the surface of a cylinder [6]. This current distribution was approximated by 4 loops of wire whose windings are separated by $\pi/6$ radians, with each loop centred about the *x* and *y* axes for a *y*-gradient, and the *x*-gradient windings rotated $\pi/4$ radians with respect to the *y*-gradient windings (Fig. 1).

A second order magnetic field coil can be shown to possess a $sin(3\theta)\hat{z}$ current distribution on the surface of a cylinder. This current distribution was approximated with 3 loops of wire whose neighbouring edges were separated by $\pi/3$ radians (Fig. 1). The magnetic fields produced by all coils were modelled using a Bio-Savart calculation such that the gradient uniformity and strength could be determined prior to winding, and were characterised using a 3-axis hall probe and NMR experiments after winding.

A robotic mapper with a 3-axis hall probe was first used to acquire a field map on the surface of a 20 mm radius sphere centred in the gradient stack. A spherical harmonic decomposition was performed on the map and the field reconstructed to generate the field and gradient maps shown in Fig. 2 for the second order coil.

A 2-D phase encoded image was obtained using this gradient stack to further characterise the fields produced by the coils. A plastic square prism container, 26.8 mm wide, 50 mm tall, filled with copper sulphate doped water, was imaged using the *x* and *y* gradient coils. With a small DC current running through the second order coil, the 2-D phase encoded image yields an echo for each pixel in space, whose phase evolution in time gives the corresponding field strength at that position due to the second order

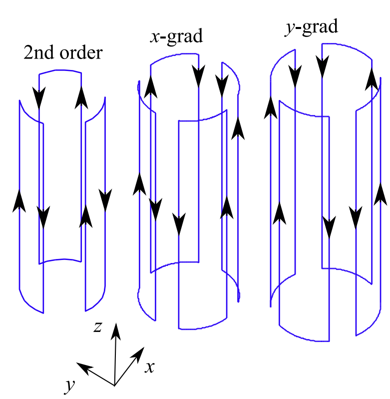

Fig. 1. Coil windings for the gradient stack, with current flow depicted by black arrows.