Excitation of Arbitrary Shapes by Gradient Optimized Random Walk in Discrete $k$-Space

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A new technique for the excitation of arbitrary shapes is proposed. It is based on a parallel sequence of small tip angle RF pulses and gradient pulses. The small tip angle rotations could yield a 90° excitation pulse within the selected excitation profile while outside the profile, the rotations cancel each other. A full theory of the completely arbitrary regional volume excitation (CARVE) method is presented and experimentally verified. In CARVE, $k$-space is discrete because the RF is applied in pulses. The discrete character of $k$-space permits an arbitrary trajectory for the $k$-space walk. The optimal random trajectory is found by minimizing the gradient load using simulated annealing. It is shown, both theoretically and experimentally, that such a trajectory is much better than any other systematic or random trajectory in $k$-space.

Key words: volume selective excitation; $k$-space trajectories; gradient load optimization.

INTRODUCTION

Volume selective experiments acquire the NMR signal from well-defined regions that cover a body part or organ under investigation. However, most well-established methods for volume selective excitation are limited to simple volumes, for example, cubes or spheres, that do not correspond to the complex shapes of organs. In the simplest methods, the volume selectivity is based on the manipulation of partial signals arising from differently oriented slices (1–11), or the inhomogeneity of the RF coils (12–16).

A more sophisticated approach is to apply shaped RF pulses in combination with shaped gradients (17–23). Such complex pulse shapes overcome the restriction of simple excitation profiles, but are very demanding on the gradient hardware. An additional limitation is that the gradient pulse shapes are designed in advance, irrespective of the excitation profile (ramp, sine, cosine) (19, 24) that limits the complexity of the excited domain.

In this article we describe the theory and provide an experimental demonstration of a new technique for completely arbitrary regional volume excitation (CARVE) (25, 26) that enables selective excitation of arbitrary shapes while minimizing the gradient hardware requirements. It is based on the application of simultaneous sequences of an amplitude modulated gradient RF (DANTE (27)) pulse and an amplitude modulated gradient pulse. CARVE operates in discrete $k$-space and thus permits the design of $k$-space trajectories of arbitrary complexity. The basic CARVE trajectory is a random walk in $k$-space whose parameters and properties can be optimized by a suitable technique. We have used the simulated annealing protocol (28, 29) to design a random trajectory that excites an arbitrarily shaped profile with minimal gradient load.

THEORY

Small-Tip-Angle Approximation in a Discrete Form

The building blocks of the CARVE sequence are short RF pulses (with flip angle $\theta$ and phase $\varphi$) and constant gradient pulses $G$ of duration $\Delta t$. The effect of the CARVE sequence on the equilibrium magnetization $M_0(r) = (0, 0, M_0(r))$ (where $\rho(r)$ is a dimensionless quantity proportional to spin density, $\rho(r) \leq 1$) can be conveniently described using rotational matrices. For simplicity, we consider only on-resonance magnetization and neglect the effects of resonance offset, chemical shift and relaxation. After the CARVE sequence with $N$ pulses, $(\theta_1, \varphi_1) \cdot G_1 \cdot (\theta_2, \varphi_2) \cdot G_2 \cdot \ldots \cdot (\theta_N, \varphi_N) \cdot G_N$, the magnetization $M(r)$ at position $r$ is given by

$$M(r) = R_{sk}(\theta_N, \varphi_N) \ldots R_{sk}(\theta_2, \varphi_2) R_{sk}(\theta_1, \varphi_1) R_{sk}(\theta_0)$$

where $\alpha_0 = \gamma \Delta t r G_1$ is an angle for which the magnetization at position $r$ rotates around the $z$ axis in a time $\Delta t$ under the influence of the gradient $G_1$. $R_{sk}(\theta_0)$ and $R_{sk}(\theta_0)$ are transformation matrices that describe this rotation and that are induced by an RF pulse with tilt angle $\theta$ and phase $\varphi$, respectively. Because of the minus sign in the basic NMR equation ($\omega_0 = -\gamma B_z$), the direction of the rotation is reversed. Thus

$$R_{sk}(\theta) = \begin{bmatrix}
\cos(\varphi) & -\sin(\varphi) & 0 \\
\sin(\varphi) & \cos(\varphi) & 0 \\
0 & 0 & 1
\end{bmatrix}$$

$$R_{sk}(\theta) = \begin{bmatrix}
\cos(\varphi) & \sin(\varphi) & 0 \\
0 & 0 & 1
\end{bmatrix}$$

$$R_{sk}(\theta) = \begin{bmatrix}
1 & 0 & 0 & 0 & \cos(\varphi) & \sin(\varphi) & 0 \\
0 & \cos(\theta) & \sin(\theta) & \sin(\varphi) & \cos(\varphi) & 0 \\
0 & -\sin(\theta) & \cos(\theta) & 0 & 0 & 1
\end{bmatrix}$$

The rotation $R_{sk}(\theta)$ is controlled by the magnetic field gradient and $R_{sk}(\theta)$ by the RF pulse. Equation [1] is an...
exact expression for the motion of the nuclear magnetization during CARVE in a model consisting of isolated spins. However, this equation is too complex to enable further theoretical consideration. Since RF pulses in CARVE are short (tip-angles are less than $10^\circ$), a small-tip-angle approximation may be used (20). In this approximation \( \cos(\theta) \approx 1, \sin(\theta) \approx \theta \) and

\[
R_{\theta \phi}(\theta) = \begin{bmatrix}
1 & 0 & -\theta \sin(\phi) \\
0 & 1 & \theta \cos(\phi) \\
\theta \sin(\phi) & -\theta \cos(\phi) & 1
\end{bmatrix}
\]  

[3]

By neglecting the higher order terms in tip-angle \( \theta \) from Eq. [1], one obtains an analytical expression for the magnetization components at the end of the CARVE sequence as

\[
M_x(r) = -M_0 \rho(r) \sum_{i=1}^{N} \alpha_i \sin(\varphi_i - \sum_{j=1}^{N} \alpha_j) 
\]

[4]

\[
M_y(r) = M_0 \rho(r) \sum_{i=1}^{N} \theta_i \cos(\varphi_i - \sum_{j=1}^{N} \alpha_j) 
\]

\[
M_z(r) = M_0 \rho(r) 
\]

This can be represented using complex number notation as

\[
M^*(r) = iM_0 \rho(r) \sum_{i=1}^{N} \Theta_i \exp(-i\gamma \Delta t) \sum_{j=1}^{N} G_j
\]

[5]

where transverse magnetization is \( M^* = M_x + iM_y \) and RF pulse \( \Theta_i = \theta_i \exp(i\varphi_i) \). Equation [5] is the discrete form of the well known small-tip-angle approximation (20). Defining a k-space vector as

\[
k_i = \gamma \Delta t \sum_{j=1}^{N} G_j 
\]

[6]

Eq. [5] simplifies to

\[
M^*(r) = iM_0 \rho(r) \sum_{i=1}^{N} \Theta_i \exp(-i\gamma k_i) 
\]

[7]

Equation [7] describes the spatial dependence of the transverse magnetization after CARVE with \( N \) RF pulses \( \Theta_i \) and \( N \) gradient pulses \( G_i \). Besides the structure of the sequence, the transverse magnetization \( M^*(r) \) also depends on the spin distribution within a volume element of the sample, \( \rho(r) \). To assess the properties of the sequence itself, this dependence on \( \rho(r) \) needs to be eliminated. The excitation profile of the CARVE sequences \( P_n(r) \) is obtained by normalizing Eq. [7] with the spatial distribution of equilibrium magnetization \( M_0 \rho(r) \)

\[
P_n(r) = \frac{M^*(r)}{iM_0 \rho(r)} = \sum_{i=1}^{N} \Theta_i \exp(-i\gamma k_i) 
\]

[8]

It is useful to consider the excitation profile \( P_n(r) \), given by Eq. [8], as a linear combination of \( N \) harmonic functions

\[
P_n(r) = \frac{1}{f} \sum_{i=1}^{N} \Theta_i \xi_i(r); \quad \xi_i(r) = f \exp(-i\gamma k_i) 
\]

[9]

where \( f \) is a normalization constant. Then harmonic functions \( \xi_i \) form a basis for the approximation of a profile of arbitrary shape.

**Arbitrary-Shaped Excitation Profile**

Let \( P(r) \) be an excitation profile of arbitrary shape defined in a box \( \mathcal{L} = \left[ -\frac{L}{2}, \frac{L}{2} \right] \) where \( L \) is the size of the \( D \)-dimensional box. Since the function of the CARVE profile is prescribed by Eq. [9], it is convenient to express \( P(r) \) over a set of the same harmonic functions, \( \xi_i \). To represent a suitable basis \( \xi_i \) must be linearly independent and spanning space \( \mathcal{L} \). Thus,

\[
\langle \xi_i, \xi_j \rangle = \int_{\mathcal{L}} \exp(i\gamma k_i) \exp(-i\gamma k_j) d\mathcal{L} = \delta_{ij}
\]

[10]

with a normalization constant \( f = \frac{2\pi}{L} \). The orthogonality of the harmonic functions \( \xi_i \) in space \( \mathcal{L} \) is accomplished if the \( k \)-space vectors satisfy the condition

\[
k_i = \frac{2\pi}{L} m_i; \quad m_i \in \mathbb{Z}^D 
\]

[11]

where \( m_i \) is an arbitrary \( D \)-dimensional integer vector (30). The conditions from Eqs. [10] and [11] specify harmonic functions as

\[
\xi_i(r) = \frac{1}{L^{D/2}} \exp\left(-\frac{2\pi i m_i r}{L}\right)
\]

[12]

These functions are periodic with a period \( L \) in every orthogonal space direction

\[
\xi_i(r) = \xi_i(r + uL); \quad u \in \mathbb{Z}^D 
\]

[13]

where \( u \) is an arbitrary \( D \)-dimensional integer vector. Thus, an infinite set of harmonic functions (Eq. [12]) form an orthonormal basis in \( \mathcal{L} \) space. Then, any ideal excitation profile \( P(r) \) can be decomposed into an infinite set of harmonic functions \( \xi_i \)

\[
P(r) = \sum_{i=1}^{\infty} \Theta_i \xi_i(r) 
\]

[14]

The coefficients \( \Theta_i \) in Eq. [14] can be calculated by projecting the ideal profile \( P \) on to the basis set of functions \( \xi_i \).
\[ \Theta_i = \frac{1}{L D^{2/3}} \left( \Theta_i, P \right) = \frac{1}{L D^{2}} \int_{D} \exp(i r k_i) P(r) \, dr \]  

[15a]

It should be noted that Eq. [15a] is the Fourier transform of an ideal profile from real space into \( k \)-space. Because in practice an ideal profile is presented in a discrete form, e.g., \( M^2 \), Eq. [15a] becomes

\[ \Theta_i = \sum_{u_i = -M^2/2}^{M^2/2-1} \sum_{u_r = -M^2/2}^{M^2/2-1} \exp \left( \frac{2 \pi i m a}{M} \right) P \left( \frac{a L}{M} \right) \]

[15b]

The magnetization profile excited by the CARVE sequence is composed of a finite number of harmonic functions (Eq. [9]) and is thus an approximation of the ideal excitation profile. When the number of pulses is infinite, the CARVE profile converges toward the ideal excitation profile

\[ \lim_{N \to \infty} P_N(r) = P_\infty(r) = P(r) \]

However, with a suitable projection method, a good approximation of an ideal excitation profile can be realized even with a finite number of pulses.

Projecting an Ideal Excitation Profile onto the CARVE Basis Functions

An ideal excitation profile \( P_\infty \) can be expressed as a sum of the CARVE profile \( P_N \) and residual \( R_N \)

\[ P_\infty(r) = P_N(r) + R_N(r) \]

[16]

To obtain the best approximation of the ideal profile with the CARVE profile, the norm of the residual has to be minimized. Since the CARVE profile is orthogonal to the residual, \( \langle R_N, P_N \rangle = 0 \), the squared norm of an ideal profile is

\[ \| P_\infty \|^2 = \langle P_\infty, P_\infty \rangle = \langle P_N, P_N \rangle + \langle R_N, R_N \rangle = \| P_N \|^2 + \| R_N \|^2 \]

[17]

Utilizing Parseval’s relation (30), Eq. [17] becomes

\[ \| P_\infty \|^2 = L^2 \sum_{l=1}^{N} | \Theta_l |^2 + L^2 \sum_{l=N+1}^{N} | \Theta_l |^2 \]

[18]

Since the norm of an ideal profile is constant, the norm of the residual is minimized when the norm of the CARVE profile is maximized. Therefore, a resemblance factor \( \eta \) \( (\eta \in [0,1]) \) may be introduced as a ratio between the squares of the norm of CARVE and the norm of the ideal excitation profile

\[ \eta = \frac{\sum_{l=1}^{N} | \Theta_l |^2}{\sum_{l=1}^{N} | \Theta_l |^2} \]

[19]

High values of \( \eta \) imply a close similarity between the ideal and CARVE profile.

For a given number of pulses \( N \) and a given excitation profile, \( N \) \( k \)-space points can be selected by maximizing \( \eta \). This is achieved by selecting \( N \) \( \Theta_l \) coefficients with the highest absolute values, out of \( M^2 \) coefficients obtained from Eq. [15b]. Corresponding \( k \)-space points select the harmonic functions on which an ideal profile has the largest projection. These \( k \)-space points are then used to calculate the gradient sequence.

The CARVE Gradient Sequence

Theoretically, the CARVE gradient sequence consists of rectangular gradient pulses of amplitude \( G_i \) and duration \( \Delta t \). During the RF pulse, gradients should be turned off. To eliminate undesired relaxation and off-resonance effects, the interval \( k \Delta t \) should be as short as possible. This may impose severe demands on the gradient hardware and render CARVE virtually impractical. However, gradient effects during the RF pulse can be neglected if (a) the small-tip-angle pulse duration, \( t_p \), is negligible compared with \( \Delta t \), \( t_p \ll \Delta t \), and (b) the frequency offset induced by the maximum gradient pulse is smaller than the pulse bandwidth, \( 2\pi/t_p \gg \gamma G_{\text{max}} L \). In practice, both conditions are easy to fulfill and consequently gradients need not be turned off during the RF pulse. Under these conditions, the gradient pulse sequence becomes a step function

\[ G_i = G_0 n_i \]

[20]

where \( G_0 \) is the magnitude of a gradient step, and \( n_i \) is an integer vector. By substituting Eq. [20] into Eq. [6] while satisfying Eq. [11] one obtains

\[ m_i = \sum_{j=1}^{N} n_j \]

[21a]

with

\[ G_0 = \frac{2\pi}{\gamma \Delta t L} \]

[21b]

The integer vectors \( m_i \) correspond to selected \( k \)-space points \( k_i \) according to Eq. [11]. A sequence of selected \( k \)-space points \( k_1 \cdot k_2 \cdot \ldots \cdot k_N \), determines a sequence of \( k \)-space integer vectors \( m_1 \cdot m_2 \cdot \ldots \cdot m_N \). Then, the sequence of gradient integer vectors \( n_1 \cdot n_2 \cdot \ldots \cdot n_N \) is calculated by taking the derivative of Eq. [21]

\[ n_N = m_N \]

\[ n_i = m_i - m_{i+1}; \quad i = N - 1, \ldots, 1 \]

[22]

Equations [20]–[22] indicate that the gradient sequence critically depends on the order of selected \( k \)-space points; i.e., the trajectory in \( k \)-space determines the magnitude of the gradients. Thus, by suitable selection of the
Construction of the CARVE Profile

A complete CARVE sequence consists of $N$ events each containing an RF pulse with angle, $\theta$, phase, $\varphi$, and $D$ gradients $G^D$, that need to be calculated for each excitation profile. For simplicity, consider a two-dimensional CARVE experiment ($D = 2$). First, the desired excitation profile, which is a binary image of a selected object, is defined as a $256 \times 256$ matrix. As an example we have chosen the figure of the character "A" constructed as a real, binary image (Fig. 1a). The next step involves the calculation of the two-dimensional discrete Fourier transform for the desired profile (a real $256 \times 256$ matrix), yielding coefficients $\Theta_n$, Eq. [15b]. For a discrete two-dimensional ideal profile where $P_{u',v'} = P_{u,v}(u^{2}/M, v^{2}/M)$ and $u', v' = -M/2, \ldots, M/2$, $1$, Eq. [15b] reduces to

$$\Theta_{m',n'} = \frac{1}{M^2} \sum_{u'=-M/2}^{M/2-1} \sum_{v'=-M/2}^{M/2-1} \exp \left( \frac{2\pi i (m'u' + m'v')}{M} \right) P_{u',v'}$$  \[23\]

It can be easily calculated by fast Fourier transformation (FFT). A $256 \times 256$ FFT yields 65,000 k-space coefficients $\Theta_n$ (Fig. 1b). These 65,000 coefficients possess all the information about the desired profile which, in the present case, is the character "A". Since a CARVE sequence with 65,000 events is impractical, it is necessary to reduce the number of events in our case to $N = 100$. This reduction obviously distorts the excitation profile. However, the difference between the ideal and CARVE profiles can be minimized by maximizing the resemblance factor Eq. [19]. This is achieved by selecting 100 k-space coefficients (out of 65,000) with the highest absolute values (Fig. 1c). The absolute values of the selected k-space coefficients are directly proportional to the tip angles $\theta_t$ of the short RF pulses, whereas their phases are equal to the phases of the pulses. Finally, using the known coefficients $\theta_t$ and $k_t$, the CARVE profile is calculated using Eq. [8] (Fig. 1d). The calculated profile represents the best approximation of the desired profile according to Eq. [19].

One should note that the actual CARVE profile is the discrete Fourier transform (DFT) of the selected $N$ coefficients.
FIG. 2. Construction of the k-space trajectory: The k-space coefficients are the same as in Fig. 1c, (a) Random trajectory, (b) spiral trajectory, (c) line trajectory, and (d) random trajectory minimized by simulated annealing, according to Eq. [24]. Because k coefficients are the same, all sequences consist of the same 100 short RF pulses. Only their order depends on the selected trajectory (Eq. [23]). However, gradient sequences in different trajectories are significantly different, since gradient magnitude depends on the selected trajectory (Eq. [20]). Gradient hardware is most loaded in the case of random (unoptimized) k-space trajectory. The load decreases in the spiral and line trajectories and becomes minimal in optimized random trajectory.
Thus, a 256 × 256 DFT generates a 256 × 256 image of the actual curve profile (Fig. 1d). This image can be used to check the quality of the approximation and to correct excitation nonuniformity in experimental NMR images.

**Construction of Gradient Sequence**

The gradient sequence is constructed from the k-space coordinates \( k = 2\pi (n^x, n^y)/L \) of selected coefficients \( k \). The procedure for selecting the coefficients \( k \) does not specify the sequence in which they are visited. Thus, all k-space trajectories are equivalent and would produce the same excitation profile provided each k-space point is visited only once. However, various trajectories have different sensitivity with regard to experimental parameters, and when experimental imperfections are taken into account, they produce different distortions to the experimental excitation profiles. The discrete character of k-space allows virtually a free choice of the trajectory used (Fig. 2).

Consequently, the problem of the trajectory design is reduced to the selection of experimental parameters for which the trajectory is optimized. Here we focus on the trajectories that minimize the load of the gradient system.

The penalty function \( E \) which expresses the gradient load can be formulated as a normalized vector sum of the applied gradients \( G_i^x \) and \( G_i^y \):

\[
E = \frac{1}{NC_0^2} \sum_{i=1}^{N} \left[ (G_i^x)^2 + (G_i^y)^2 \right] \quad [24a]
\]

or with regard to Eq. [20]

\[
E = \frac{1}{N} \sum_{i=1}^{N} \left[ (n_i^x)^2 + (n_i^y)^2 \right] \quad [24b]
\]

An obvious way to minimize gradient load is to increase duration of the gradient pulses, \( \Delta t \), Eq. [21b]. However, this prolongs the CARVE sequence, and therefore increases magnetization relaxation effects that cause distortions in the excited profile. A much better approach is to keep the pulse times constant and to search for a trajectory that minimizes the penalty function (Eq. [24]).

**Table 1**

<table>
<thead>
<tr>
<th>k-Space trajectory</th>
<th>Penalty function ( E )</th>
<th>( \Delta E )</th>
<th>( E ) in % of ( E_{\text{MIN}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random</td>
<td>94.2</td>
<td>9.71</td>
<td>5.65</td>
</tr>
<tr>
<td>Spiral</td>
<td>21.3</td>
<td>4.61</td>
<td>2.88</td>
</tr>
<tr>
<td>Line</td>
<td>5.99</td>
<td>2.45</td>
<td>1.42</td>
</tr>
<tr>
<td>Random, optimized by</td>
<td>2.97</td>
<td>1.72</td>
<td>1.00</td>
</tr>
</tbody>
</table>

by simulated annealing where the penalty function is reduced 30 times compared with the random unoptimized trajectory (Fig. 2d).

**How CARVE Works**

The mechanism of CARVE can be most easily understood by analyzing the trajectories of the magnetization during the sequence. Figure 3 shows trajectories and the transverse magnetization buildup for the regions within (Fig. 3a) and outside the excitation profile (Fig. 3b). For both regions, applied small tip-angle rotations are identical. The difference in trajectories is produced by the gradients that determine the position of the magnetization at the moment of a short pulse. Within the excitation profile, short RF pulses almost always rotate the magnetization away from the z-axis, which causes an increase in both the tip-angle and transverse magnetization. A properly designed sequence of gradient steps produces rotations of the magnetization around the z-axis that enable constructive superposition of magnetization flips. Thus, the final flip-angle approaches 90°. However, the same sequence of gradient pulses outside the excitation profile produces z-axis rotations that cause destructive superposition of magnetization flips. Flips away from the z-axis are compensated by similar flips in the opposite direction at some latter interval. The result is that the magnetization after the whole sequence is predominantly oriented along the z-axis and the resulting flip angle is close to zero. Note that there are significant differences among the magnetization trajectories at different positions φ-φ either within (Fig. 3a) or outside the excitation profile (Fig. 3b). The magnetization components at the gradient center (Fig. 3b) do not rotate in the x’y’ plane whereas components from the gradient center rotate many times before acquiring a final position at the end of CARVE—along the z-axis if outside the profile (Fig. 3b θ) or along the y’-axis if inside the profile (Fig. 3a θ).

**Off-Resonance Effects**

The presented theory, in which the excited profile is independent of the k-space trajectory, is valid only when the nuclei are exactly on-resonance. In practice this condition is not fulfilled, especially in samples with a large spread of chemical shifts. For off-resonance nuclei, the efficacy of CARVE critically depends on the k-space trajectory design. For example, when the k-space trajectory progresses from one part of k-space to the other (line k-space trajectory), the off-resonance produces a shift proportional to the resonance offset. In random k-space trajectories, off-resonance effects produce a blurred excitation profile (31). Thus, besides spatial selectivity, the CARVE sequence is also frequency dependent.

Figure 4 shows magnetization trajectories in the sequence from Fig. 2d, with different resonance offsets. With an increase of the resonance offset, the resulting tip angle within the profile decreases (Fig. 4a) whereas outside the profile the tip angle increases (Fig. 4b). This results in an almost random off-resonance excitation profile even at modest offsets. The loss of spatial selectivity is caused by the additional time evolution of the off-resonance magnetization. Fraction of magnetization ex-
tion spectrometer equipped with microimaging accessories. The sample was a 5-mm NMR tube filled with water. For simplicity, two-dimensional CARVE sequences were implemented by use of \( G_x \) and \( G_y \) gradients. The sample tube was oriented with its long axis along the z-direction, Fig. 5a. The excited magnetization profiles were visualized by a standard gradient-echo imaging sequence in which the initial 90° excitation pulse was replaced by a CARVE sequence (Fig. 5b).

Since the sample is uniform along the z-axis, xy-slice selection was excluded from the imaging sequence. CARVE profiles were imaged with 5-mm field of view on a matrix 256 × 256, using the following parameters: spectral width, 50 kHz, with two scans, repetition time 1 s and “echo-time” equal to time of the CARVE sequence + 8 ms. To maintain linearity between the RF pulse duration and tip angle, a linear transmitter was used (transmitter gain 27 dB) with \( t_{\text{RF}} = 80 \mu s \). Thus, individual RF pulses were in the range 0.5–5 \( \mu s \).

Simulated annealing for random trajectory optimization was performed using Eq. [24] as the penalty functions with initial “energy” \( kT \) equal to the value of penalty function for an unoptimized random trajectory. The temperature was reduced by a factor of 0.999 every 100 cycles or after 10 successive unsuccessful attempts to find a trajectory with lower energy. If a trajectory with lower energy was found, it was accepted; if not, the Boltzmann probability factor of the energy difference of the current and previous trajectory, \( \exp [-\frac{(E_{\text{current}} - E_{\text{previous}})}{kT}] \), was compared with a random number [0,1]. If the Boltzmann factor was larger than the random number, a new trajectory was accepted. The search was terminated when \( kT < 10^{-8} \). New trajectories were generated by swapping two randomly chosen coefficients \( k_x, k_y \).

**RESULTS**

Influence of the k-Space Trajectory

We conducted several experiments to demonstrate and verify various aspects of CARVE. First, we demonstrate that the overall CARVE profile is independent of the k-space trajectory when the sample is on-resonance, but that the profile quality depends on the trajectory optimi-
Signal. They can be used to calculate an image of the transverse magnetization phase from the relation \( M^* = M_x + iM_y = M^* \exp(i\theta) \). Since the ideal excitation profile is real, magnetization is expected to be excited predominantly in \( y' \) direction, so that angle \( \theta \) is either 90° or -90°. Figure 7 shows pairs of theoretical (left) and experimental (right) images: a) magnitude of transverse magnetization, \( M^* \), b) \( M_x \), c) \( M_y \), d) sine of transverse magnetization phase angle: \( \sin(\theta) = M_y / M^* \). A comparison shows a great deal of similarity between the theoretical and the experimental CARVE images. The CARVE profile resembles both the magnitude mode and the phase sensitive mode. Thus, in experimental CARVE profile, the phase uniformity is preserved, as theoretically predicted.

**Influence of the Number of Pulses**

In the last experiment, the dependence of the CARVE profile on the number of pulses was tested. The resemblance between the ideal and excited profile is predominantly by the number of pulses. CARVE images with a different number of events were generated for the ideal excitation profile from Fig. 1. In all sequences, \( k \)-space trajectories were optimized by simulated annealing. Figure 8 shows calculated CARVE profiles (left) and experimental profiles (right) obtained with: a) \( N = 50 \), b) \( N = 100 \), c) \( N = 150 \), and d) \( N = 200 \) events. It is clear that with a larger number of pulses, the CARVE profile approximates quite well the ideal profile as expected from the theory. Resemblance factors (Eq. [19]) for subsequent experiments are: a) 0.66, b) 0.78, c)

**Phase Uniformity**

Next, we verify that the phase of the experimental CARVE profile is well behaved as predicted by Eq. [4]. The CARVE experiment from Fig. 6d, with \( k \)-space trajectory generated by simulated annealing, is examined. Because of pure phase detection, the images of the \( M_x \) and \( M_y \) components can be extracted from the acquired...
pulse combined with a single static field gradient selects a plane (2); two selective RF pulses, and two static field gradients selectively excite a cross-section of the respective planes, and three perpendicular gradients combined with selective RF pulses excite a cube (7, 11). Thus, selective excitation of shapes more complex than cubes requires more combinations of RF pulses and gradients in analogy with carving, where more complex objects require more cuts.

In CARVE, "cuts" are defined by a set of \( N \) orthonormal harmonic functions (Eq. [9]). The larger the number of functions, the more complex the profile that can be excited. Since an arbitrarily shaped profile can be represented exactly only with an infinite set of harmonic functions (Eq. [14]), the CARVE profile is always only an approximation of an ideal one. Thus, besides the total number of harmonic functions, the quality of the approximation depends on the way these functions are selected out of infinite set. We have introduced the resemblance factor, \( \eta \), as a means to compare different approximations (Eq. [19]).

Many different resemblance factors can be defined, based on various criteria that express the distortion of the ideal profile on casting it into the CARVE mold. The resemblance factors in Eq. [19] use the norm of the CARVE profile as a criterion. Selected are coefficients that minimize the "volume" difference of the two profiles. However, such a resemblance factor may be insensitive to the local deviations of the CARVE profile from an ideal one. Furthermore, this criterion may introduce undesired amplitude deviations; in an attempt to minimize the differences in the total "volumes", overestimation of the function in one domain fosters its underestimation in the other. It is easy to envisage that other criteria, rather than similarity of profile volumes, might produce a resemblance factor more suitable than the one expressed by Eq. [19].

As shown in the theory presented here, because of the pulsed RF excitation, CARVE operates in discrete \( k \)-space. The most important consequence of the discrete character of CARVE is the freedom in the design of the \( k \)-space trajectory. In CARVE, \( k \)-space points are visited in "jumps." This relieves CARVE from possible problems of trajectory crossings, and offers full freedom in designing the sequence by which selected \( k \)-space points are

FIG. 6. Experimental CARVE of the profile defined in Fig. 1 recorded with the setup shown in Fig. 5 using CARVE sequences from Fig. 2. (a) random trajectory (Fig. 2a); (b) spiral trajectory (Fig. 2b); (c) line trajectory (Figs. 2c and 2d); (d) optimized random trajectory (Fig. 2d). All CARVE sequences consisted of 100 short RF pulses, separated by \( \Delta t = 500 \mu s \) and with total tip angle 90°. Imaging field of view was equal to one period of excitation profile, which was set to \( L = 5 \) mm, with gradient step unit \( G_0 = 9.4 \) mT/m.

0.83, and d) 0.87. An increase in the value of the resemblance factor does not guarantee improvements in the experimental image. A direct correlation between the image quality and the number of pulses holds only within the range of linearity of the gradient system and negligible relaxation during the sequence. Experimentally, beyond a certain number of pulses, gradient and relaxation artifacts increase and the quality of the image remains constant or even deteriorates. This is evident from a comparison of the experimental images in Figs. 8c and 8d. It is hard to tell whether the image recorded with \( N = 200 \) is better than the one with \( N = 150 \).

DISCUSSION

The selective excitation of an arbitrary shaped profile achieved by CARVE offers new possibilities in MR imaging and spectroscopy. These range from the removal of aliasing when zooming into smaller regions of interest, to the selective recording of the NMR spectrum from a chosen organ or body part. In general, the shape of the selected region is determined by the number of RF and gradient pulse pairs. For example, a single selective RF
FIG. 7. Phase uniformity of the CARVE sequence from Fig. 2d. Excited profile is displayed with four image pairs: (a) the magnitude of transverse magnetization \( M^* \), (b) \( M_T \) magnetization, (c) \( M_s \) magnetization, and (d) sine of transverse magnetization phase angle: \( \sin(\theta) = M_s / M^* \). Left image of each pair is theoretical and right, experimental.

FIG. 8. Dependence of excited profiles on the number of pulses. CARVE sequences of profile from Fig. 1a were calculated and experimentally recorded with a different number of pulses: (a) \( N = 50 \), (b) \( N = 100 \), (c) \( N = 150 \), and (d) \( N = 200 \). Each gradient sequence was optimized by simulated annealing. Left, theoretical and right experimental images. Experimental parameters were as in Fig. 2.

visited. Theoretically, the order of selected \( k \)-points is irrelevant. However, in practice different sequences may have different demands on the gradient system and consequently may produce experimental profiles of different quality. Thus, the search for the optimal trajectory is an important part of the CARVE implementation.

To find an optimal trajectory one needs to define a method and a criterion for the search. Among available methods (Monte Carlo, Simplex, Taboo Search, etc.), we have selected simulated annealing protocol because of its efficacy in avoiding local minima and its ease of implementation. As a criterion for evaluating the quality of the trajectory, we have chosen the total gradient load that is expressed by the corresponding penalty function (Eq. [24]). The square root of the penalty function represents the average integer gradient vector, which is a direct measure of the average gradient load (Eq. [20]). As shown in Table 1, optimization of a random trajectory by simulated annealing results in an almost sixfold reduction of the gradient load. The importance of such a reduction can be best judged by a comparison of the CARVE images obtained by the two random trajectories (Figs. 6a and 6d). Whereas the CARVE profile from an unoptimized random trajectory is hardly recognizable (Fig. 6a), the one generated by optimized random trajectory is almost identical to the theoretical profile (Figs. 6d and 7). Gradient imperfections are the principal sources of the profile distortions, but the type of imperfection may vary from one gradient system to another. Then, it is useful to seek
the best trajectory by applying several different penalty functions. The most important parameter that needs to be optimized can be found empirically. For example, if gradient switching time is a limiting parameter rather than the overall gradient load, the penalty function is

\[ E = \frac{1}{NG_0^2} \sum_{i=1}^{N} \left[ \left(G_i^T - G_i^F\right)^2 + \left(G_i^T - G_i^F\right)^2 \right] \]  

[25]

Additional cross-terms, \( G_{i-1} \cdot G_i \), express correlation between successive gradient levels. This penalty function highly favors trajectories with minimized jumps between successive levels, but is insensitive to total gradient load. It is almost zero for constant gradients, irrespective of their magnitude. A proper balance between the average load and the sizes of gradient jumps can be established by weighing of cross- and square terms in Eq. [25].

Simulated annealing has already been used for searching the optimal RF pulse profile (32–34). It has also been applied for the optimization of k-space trajectory in the design of spatial and spectral selective excitation (25, 26). However, its most important application might be for the imaging trajectory optimization in rapid scanning methods. For example, in complete analogy with CARVE optimization, single shot stochastic imaging technique (31) may be improved by the k-space trajectory optimization using simulated annealing protocol described here.

CARVE is also frequency-dependent, because it uses a long train of small tip-angle RF pulses. Contrary to DANTE, its spectral width is difficult to assess; the pulses are randomly modulated in both phase and amplitude. However, it is easy to predict CARVE properties for exact on-resonance magnetization. In the \( x'y'z \) frame, on-resonance magnetization does not evolve in the course of time (does not rotate around z-axis). Rotation about the z-axis is exclusively caused by applied gradients, as expressed by Eq. [2]. Then, the magnetization trajectories are as described in presented on-resonance theory. At the end of CARVE, transverse magnetization is created within the excitation profile and longitudinal outside it. Deviations from the on-resonance condition (caused by chemical shifts, relaxation, static field gradients, etc.) introduce additional time evolution of transverse magnetization. This is equivalent to additional rotations around the z-axis, which now interferes with rotations induced by gradients. Since the gradient rotations are random in time, in reverse, time evolution is random as observed from the gradient sequence. The total effect is that the presence of any time evolution in the \( x'y' \) plane interferes destructively with gradient evolution, yielding a random response to the CARVE sequence. In essence, CARVE behaves like a low-pass filter for resonance frequencies. This is in complete analogy with a method used in high resolution spectroscopy to filter out zero-quantum coherence (high frequency components) from longitudinal magnetization (zero frequency component) (35, 36). This is also analogous to stochastic imaging technique (31).

A remarkable property of CARVE is the phase uniformity across the excitation profile (Fig. 7). Phase uniformity enables the profile to be represented in the phase sensitive mode, thus providing much better resolution and signal-to-noise ratio than an absolute value representation (37). Also, the imaginary part of the CARVE profile can be used to assess the overall quality of CARVE. Theoretically, the imaginary part is a regular pattern of very small deviations from zero, thus, empirical imperfections easily would be noticed. The most important consequence of phase uniformity is the possibility to average profiles from several CARVE experiments, performed with slightly different random trajectories. Experimental imperfections manifest as a random deviation from an expected profile. In experiments repeated with slightly different trajectories, experimental imperfections co-add like noise whereas the expected profiles co-add linearly. Thus experimental imperfections can be reduced \( \sqrt{n} \) times in \( n \) repeated experiments, in complete analogy with coherent signal averaging. Without phase uniformity, that would not be the case.

An extension of the presented method to the third dimension is obvious. The only limitation in the 3D case is that with 150–200 basis functions, only moderately complex 3D objects can be properly presented. Possible solutions of this limitation and implementation of the method to 3D will be published elsewhere. For example, linearity of the CARVE sequence permits co-addition of two or more experiments. Then, \( N_1 \times N_2 \) basis functions can be distributed among \( N_1 \) experiments with \( N_2 \) functions. Choice of \( N_1 \) and \( N_2 \) depends on the particular goal because they define both the spatial resolution and the spectral bandwidths of the excited profile.

CONCLUSION

We presented an on-resonance theory for the excitation of an arbitrarily shaped profile and verified it with a series of two-dimensional excitation experiments. CARVE proved to be very efficient on samples that have single line NMR spectra and are well shimmed and set on-resonance. Under such conditions a rather complex two-dimensional profile can be excited with a CARVE sequence of 100–200 pulses.

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