Quantum-mechanical generalization of the Extended Phase Graph method (QuaM-EPG) for the simulation of coupled spin systems under SSFP excitation

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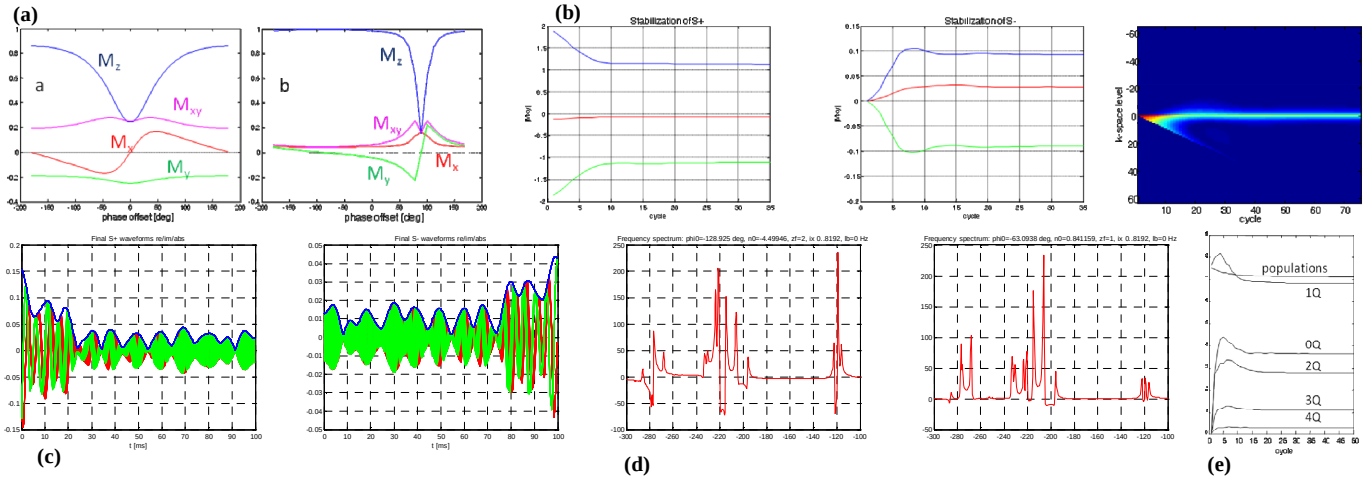
Introduction: The nonbalanced steady-state free precession acquisition mode (nb-SSFP) may become an alternative for fast proton MR spectroscopic imaging of metabolites [1], particularly in high field: unlike echo-planar techniques, SSFP is not hampered by too high sampling rates and is compatible with low flip angle excitation. It may be further supported by shortened acquisition, water-gap excitation, and non-Fourier data analysis. Nb-SSFP has to be preferred to the balanced version in order to avoid the banding artifact. For the assessment of the applicability of SSFP for the detection and for the quantification of metabolites with coupled spin systems, a suitable algorithm for predicting the excitation and spectra is needed. The Extended Phase Graph (EPG) approach [2] can efficiently handle periodic excitation, but it is well suited for isolated spin- ½ nuclei only and is inapplicable directly to coupled spin systems. For such systems, full quantum mechanical treatment employing the density operator is necessary. Such a calculation alone, however, does not answer the questions about the complex echoes arising in multipulse sequences like SSFP. Because of its role in SSFP, relaxation may not be neglected. We present a combination and extension of the two approaches, QuaM-EPG, which also adds the support for spectroscopic simulations.

Methods: The EPG method is an extension of the Bloch model such that k-space stratification of the coherence transfer pathways (CTP) at certain time instants is utilized for tracking divergent and reconvergent CTPs. Its assumptions are: (a) each isochromat is characterized by a single-quantum free precession angle Φ during each cycle, which may be due to gradients, static field inhomogeneity or chemical shift, (b) the magnetization is observed only at such instants that the phase of any CTP related to the same isochromat changes by an integral multiple of Φ between such instants, so that any observed magnetization component can be expressed by Fourier series $M_Q(\Phi) = \Sigma_{n=-\infty}^{\infty} Q_k \exp(in\Phi)$, (c) the magnetization profile $\boldsymbol{M}(\Phi)$, with a period of 2π, is represented by its Fourier coefficients (F_k for M_{xy}, Z_k for M_z in [2]), (d) the two supported types of evolution – hard RF pulse or free precession – are described analytically by a transition matrix linking the Fourier coefficients, and (e) the signal amplitude is found as F_0, the nonmodulated component of the transverse magnetization. QuaM-EPG translates the essence of these postulates in the density-matrix model and at the same time, it isolates the coherence level separation from the natural phase evolution so that spectroscopic information is retained. In QuaM-EPG, (a) each isochromat is characterized by its natural parameters (local B_0, chemical shifts, J-coupling constants, position, Redfield relaxation matrix), some of which may be taken as variables (b) the observation may be continuous because the echo isolation at Fourier level 0 is achieved by introducing an artificial data dimension associated with one F_z rotation by an angle $\Phi = n.2\pi/N$ per cycle, which does not interfere with normal evolution and properly represents the different sensitivity of MQCs to gradients, (c) the density matrix elements, which are periodic functions of Φ, are handled as vectors of samples for $\Phi \in \langle -\pi, \pi \rangle$, thanks to which (d) standard spin system calculation may be applied throughout the calculation without analytical derivations or special algebra, and (e) the signal M_{xy} is found as $\mathrm{Tr}\{F_+ \sigma_\lambda\}$, where $F_+ = F_x + iF_y$ and σ_λ is the density matrix obtained by Fourier transforming the appropriate elements of density matrix vectors over Φ and picking the Fourier component λ that becomes coherent in the target signal type. In case of nb-SSFP either $\lambda=0$ for the coherence-losing S_+ signals (artificial rotation before RF pulses) or $\lambda=-1$ for the coherence-gaining signals S_- (artificial rotation after RF pulses). The density matrix evolution including relaxation has been implemented as a finite-element calculation in the operator space, approximating the simultaneous excitation and relaxation by consecutive evolution. The superoperator space has been avoided by taking the sparsity and near diagonality of the Redfield relaxation matrix in account. The algorithm prototype has been implemented in Matlab (The MathWorks, Inc., USA).

Results: Numerous examples of the application of this approach may be given: (a) Banding patterns in balanced SSFP and their RF-phase sensitivity. (b) Stabilization of the SSFP excitation. (c) S+ and S− signals. (d) Sensitivity of spectral patterns to miscellaneous parameters (flip angles). (e) Passage of MQC between cycles.



Discussion: SSFP-based MRSI faces several challenges, such as water suppression without the usual presaturation, shorter signals that would cause artifacts in Fourier processing, increased quantification uncertainty with short signals etc. The newly proposed algorithm, QuaM-EPG, shows a way of simulating spectroscopic SSFP sequences with coupled spin systems. Continuous signals or evolution of quantum-mechanical coherences may be obtained. It is an advantage that a standard simulation core can be used in QuaM-EPG – the SSFP-specific functionality comes as a superstructure acting upon an array of density matrices, whose evolution differs from the natural one only by one nonselective z-rotation per cycle. Due to this feature, QuaM-EPG may be found a useful alternative to EPG itself, particularly if questions about selective excitation and/or relaxation in cyclic sequences arise or if continuous observation is preferred.This algorithm is going to be implemented in the jMRUI [3] spectrum simulation package.

[1] Schuster C, Dreher W, Geppert C, Leibfritz D, Magn. Reson. Med. 57:82–89 (2007); [2] Hennig J, Weigel M, Scheffler K, Magn. Reson. Med. 51:68-80 (2004); [3] Naressi A, Couturier C, Devos JM, Janssen M, Mangeat C, de Beer R, Graveron-Demilly D, MAGMA 12:141-152 (2001).

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