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Mathematical Analysis of Generation and Elimination of Intersequence Stimulated Echo in Double-Quantum Filtering

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In double-quantum filtering (DQF) with fast repetition cycle, an intersequence stimulated echo (ISTE) can be generated by two consecutive DQF pulse sequences (*1*). The ISTE can pass through the double-quantum filtering, resulting in breakthrough of the single-quantum (SQ) signal. A technique for eliminating the ISTE has been developed by the authors in Ref. (*1*), using the partition method and computer simulations. In this Note, we will supplement Ref. (*1*) by providing a mathematical analysis based on the density and tensor operators (*2*). Furthermore, the same elimination technique will be shown to be valid for the other DQF schemes introduced by the authors (*3*).

The reason ISTE passes through DQF is that the phase of ISTE has the same property as that of the DQ signal [for a general discussion of the DQ signal we refer the reader to Ref. (*3*)]. The elimination technique for ISTE consists in making the phase property of ISTE different from that of the DQ signal by changing the phase-cycling direction in DQF. To analyze the effects of an RF pulse (θ, ϕ) on the phase of the signal, the irreducible tensor operator T_{lm} is convenient because the phase of an NMR signal can be explicitly described as

$$T_{lm} \xrightarrow{(\theta,\ \phi)} \sum_{m'=-l}^{l} d^{l}_{m'm}(\theta)\exp[i(m - m')\phi]T_{lm'}, \quad [1]$$

where l denotes the rank of tensors, m and m' denote quantum numbers (or coherence orders) before and after application of the RF pulse, and $d^{l}_{m'm}(\theta)$ denotes the reduced rotation-matrix element (*4*).

The DQF pulse sequence with nonrefocused preparation (τ_{P}) and evolution (τ_{E}) times may be expressed as

$$(\theta_1,\ \phi_1)—\tau_{\mathrm{P}}—(\theta_2,\ \phi_2)—\tau_{\mathrm{E}}—(\theta_3,\ \phi_3)—\mathrm{Acq}(t_2,\ \phi_{\mathrm{R}}), \quad [2]$$

where ϕ_n denotes the phase angle of each RF pulse with flip angle θ_n, t_2 is the acquisition (or detection) time, and ϕ_{R} is the receiver phase.

The generation of ISTE in two consecutive DQF pulse sequences (Fig. 1A) can be described by use of a flow chart (Fig. 1B) of the tensors involved. In the (n − 1)th sequence, SQ tensors $T_{l,\pm 1}$ during the evolution time are converted into zero-quantum (ZQ) tensors T_{l0} by a readout RF pulse (θ_3, ϕ_3). These ZQ tensors correspond to the spin state after application of the second 90° RF pulse in the stimulated-echo pulse sequence (*5*). During the recycle or intersequence delay (τ_{D}), the phases of the ZQ tensors remain constant. Hence, when longitudinal relaxation is not complete during the intersequence delay, the spin accumulates a phase in the nth sequence in addition to the phase induced in the (n − 1)th sequence. Therefore, the spin's phase is doubled and, consequently, the ISTE passes through the DQF.

The mathematical analysis will follow the derivation in Ref. (*3*), but will be focused on the tensors leading to an ISTE as described in Fig. 1B. For $\theta_1 = \frac{1}{2}\pi$, the density operator $\sigma(0^-)$, corresponding to the equilibrium state before application of the first RF pulse at $t = 0$, may be written as

$$\sigma(0^-) = \sqrt{5}T_{10}. \quad [3]$$

The superscripts − and + in expressions such as $\sigma(t^-)$ and $\sigma(t^+)$ denote the density operator before and after application of the RF pulse at time t, respectively ($t = 0$ in Eq. [3]). Following application of the RF pulse ($\frac{1}{2}\pi$, ϕ_1) at $t = 0$, density operator $\sigma(0^+)$ consists of two SQ components, i.e.,

$$\sigma(0^+) = \sqrt{\tfrac{5}{2}}\{-\exp[-i\phi_1]T_{11} + \exp[i\phi_1]T_{1\bar{1}}\}, \quad [4]$$

where $\bar{m}$ denotes $-m$ ($m = 1$ in Eq. [4]).

During the preparation time, the first-rank tensors in Eq. [4] evolve into tensors with ranks ranging from 1 to 3 through the function $f^{(1)}_{l1}(\tau_{\mathrm{P}})$, but the quantum numbers of the tensors are retained. Therefore, just before application of the RF pulse (θ_2, ϕ_2) at $t = \tau_{\mathrm{P}}$, density operator $\sigma(\tau_{\mathrm{P}}^-)$ becomes a superposition of density operators for tensors with different ranks, i.e.,

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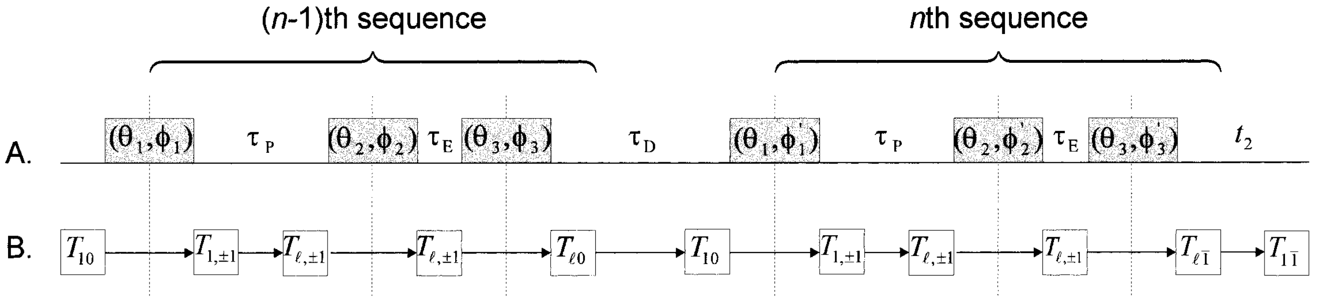

FIG. 1. (A) Two consecutive DQF pulse sequences and (B) a flow chart for the tensors leading to ISTE. θ_n, RF flip angle; ϕ_n, RF phase; τ_P, preparation time; τ_E, evolution time; τ_D, recycle (or intersequence) delay.

$$\sigma(\tau_P^-) = \sum_{l=1}^{3} \sigma_l(\tau_P^-), \quad [5]$$

where

$$\sigma_l(\tau_P^-) = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P)\{-\exp[-i\phi_1]T_{l1} + \exp[i\phi_1]T_{l\bar{1}}\}. \quad [6]$$

For simplicity and without loss of generality, the carrier frequency of the NMR system is assumed to be on-resonance (*6*).

Application of a DQ-creation RF pulse (θ_2, ϕ_2) at $t = \tau_P$ converts the SQ tensors in Eq. [6] into tensors with quantum numbers ranging from $m = -l$ to l. Therefore, density operator $\sigma_l(\tau_P^+)$ can be decomposed into m-quantum density operators $\sigma_{lm}(\tau_P^+)$, i.e.,

$$\sigma_l(\tau_P^+) = \sum_{m=0}^{l} \sigma_{lm}(\tau_P^+), \quad [7]$$

where $\sigma_{lm}(\tau_P^+)$ involves the lth-rank tensors for both m and $-m$.

Since ISTE is derived from SQ tensors ($m = \pm 1$), the derivation can be simplified by focusing only on these tensors. The density operator $\sigma_{l1}(\tau_P^+)$ for the lth-rank SQ tensors can be grouped into terms involving T_{l1} and $T_{l\bar{1}}$ by the expression

$$\sigma_{l1}(\tau_P^+) = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P)(C_{l1}T_{l1} + C_{l\bar{1}}T_{l\bar{1}}), \quad [8]$$

where

$$C_{l1} = \exp[-i\phi_1]\{-d_{11}^l(\theta_2) + d_{1\bar{1}}^l(\theta_2)\exp[-i2\phi_P]\} \quad [9]$$

and

$$C_{l\bar{1}} = -\exp[i\phi_1]\{-d_{11}^l(\theta_2) + d_{1\bar{1}}^l(\theta_2)\exp[i2\phi_P]\}. \quad [10]$$

In Eqs. [9] and [10], the RF phases involved in the preparation time have been simplified by collectively defining

$$\phi_P = -\phi_1 + \phi_2. \quad [11]$$

Furthermore, in deriving Eqs. [9] and [10], the identities

$$d_{MN}^l(\theta) = (-1)^{M-N} d_{\overline{MN}}^l(\theta) \quad [12]$$

and

$$d_{MN}^l(\theta) = d_{\overline{NM}}^l(\theta) \quad [13]$$

have been employed to show the similarity between C_{l1} and $C_{l\bar{1}}$ (*4*).

By restricting the RF phases to

$$\phi_P = \frac{k}{2}\pi \quad [14]$$

with integer k, $\exp[i2\phi_P]$ and $\exp[-i2\phi_P]$ become identical, i.e.,

$$\exp[i2\phi_P] = \exp[-i2\phi_P] = (-1)^k. \quad [15]$$

Under condition [15], Eqs. [9] and [10] may be rewritten as

$$C_{l1} = \exp[-i\phi_1]P_{l1}(\phi_P, \theta_2) \quad [16]$$

and

$$C_{l\bar{1}} = -\exp[i\phi_1]P_{l1}(\phi_P, \theta_2), \quad [17]$$

respectively, where

$$P_{l1}(\phi_P, \theta_2) = -d_{11}^l(\theta_2) + d_{1\bar{1}}^l(\theta_2)\exp[i2\phi_P]. \quad [18]$$

In Eqs. [16]–[18] and succeeding equations, ϕ_P is retained instead of k to emphasize its physical meaning. Substitution of C_{l1} and $C_{l\bar{1}}$ in Eq. [8] with Eqs. [16] and [17] yields

$$\sigma_{l1}(\tau_P^+) = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) P_{l1}(\phi_P, \theta_2)\{\exp[-i\phi_1]T_{l1} - \exp[i\phi_1]T_{l\bar{1}}\}. \quad [19]$$

After SQ relaxation during the evolution time through the function $f_{ll}^{(1)}(\tau_E)$, the density operator becomes

$$\sigma_{l1}(\tau_P + \tau_E^-) = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) P_{l1}(\phi_P, \theta_2) \times \{\exp[-i\phi_1]T_{l1} - \exp[i\phi_1]T_{l\bar{1}}\}. \quad [20]$$

Following application of the readout RF pulse (θ_3, ϕ_3) at $t = \tau_P + \tau_E$, the SQ tensors in Eq. [20] are converted into tensors with the same rank l, but with quantum numbers ranging from $m = -l$ to l. Since only the ZQ tensors lead to an ISTE in the nth sequence, the density operator for T_{l0} is next considered as

$$\sigma_{l1}(\tau_P + \tau_E^+) = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) d_{01}^{l}(\theta_3) P_{l1}(\phi_P, \theta_2) A(\phi_1, \phi_3) T_{l0}, \quad [21]$$

where

$$A(\phi_1, \phi_3) = \exp[i(-\phi_1 + \phi_3)] + \exp[i(\phi_1 - \phi_3)]. \quad [22]$$

In deriving Eqs. [21] and [22], the following identity has been applied (*4*):

$$d_{0\bar{1}}^{l}(\theta_3) = -d_{01}^{l}(\theta_3). \quad [23]$$

With the collective definition of the RF phases involved in the evolution time as

$$\phi_E = -\phi_2 + \phi_3, \quad [24]$$

the phase terms in Eq. [22] can be expressed in terms of ϕ_P and ϕ_E as

$$-\phi_1 + \phi_3 = -\phi_1 + \phi_2 - \phi_2 + \phi_3 = \phi_P + \phi_E. \quad [25]$$

Then, Eq. [22] may be rewritten as

$$A(\phi_P, \phi_E) = A(\phi_1, \phi_3) = \exp[i(\phi_P + \phi_E)] + \exp[-i(\phi_P + \phi_E)]. \quad [26]$$

During the intersequence delay, the ZQ tensors relax longitudinally through the function $f_{1l}^{(0)}(\tau_D)$, for example (*7, 8*),

$$f_{11}^{(0)}(\tau_D) = \tfrac{1}{5}[4\exp(-\tau_D/T_{1s}) + \exp(-\tau_D/T_{1f})] \quad [27]$$

and

$$f_{13}^{(0)}(\tau_D) = \tfrac{2}{5}[-\exp(-\tau_D/T_{1s}) + \exp(-\tau_D/T_{1f})]. \quad [28]$$

The density operator for the ZQ tensors before the nth sequence is

$$\sigma_{l1}(T_R^-) = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) f_{1l}^{(0)}(\tau_D) d_{01}^{l}(\theta_3) P_{l1}(\phi_P, \theta_2) A(\phi_P, \phi_E) T_{10}, \quad [29]$$

where T_R is the repetition time defined as

$$T_R = \tau_P + \tau_E + \tau_D. \quad [30]$$

In Eq. [29], the phase induced on the ZQ tensors in the $(n - 1)$th sequence is contained in $P_{l1}(\phi_P, \theta_2)$ and $A(\phi_P, \phi_E)$. When the ZQ tensors do not relax fully during the intersequence delay, the phase induced in the $(n - 1)$th sequence is transferred to the nth sequence, i.e., the next sequence. For simplicity, let us define

$$W = \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) f_{1l}^{(0)}(\tau_D) d_{01}^{l}(\theta_3), \quad [31]$$

and rewrite Eq. [29] as

$$\sigma_{l1}(T_R^-) = W P_{l1}(\phi_P, \theta_2) A(\phi_P, \phi_E) T_{10}. \quad [32]$$

Next, we analyze the tensors leading to an ISTE in the nth sequence, where the RF phases are denoted with a prime, i.e., ϕ_1', ϕ_2', ϕ_3', ϕ_P', ϕ_E', and ϕ_R'. Following the same derivation as in the $(n - 1)$th sequence, the density operator for the SQ tensors before application of readout RF pulse (θ_3, ϕ_3') may be written as

$$\sigma_{l1}(T_R + \tau_P + \tau_E^-) = W P_{l1}(\phi_P, \theta_2) A(\phi_P, \phi_E) \sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) P_{l1}(\phi_P', \theta_2) \times \{\exp[-i\phi_1']T_{l1} - \exp[i\phi_1']T_{l\bar{1}}\}. \quad [33]$$

After application of the readout RF pulse, only the tensors with a quantum number -1 lead to detectable NMR signals during the acquisition time t_2. The density operator for SQ tensor $T_{l\bar{1}}$ may be written as

$$\sigma_{l1}(T_R + \tau_P + \tau_E^+) = W\sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) P_{l1}(\phi_P, \theta_2) P_{l1}(\phi'_P, \theta_2) \times A(\phi_P, \phi_E) B_l(\phi'_P, \phi'_E, \theta_3) \exp[i\phi'_3] T_{l\bar{1}}, \quad [34]$$

where

$$B_l(\phi'_P, \phi'_E, \theta_3) = d^l_{1\bar{1}}(\theta_3)\exp[i(\phi'_P + \phi'_E)] - d^l_{11}(\theta_3)\exp[-i(\phi'_P + \phi'_E)], \quad [35]$$

and the phase terms in Eq. [35] have been arranged by use of Eq. [25].

During the acquisition time in the intersequence delay, the lth-rank SQ tensor $T_{l\bar{1}}$ will evolve into the first-rank SQ tensor $T_{1\bar{1}}$ by

$$T_{l\bar{1}} \xrightarrow{t_2} f_{1l}^{(1)}(t_2) T_{1\bar{1}}. \quad [36]$$

Then, the density operator for $T_{1\bar{1}}$ may be written as

$$\sigma_{l1}(t_2) = W\sqrt{\tfrac{5}{2}} f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) f_{1l}^{(1)}(t_2) P_{l1}(\phi_P, \theta_2) P_{l1}(\phi'_P, \theta_2) \times A(\phi_P, \phi_E) B_l(\phi'_P, \phi'_E, \theta_3) \exp[i\phi'_3] T_{1\bar{1}}. \quad [37]$$

The detectable NMR signal $S_{l1}(t_2)$ for ISTE is given by

$$S_{l1}(t_2) = -\sqrt{10}\,\mathrm{Tr}\{\sigma_{l1}(t_2) T_{11}\}\exp[i\phi_R]. \quad [38]$$

Provided that the tensor operators are orthogonal and normalized, i.e.,

$$\mathrm{Tr}\{T_{1\bar{1}} T_{11}\} = -1, \quad [39]$$

the acquired ISTE signal $S_{l1}(t_2)$ may be written as

$$S_{l1}(t_2) = W' f_{1l}^{(1)}(t_2) P_{l1}(\phi_P, \theta_2) P_{l1}(\phi'_P, \theta_2) A(\phi_P, \phi_E) \times B_l(\phi'_P, \phi'_E, \theta_3) \exp[i(\phi'_3 + \phi_R)], \quad [40]$$

where

$$W' = 5 f_{l1}^{(1)}(\tau_P) f_{ll}^{(1)}(\tau_E) W. \quad [41]$$

To analyze the phase of the ISTE, the relation of RF phases in the phase-cycling scheme needs to be considered for the two consecutive sequences. In DQF, since the phase of the DQ signal is a function of $2\phi_E$, the selection of DQ signals is achieved by use of the phase-cycling scheme with

$$\phi_E = \pm \frac{n}{2}\pi \quad [42]$$

and

$$\phi_R = 2\phi_E = n\pi, \quad [43]$$

where n is an integer (*9*). On the other hand, the phase ϕ_P set by Eq. [14] is constant throughout the phase cycles in general, i.e.,

$$\phi'_P = \phi_P. \quad [44]$$

Therefore, Eq. [40] may be rewritten as

$$S_{l1}(t_2) = W' f_{1l}^{(1)}(t_2)[P_{l1}(\phi'_P, \theta_2)]^2 A(\phi'_P, \phi_E) \times B_l(\phi'_P, \phi'_E, \theta_3)\exp[i(\phi'_3 + \phi'_R)]. \quad [45]$$

From Eq. [42], the relations between RF phases ϕ_E and ϕ'_E may be either

$$\phi'_E = \phi_E + \frac{\pi}{2} \quad [46]$$

or

$$\phi'_E = \phi_E - \frac{\pi}{2}. \quad [47]$$

In other words, the RF phase ϕ_E can be cycled in the positive or negative direction. For these two cases denoted with superscripts + and −, respectively, the received ISTE may be written as

$$S_{l1}(t_2)^{\pm} = W' f_{1l}^{(1)}(t_2)[P_{l1}(\phi'_P, \theta_2)]^2 C_l(\phi'_P, \phi'_E, \theta_3)^{\pm} \times \exp[i(\phi'_3 + \phi'_R)], \quad [48]$$

where $C_l(\phi'_P, \phi'_E, \theta_3)^{\pm}$ includes the factors determining the phase of ISTE as

$$C_l(\phi'_P, \phi'_E, \theta_3)^{\pm} = A\left(\phi'_P, \phi'_E \mp \frac{\pi}{2}\right) B_l(\phi'_P, \phi'_E, \theta_3). \quad [49]$$

Substitution of $A(\phi'_P, \phi'_E \mp \pi/2)$ and $B_l(\phi'_P, \phi'_E, \theta_3)$ in Eq. [49] with Eqs. [26] and [35], respectively, results in

$$C_l(\phi'_P, \phi'_E, \theta_3)^{\pm} = D_l(\phi'_P, \phi'_E, \theta_3)\exp\left[\pm i\,\frac{\pi}{2}\right], \quad [50]$$

where

$$D_l(\phi'_P, \phi'_E, \theta_3) = d^l_{11}(\theta_3) + d^l_{1\bar{1}}(\theta_3) - d^l_{11}(\theta_3)\exp[-i(2\phi'_P + 2\phi'_E)] - d^l_{1\bar{1}}(\theta_3)\exp[i(2\phi'_P + 2\phi'_E)]. \quad [51]$$

The phases of the two terms in Eq. [51] are proportional to $2\phi'_E$ in the same way as that of the actual DQ signal [details about the DQ signal can be found in Ref. (*3*)]. Therefore, the ISTE can pass through DQF in the same manner as the actual DQ signal.

The technique for eliminating the ISTE can be derived from Eq. [50]. We start by noting that the function $D_l(\phi'_P, \phi'_E, \theta_3)$ in Eq. [51] is not sensitive to the cycling direction of the RF phase ϕ'_E. Therefore, if two signals are acquired with the phase cycling in Eqs. [46] and [47], respectively, the summation of $C_l(\phi'_P, \phi'_E, \theta_3)^+$ and $C_l(\phi'_P, \phi'_E, \theta_3)^-$ yields

$$\begin{aligned} C_l(\phi'_P, \phi'_E, \theta_3)^+ + C_l(\phi'_P, \phi'_E, \theta_3)^- &= \mathrm{D}_l(\phi'_P, \phi'_E, \theta_3)\left\{\exp\left[i\,\frac{\pi}{2}\right] + \exp\left[-i\,\frac{\pi}{2}\right]\right\} \\ &= D_l(\phi'_P, \phi'_E, \theta_3) 2\cos\left(\frac{\pi}{2}\right) \\ &= 0. \end{aligned} \quad [52]$$

Hence, from Eqs. [48] and [52],

$$S_{l1}(t_2)^+ + S_{l1}(t_2)^- = 0. \quad [53]$$

Thus, the ISTE is clearly canceled out.

The preceding equations have been derived for arbitrary flip angles θ_2 and θ_3 of the creation and readout RF pulses, respectively. Furthermore, the RF phases in Eqs. [14] and [42] are also inclusive for all the other new DQF schemes (*3*). Therefore, the result presented in Eq. [53] is valid for the conventional as well as the other DQF schemes; i.e., the technique presented in Ref. (*1*) and analyzed in this Note can be used to eliminate the SQ breakthrough due to ISTE in any of the DQF schemes.

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