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Get["QUADRUPOLE"];

(*
 One-dimensional SPAM MQMAS of a spin I = 5/2,
 Three pulse sequence with three x phases,
 3Q echo amplitude optimization with the second pulse,
 Coherence pathway 0Q → 3Q → (1Q, 0Q, and -1Q) → -1Q,
 Wolfram Mathematica 5.0,
 Author: R. HAJJAR
 *)

(*------------ Nucleus ------------*)
quadrupoleSpin = 2.5;
larmorFrequencyMhz = 208.61889974; (* Al-27 with 800 MHz NMR spectrometer *)

(*----- Quadrupole interaction ----*)
quadrupoleOrder = 2;
QCCMHz = 5;       η = -1;

(*--- Rotor Euler angles in PAS ---*)
αPR = 0;     βPR = 0;       γPR = 0;

(*----------- Parameters ----------*)
startOperator = Iz;
ωRFkHz = 90;    (* strong RF pulse strength in kHz unit *)
ωRF3kHz = 9.3; (* weak RF pulse strength in kHz unit *)
spinRatekHz = 5;
powderFile = "rep100_simp";
numberOfGammaAngles = 10;
t1 = 4;    (* the first-pulse duration in microsecond unit *)
t2 = 4;    (* the second-pulse duration in microsecond unit *)
t3 = 9;    (* the third-pulse duration in microsecond unit *)
Δt = 0.25;    (* pulse duration increment in microsecond unit *)
np = t1 / Δt;  (* number increment of the first-pulse duration *)

(*--------- Pulse sequence ---------*)
elements1 = {{2, 5}};   (* 3Q matrix element *)
coherence2 = {1, 0, -1}; (* ±1Q and 0Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz]; (* first pulse with x phase *)
         store[2];
        filterElt[elements1]; (* 3Q coherence pathway selection *)
     pulse[t2, ωRFkHz]; (* second pulse with x phase *)
         filterCoh[coherence2]; (* ±1Q and 0Q coherence pathway selection *)
     pulse[t3, ωRF3kHz]; (* third pulse with x phase *)
        acq[p];
         recall[2];
   }];
 );
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(*--- Execute, plot, and save simulation
  in "spam_P1_3Qxxx" file -----------*)
run;
tabgraph["spam_P1_3Qxxx"];

(* ------------------------------------ *)
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Rang	t(μs)	intensity
0	0	0.
1	0.25	$-7.255596791\times10^{-6}$
2	0.5	−0.000203658701
3	0.75	−0.001237129471
4	1.	−0.00385172575
5	1.25	−0.008141478133
6	1.5	−0.01342723619
7	1.75	−0.01872429868
8	2.	−0.02331784361
9	2.25	−0.02702438877
10	2.5	−0.02998142307
11	2.75	−0.03244765353
12	3.	−0.03475806269
13	3.25	−0.03714699481
14	3.5	−0.03965910557
15	3.75	−0.04225966804
16	4.	−0.04494629298