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Get["QUADRUPOLE"];

(*
 One-dimensional SPAM MQMAS of a spin I = 5/2,
 Three pulse sequence with three x phases,
 3 Q echo amplitude optimization with the second pulse,
 All the 3 Q coherences are considered,
 Coherence pathway 0 Q → 3 Q → (1 Q, 0 Q, and -1 Q) → -1 Q,
 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 = t2 / Δt;  (* number increment of the second-pulse duration *)

(*--------- Pulse sequence ---------*)
coherence1 = {3};       (* 3 Q matrix coherences *)
coherence2 = {1, 0, -1}; (* ±1 Q and 0 Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  pulse[t1, ωRFkHz];     (* first pulse with x phase *)
     filterCoh[coherence1];   (* 3 Q coherence pathway selection *)
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz]; (* second pulse with x phase *)
        store[2];
        filterCoh[coherence2]; (* ±1 Q and 0 Q 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_P2_3QxxxS" file -------------*)
run;
tabgraph["spam_P2_3QxxxS"];

(* ------------------------------------ *)
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Rang	t(μs)	intensity
0	0	0.
1	0.25	−0.0134092809
2	0.5	−0.05277347644
3	0.75	−0.1046151101
4	1.	−0.1485227615
5	1.25	−0.1699290563
6	1.5	−0.1658531604
7	1.75	−0.1421014085
8	2.	−0.1083333979
9	2.25	−0.07429010261
10	2.5	−0.04773821507
11	2.75	−0.03286683273
12	3.	−0.02921117503
13	3.25	−0.03280996595
14	3.5	−0.03914424156
15	3.75	−0.04552316416
16	4.	−0.0516873895