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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 = t3 / 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 *)
  pulse[t2, ωRFkHz];     (* second pulse with x phase *)
      filterCoh[coherence2]; (* ±1 Q and 0 Q coherence pathway selection *)
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRF3kHz]; (* third pulse with x phase *)
        store[2];
        acq[p];
        recall[2];
   }];
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 );

(*--- Execute, plot, and save simulation
  in "spam_P3_3QxxxS" file -------------*)
run;
tabgraph["spam_P3_3QxxxS"];

(* ------------------------------------- *)
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Rang	t (μs)	intensity
0	0	−0.03967672866
1	0.25	−0.04016984266
2	0.5	−0.04057043626
3	0.75	−0.04086439109
4	1.	−0.04106820629
5	1.25	−0.04121254595
6	1.5	−0.04132453322
7	1.75	−0.04142132695
8	2.	−0.04151428345
9	2.25	−0.04161346793
10	2.5	−0.04172555518
11	2.75	−0.04184881512
12	3.	−0.04197405803
13	3.25	−0.04209410489
14	3.5	−0.04221376484
15	3.75	−0.04234983156
16	4.	−0.04251984155
17	4.25	−0.0427299185
18	4.5	−0.04297376511
19	4.75	−0.04324380597
20	5.	−0.04354272933
21	5.25	−0.04388271037
22	5.5	−0.0442720407
23	5.75	−0.04470257534
24	6.	−0.04515207285
25	6.25	−0.04560138799
26	6.5	−0.04605112755
27	6.75	−0.04652162819
28	7.	−0.04703537074
29	7.25	−0.04759729519
30	7.5	−0.04818995602
31	7.75	−0.04878656577
32	8.	−0.04936951728
33	8.25	−0.04993910141
34	8.5	−0.05050798581
35	8.75	−0.05108914302
36	9.	−0.0516873895