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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 = t3 / Δt;  (* number increment of the second-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 := (
  pulse[t1, ωRFkHz];     (* first pulse with x phase *)
     filterElt[elements1];  (* 3Q coherence pathway selection *)
  pulse[t2, ωRFkHz];     (* second pulse with x phase *)
      filterCoh[coherence2]; (* ±1Q and 0Q 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_3Qxxx" file -----------*)
run;
tabgraph["spam_P3_3Qxxx"];

(* ------------------------------------ *)
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Rang	t(μs)	intensity
0	0	−0.03365329788
1	0.25	−0.03398480198
2	0.5	−0.03423350811
3	0.75	−0.03438558135
4	1.	−0.03445778848
5	1.25	−0.03448085099
6	1.5	−0.0344817151
7	1.75	−0.03447721748
8	2.	−0.0344783431
9	2.25	−0.03449477256
10	2.5	−0.03453277047
11	2.75	−0.03459016837
12	3.	−0.03465735118
13	3.25	−0.034726781
14	3.5	−0.03480297844
15	3.75	−0.03490244729
16	4.	−0.03504232758
17	4.25	−0.035228191
18	4.5	−0.03545309458
19	4.75	−0.0357088615
20	5.	−0.03599776269
21	5.25	−0.03633183279
22	5.5	−0.03671951299
23	5.75	−0.03715301423
24	6.	−0.03761054803
25	6.25	−0.03807357004
26	6.5	−0.03854376231
27	6.75	−0.03904340809
28	7.	−0.03959780442
29	7.25	−0.04021484517
30	7.5	−0.04087882104
31	7.75	−0.04156202612
32	8.	−0.04224260126
33	8.25	−0.04291410975
34	8.5	−0.04358253311
35	8.75	−0.04425750607
36	9.	−0.04494629298