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Get["QUADRUPOLE"];

(*
One-dimensional z-filtered MQMAS of a spin I = 5/2,
Three pulse sequence,
3 Q echo and -3 Q antiecho amplitude optimization with the third pulse,
Coherence pathway 0 Q → ±3 Q → 0 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 third-pulse duration *)

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

fsimulation := (
  pulse[t1, ωRFkHz]; (* first pulse *)
  filterElt[elements1]; (* ±3 Q coherence pathway selection *)
  pulse[t2, ωRFkHz]; (* second pulse *)
  filterCoh[coherence2]; (* 0 Q coherence pathway selection *)
  acq0;

  For[p = 1, p ≤ np, p++, {
    pulse[Δt, ωRF3kHz]; (* third pulse *)
    acq[p];
  }];
);

(*--- Execute, plot, and save simulation

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in "zfilter_P3" file -----*)
run;
tabgraph["zfilter_P3"];
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(* ----- *)
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Rang	t (μ s)	intensity
0	0	0.
1	0.25	-0.0007129352993
2	0.5	-0.001433705113
3	0.75	-0.002165686894
4	1.	-0.002906224332
5	1.25	-0.003648460088
6	1.5	-0.004384546413
7	1.75	-0.00510775821
8	2.	-0.005812808853
9	2.25	-0.006495587637
10	2.5	-0.007153618317
11	2.75	-0.007786967697
12	3.	-0.008398134973
13	3.25	-0.008990160432
14	3.5	-0.009564116213
15	3.75	-0.01011811309
16	4.	-0.01064876055
17	4.25	-0.01115377594
18	4.5	-0.01163342335
19	4.75	-0.01208974372
20	5.	-0.01252475249
21	5.25	-0.01293959077
22	5.5	-0.01333524813
23	5.75	-0.01371355034
24	6.	-0.01407679773
25	6.25	-0.01442605853
26	6.5	-0.01475987204
27	6.75	-0.01507498589
28	7.	-0.01536874034
29	7.25	-0.01564097868
30	7.5	-0.0158937954
31	7.75	-0.01612949109
32	8.	-0.01634864614
33	8.25	-0.01654985374
34	8.5	-0.01673097
35	8.75	-0.01689065135
36	9.	-0.01702925149

