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Get["QUADRUPOLE"];

(*
One-dimensional z-filtered MQMAS of a spin I = 5/2,
Three pulse sequence,
3Q echo and -3Q antiecho amplitude optimization with the first pulse,
Coherence pathway 0Q → ±3Q → 0Q → -1Q,
Coherences belonging to the same pathway are considered,
Wolfram Mathematica 5.0,
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*)

(*----- 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 = "repl00_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 -----*)
coherencel = {-3, 3}; (* ±3Q coherences *)
coherence2 = {0};     (* 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 *)
    store[2];
    filterCoh[coherencel]; (* ±3Q coherence pathway selection *)
    pulse[t2, ωRFkHz]; (* second pulse *)
    filterCoh[coherence2]; (* 0Q coherence pathway selection *)
    pulse[t3, ωRF3kHz]; (* third pulse *)
    acq[p];
    recall[2];
  }];
)

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);  
  
(*--- Execute, plot, and save simulation  
in "zfilter_P1S" file -----*)  
run;  
tabgraph["zfilter_P1S"];  
  
(* ----- *)
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Rang	t (μ s)	intensity
0	0	0.
1	0.25	$-2.796152396 \times 10^{-6}$
2	0.5	-0.00007925667121
3	0.75	-0.0005124262903
4	1.	-0.001712121583
5	1.25	-0.003858724428
6	1.5	-0.00682857892
7	1.75	-0.01020744627
8	2.	-0.01350547668
9	2.25	-0.0164370072
10	2.5	-0.01889948748
11	2.75	-0.02088366752
12	3.	-0.02244126661
13	3.25	-0.02362032572
14	3.5	-0.02440619022
15	3.75	-0.02482844816
16	4.	-0.02501123257

