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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 first pulse,
 Coherence pathway 0 Q → ±3 Q → 0 Q → -1 Q,
 Coherences belonging to the same pathway are considered,
 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 = t1 / Δt;  (* number increment of the first-pulse duration *)

(*--------- Pulse sequence ---------*)
coherence1 = {-3, 3}; (* ±3 Q coherences *)
coherence2 = {0};      (* 0 Q 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[coherence1]; (* ±3 Q coherence pathway selection *)
     pulse[t2, ωRFkHz];  (* second pulse *)
        filterCoh[coherence2]; (* 0 Q 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 (μs)	intensity
0	0	0.
1	0.25	$-2.796152396\times10^{-6}$
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