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Get["QUADRUPOLE"];

(*
 One-dimensional SPAM MQMAS of a spin I = 5/2,
 Three pulse sequence with x, x, and -x phases,
 3Q echo amplitude optimization with the second pulse,
 Coherence pathway 0Q → 3Q → -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 = t2 / Δt;  (* number increment of the second-pulse duration *)

(*--------- Pulse sequence ---------*)
elements1 = {{2, 5}}; (* 3Q matrix element *)
coherence2 = {-1};    (* -1Q 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 *)
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz];  (* second pulse with x phase *)
        store[2];
        filterCoh[coherence2]; (* -1Q coherence pathway selection *)
     pulse[t3, -ωRF3kHz]; (* third pulse with -x phase *)
        acq[p];
        recall[2];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "spam_P2_3Q-1Qxx-x" file ----------*)
run;
tabgraph["spam_P2_3Q-1Qxx-x"];

(* ------------------------------------ *)
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Rang	t (μs)	intensity
0	0	0.
1	0.25	−0.0001137674134
2	0.5	−0.001603564251
3	0.75	−0.006623588442
4	1.	−0.01589306106
5	1.25	−0.02753651111
6	1.5	−0.03802983527
7	1.75	−0.04408064202
8	2.	−0.04398299478
9	2.25	−0.0379960278
10	2.5	−0.02805475162
11	2.75	−0.01712148162
12	3.	−0.008205879735
13	3.25	−0.003290487197
14	3.5	−0.002742284687
15	3.75	−0.005548700715
16	4.	−0.01012290866