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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,
 -3 Q antiecho amplitude optimization with the second-pulse duration,
 Coherence pathway 0 Q → -3 Q → (1 Q, 0 Q, and -1 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 = t1 / Δt;  (* number increment of the first-pulse duration*)

(*--------- Pulse sequence ---------*)
elements1 = {{5, 2}};    (* -3 Q matrix element *)
coherence2 = {1, 0, -1}; (* ±1 Q and 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 with x phase *)
        store[2];
       filterElt[elements1]; (* -3 Q coherence pathway selection *)
     pulse[t2, ωRFkHz];   (* second pulse with x phase *)
        filterCoh[coherence2]; (* ±1 Q and 0 Q coherence pathway selection *)
     pulse[t3, -ωRF3kHz]; (* third pulse with -x phase *)
       acq[p];
        recall[2];
   }];
 );
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(*--- Execute, plot, and save simulation
  in "spam_P1_-3Qxx-x" file -----------*)
run;
tabgraph["spam_P1_-3Qxx-x"];

(* ------------------------------------ *)
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Rang	t(μs)	intensity
0	0	0.
1	0.25	$7.924622464 \times 10^{-6}$
2	0.5	0.0002240724299
3	0.75	0.001378791054
4	1.	0.004377906361
5	1.25	0.009504306276
6	1.5	0.01619873893
7	1.75	0.02342991008
8	2.	0.03022938645
9	2.25	0.03604793428
10	2.5	0.04072912412
11	2.75	0.04443903396
12	3.	0.04759563155
13	3.25	0.05056637037
14	3.5	0.0534930754
15	3.75	0.0563881051
16	4.	0.0592659267