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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, -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 = t3 / Δt;  (* number increment of the third-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 := (
  pulse[t1, ωRFkHz];      (* first pulse with x phase *)
     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 *)
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, -ωRF3kHz]; (* third pulse with -x phase *)
        store[2];
       acq[p];
        recall[2];
   }];
 );
```

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(*--- Execute, plot, and save simulation
  in "spam_P3_-3Qxx-x" file -----------*)
run;
tabgraph["spam_P3_-3Qxx-x"];

(* ------------------------------------ *)
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Rang	t(μs)	intensity
0	0	0.06084622189
1	0.25	0.0611737721
2	0.5	0.06151784546
3	0.75	0.06192677445
4	1.	0.06240882934
5	1.25	0.06294352878
6	1.5	0.06349606485
7	1.75	0.06402579168
8	2.	0.06449353021
9	2.25	0.06487437943
10	2.5	0.0651711321
11	2.75	0.06541430388
12	3.	0.0656422931
13	3.25	0.06587402109
14	3.5	0.06609632214
15	3.75	0.06627679576
16	4.	0.06638981972
17	4.25	0.0664319363
18	4.5	0.06641442974
19	4.75	0.06634432324
20	5.	0.06621580646
21	5.25	0.06602133421
22	5.5	0.0657690034
23	5.75	0.0654845556
24	6.	0.06519220082
25	6.25	0.0648918987
26	6.5	0.06455665824
27	6.75	0.06415500352
28	7.	0.06367909054
29	7.25	0.06315315328
30	7.5	0.06261619026
31	7.75	0.06209570198
32	8.	0.06159307415
33	8.25	0.06108716317
34	8.5	0.0605472353
35	8.75	0.05994521618
36	9.	0.0592659267