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Get["QUADRUPOLE"];

(*
 One-dimensional two-pulse MQMAS of a spin I = 5/2,
 3 Q echo and -3 Q antiecho amplitude optimization with the second pulse,
 Coherence pathway 0 Q → ±3 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 = 100;     (* RF pulse strength in kHz unit *)
spinRatekHz = 15;
powderFile = "rep100_simp";
numberOfGammaAngles = 10;
t1 = 4;     (* the first-pulse duration in microsecond unit *)
t2 = 4;     (* the second-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}, {5, 2}}; (* ±3 Q matrix elements *)
detectElt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  pulse[t1, ωRFkHz];     (* first pulse *)
  filterElt[elements1]; (* ±3 Q coherence pathway selection *)

  acq0;
  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz]; (* second pulse *)
     acq[p];
   }];
 );

(*--- Execute, plot, and save simulation
  in "twoPulse_P2" file -----------*)
run;
tabgraph["twoPulse_P2"];

(* ----------------------------------- *)
```

Rang	t (μs)	intensity
0	0	0.
1	0.25	0.02521224919
2	0.5	0.07693055193
3	0.75	0.1099626208
4	1.	0.09970119991
5	1.25	0.0570143255
6	1.5	0.0105948941
7	1.75	−0.01759249214
8	2.	−0.02148056633
9	2.25	−0.006281997594
10	2.5	0.01724960981
11	2.75	0.03701230806
12	3.	0.04524591779
13	3.25	0.04244521623
14	3.5	0.03372836712
15	3.75	0.02306165688
16	4.	0.01255684181