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Get["QUADRUPOLE"];

(*
One-dimensional two-pulse MQMAS of a spin I = 5/2,
-3Q antiecho amplitude optimization with the second pulse,
Coherence pathway 0Q → -3Q → -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 = 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 = {{5, 2}}; (* -3Q matrix elements *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

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

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

(*--- Execute, plot, and save simulation
in "twoPulseAntiecho_P2" file -----*)
run;
tabgraph["twoPulseAntiecho_P2"];

(* ----- *)

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Rang	t (μ s)	intensity
0	0	0.
1	0.25	0.0255761992
2	0.5	0.08192560901
3	0.75	0.1297272394
4	1.	0.1443789654
5	1.25	0.1286972157
6	1.5	0.1007257322
7	1.75	0.07610453079
8	2.	0.06142050461
9	2.25	0.05701418998
10	2.5	0.05972096762
11	2.75	0.06437221499
12	3.	0.06721789592
13	3.25	0.06881496661
14	3.5	0.07124424203
15	3.75	0.0740261482
16	4.	0.07492458534

