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Get["QUADRUPOLE"];

(*
One-dimensional two-pulse MQMAS of a spin I = 5/2,
3Q echo amplitude optimization with the second pulse,
Coherence pathway 0Q → 3Q → -1Q,
Wolfram Mathematica 5.0,
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*)

(*----- 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}}; (* +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 "twoPulseEcho_P2" file -----*)
run;
tabgraph["twoPulseEcho_P2"];

(* ----- *)

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Rang	t (μs)	intensity
0	0	0.
1	0.25	-0.000363950009
2	0.5	-0.00499505708
3	0.75	-0.01976461861
4	1.	-0.04467776548
5	1.25	-0.07168289018
6	1.5	-0.09013083809
7	1.75	-0.09369702292
8	2.	-0.08290107093
9	2.25	-0.06329618758
10	2.5	-0.0424713578
11	2.75	-0.02735990692
12	3.	-0.02197197813
13	3.25	-0.02636975038
14	3.5	-0.03751587491
15	3.75	-0.050964449132
16	4.	-0.06236774353

