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Get["QUADRUPOLE"];

(*
One-dimensional two-pulse MQMAS of a spin I = 5/2,
3Q echo and -3Q antiecho amplitude optimization with the first 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 = 1;    (* the second-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 = {{2, 5}, {5, 2}}; (* ±3Q matrix elements *)
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 *)
    store[1];             (* save propagator *)
    filterElt[elements1]; (* ±3Q coherence pathway selection *)

    pulse[t2, ωRFkHz];    (* second pulse *)
    acq[p];
    recall[1]              (* recall propagator *)
  }];
);

(*--- Execute, plot, and save simulation
in "twoPulse_P1" file -----*)
run;
tabgraph["twoPulse_P1"];

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(* ----- *)

Rang	t (μ s)	intensity
0	0	0.
1	0.25	0.00001412718276
2	0.5	0.0004081283236
3	0.75	0.002577723198
4	1.	0.00841576114
5	1.25	0.0187634475
6	1.5	0.03247939763
7	1.75	0.04707080741
8	2.	0.06026537494
9	2.25	0.07097105318
10	2.5	0.07910153785
11	2.75	0.08505105268
12	3.	0.08940696677
13	3.25	0.09279090056
14	3.5	0.09562326696
15	3.75	0.09797406538
16	4.	0.09970119991

