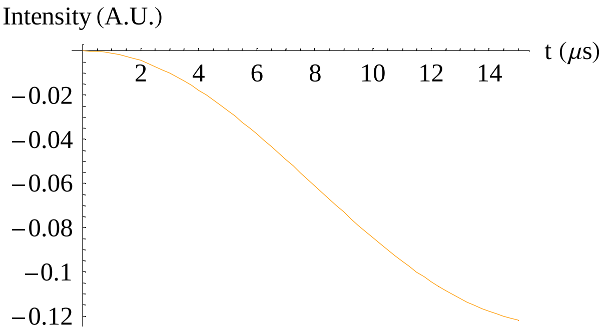
```
Get["QUADRUPOLE"];

(*
 One-dimensional phase-modulated shifted-echo MQMAS of a spin I = 5/2,
 Three-pulse sequence,
 3 Q echo amplitude optimization with the third pulse,
 Coherence transfer pathway 0 Q → 3 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 = 100;  (* strong RF pulse strength in kHz unit *)
ωRF3kHz = 10;  (* weak 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 *)
t3 = 15;   (* 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 ---------*)
coherence1 = {3};     (* 3 Q coherences *)
coherence2 = {1};     (* 1 Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  pulse[t1, ωRFkHz];      (* first pulse *)
     filterCoh[coherence1];  (* 3 Q coherence pathway selection *)
  pulse[t2, ωRFkHz];      (* second pulse *)
     filterCoh[coherence2];  (* 1 Q coherence pathway selection *)

  acq0;
  For [p = 1, p ≤ np,  p++, {
     pulse[Δt, ωRF3kHz];   (* third pulse *)
     acq[p];
   }];
 );

(*--- Execute, plot, and save simulation
```

```
  in "shifted_echo_P3" file ----------------*)
run;
tabgraph["shifted_echo_P3"];

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

```
powderFile: rep100_simp
```

Rang	t(μs)	intensity
0	0	0.
1	0.25	−0.00006938196006
2	0.5	−0.0002650404243
3	0.75	−0.0005885360369
4	1.	−0.001054359172
5	1.25	−0.001673129044
6	1.5	−0.002446381796
7	1.75	−0.003371457196
8	2.	−0.004446009041
9	2.25	−0.005666487117
10	2.5	−0.007025023283
11	2.75	−0.0085113378
12	3.	−0.01011885502
13	3.25	−0.01184767343
14	3.5	−0.01370013484
15	3.75	−0.01567355939
16	4.	−0.01775825035
17	4.25	−0.01994288568
18	4.5	−0.0222211769
19	4.75	−0.02459268653
20	5.	−0.02705745457
21	5.25	−0.02961045077
22	5.5	−0.03224122186
23	5.75	−0.0349381634
24	6.	−0.03769262908
25	6.25	−0.04049941557
26	6.5	−0.0433543259
27	6.75	−0.04625180124
28	7.	−0.0491845306
29	7.25	−0.05214456894
30	7.5	−0.05512443575
31	7.75	−0.05811737645
32	8.	−0.06111713202
33	8.25	−0.06411779359
34	8.5	−0.0671138025
35	8.75	−0.07009966035
36	9.	−0.07306896823
37	9.25	−0.07601323703
38	9.5	−0.07892182992
39	9.75	−0.08178397148
40	10.	−0.08459145098
41	10.25	−0.08733972877
42	10.5	−0.09002624454
43	10.75	−0.0926470763
44	11.	−0.09519503295
45	11.25	−0.0976606056
46	11.5	−0.100034418
47	11.75	−0.1023087066
48	12.	−0.1044773708
49	12.25	−0.1065362854
50	12.5	−0.1084845345
51	12.75	−0.1103245092
52	13.	−0.1120585693
53	13.25	−0.1136843154
54	13.5	−0.1151935661
55	13.75	−0.1165780535
56	14.	−0.1178365236
57	14.25	−0.1189754953
58	14.5	−0.1200011653
59	14.75	−0.1209095953
60	15.	−0.1216860303


Intensity (A.U.)
t (μs)
2
4
6
8
10
12
14
−0.02
−0.04
−0.06
−0.08
−0.1
−0.12