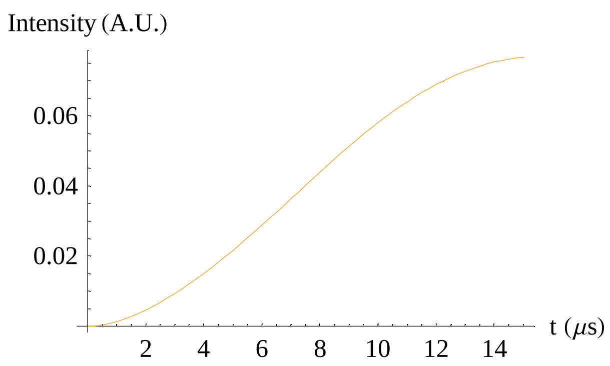
```
Get["QUADRUPOLE"];

(*
 One-dimensional phase-modulated shifted-antiecho 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 = 1.75;  (* 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_antiecho_P3" file ----------------*)
run;
tabgraph["shifted_antiecho_P3"];

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

Rang	t(μs)	intensity
0	0	0.
1	0.25	0.00007899758294
2	0.5	0.0003204186059
3	0.75	0.0007213867017
4	1.	0.001267838728
5	1.25	0.001940156801
6	1.5	0.002720315118
7	1.75	0.003596420923
8	2.	0.004562520206
9	2.25	0.00561500536
10	2.5	0.006749118864
11	2.75	0.007958278441
12	3.	0.009236096822
13	3.25	0.01057862205
14	3.5	0.01198443868
15	3.75	0.01345249678
16	4.	0.01497971555
17	4.25	0.01656052235
18	4.5	0.01818856936
19	4.75	0.01985887576
20	5.	0.02156844654
21	5.25	0.02331510027
22	5.5	0.02509596825
23	5.75	0.02690717697
24	6.	0.0287447098
25	6.25	0.03060509211
26	6.5	0.03248488979
27	6.75	0.03437952865
28	7.	0.03628282664
29	7.25	0.0381878932
30	7.5	0.04008863318
31	7.75	0.04198064066
32	8.	0.04386099269
33	8.25	0.04572737643
34	8.5	0.04757695529
35	8.75	0.04940521212
36	9.	0.05120553782
37	9.25	0.05297022615
38	9.5	0.05469267593
39	9.75	0.05636922257
40	10.	0.05799839659
41	10.25	0.05957788021
42	10.5	0.06110208926
43	10.75	0.0625634502
44	11.	0.06395657192
45	11.25	0.0652812185
46	11.5	0.06654072454
47	11.75	0.06773690464
48	12.	0.06886640963
49	12.25	0.06992232822
50	12.5	0.07090015308
51	12.75	0.07180216517
52	13.	0.07263579307
53	13.25	0.07340651393
54	13.5	0.07411154553
55	13.75	0.07474081402
56	14.	0.07528510027
57	14.25	0.07574297621
58	14.5	0.07612001027
59	14.75	0.07642175872
60	15.	0.07664773228


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