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Notes to program I/Q pairs of PSMIII

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Revision History
June 17, 2018 ... Preliminary Version
Aug   8, 2018 ... First Revision, updated range of Nc, added WURST adiabatic programing, corrections or errors (in previous information) are highlighted in red and marked with a *

Facts and Notation
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 -Number of I/Q pairs is 2048
 -I/Q pair amplitude is bipolar 10 bit -> amplitude programing will be scaled to Fi(n)=[511*Fi'(n)], where Fi'(n) ranges from (-1,1) and [ ]=nearest integer.
  All I/Q mod functions will have this "full scale" programing.  If the amplitude of the pulse needs to vary, use the channel's output scale factor. This preserves the fidelity of the modulation envelope.
*-The current maximum_value_of_Nc = Ncmax = 4095
*-the I/Q data pair is clocked out at (Nc+1)*50ns,  where Nc ranges from 0->Ncmax
*-the longest modulated pulse available is Ncmax*2048*50ns=419.328ms
 -Tp(ms) is the calculated length of the pulse in real time. Tpc(ms) is the calculated length of the pulse rounded up to the next (Nc+1)50ns
 -fo is the central frequency, f1(kHz) is the frequency of Li precession =.63015kHz/G * B1rot(G), Δf (kHz) is the requested bandwidth of the pulse modulation, Δfs(kHz) is the scanned freq range for the wurstN pulse
  (note: to achieve population inversion over the requested bandwidth Δf for either the GaussianHermite or csech functions, a minimum value of f1>Δf is required. This is not true for the wurstN.
 -Each modulation function can be written as Fi(n)=511*[F'i{b_i*(t-Tpc/2)/(Tpc/2)}]=[511*Fi'{b_i*2*(2n-Niq-1)/(2*(Niq-1))}]; (slightly more accurate than the definition in the PSMii documentation)
   where the F'i is a function whose value is in the range (-1,1) and 2*(2n-Niq-1)/(2*(Niq-1)) is the discreet normalized time which goes from -1->1 as (t-Tpc2)/Tpc/2 goes from -Tpc/2 to+Tpc/2
   Tp is the nominal length/time of the pulse determined by the required linewidth, and Tpc is the calculated length of the pulse rounded to the next (Nc+1*50ns)
   t discreetly ranges from 0 to Tpc whereas the iq index n ranges from 1 to Niq.
   Niq is the number of iq pairs (i.e. the I&Q data Memory Length) with n ranging from 1 to Niq.
   b_i is chosen so that at t=0,Tp (or n=1,Nqi) F'i(b_i)=.01 ....  i.e. that actual digitally modulated pulse amplitude goes from .01->1->.01 which contributes to the defined pulse length Tpc
    However, for the WURST pulse amplitude, which goes from 0 -> 0 in the first and last bins modulation bins, i.e. when n=1 or = Niq, we leave b_wurstN=1
*  b_csech = 5.2983   I'csech(x)=sech(x)*cos(u*ln(sech(x)))  Q'sech(x)=sech(x)*sin(u*ln(sech(x))), with u=5 (positive sign on Q’ is because ln(sech) is negative
                                                                                                             … which means freq sweep in the pulse modulation is from low to high, i.e. fo-Δf/2 to fo+Δf/2)
     References: Zhang et al, Full Analytical Solution of the Bloch Equation When Using a Hyperbolic-Secant Driving Function, Magnetic Resonance in Medicine 77:1630-1638(2017)
                 Siegel et al, Sensitivity Enhancement of NMR Spectra of Half-Integer Quadrupolar Nuclei in the Solid State via Population Transfer, Concepts in Magnetic Resonance Part A, Vol. 26A(2) 47â€“61 (2005)
                 Silver et al, Selective Spin inversion in nuclear magnetic resonance and coherent optics through an exact solution of the Block-Riccati equation, Phys. Rev. A, Vol. 31, No. 4 (1985)
                 Rosenfeld et al, Is the sech/tanh Adiabatic Pulse Really Adiabatic?, JMR 132, 102-108 (1998)
   b_ghermite = 2.5   I'ghermite(x)=(1-x^2)*exp(-(x^2)) Q'ghermite=0
   b_wurstN = 1       I’wurstN(x)=(1-(abs(sin(pi*x/2)))^N)*cos((Qo/8)*((Δfs/f1)^2)*(x^2))  Q’wurst(x)=-(1-(abs(sin(pi*x/2)))^N)*sin((Qo/8)*((Δfs/f1)^2)*(x^2)), Qo=5, for N=40 Δfs=Δf*1.3, for N=80 Δfs=Δf*1.2
     References: O’Dell, The WURST kind of pulses in solid-state NMR, Solid State Nuclear Magnetic Resonance 55-56 (2013) https://www.journals.elsevier.com/solid-state-nuclear-magnetic-resonance

Calculation of Tp: (and other needed parameters)
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 Note:  The calculation for Tp is dependent on the relationship between the needed irradiation line width Δf and the function chosen & the fulfilling of the adiabatic sweep condition for the wurst pulse
 For the csech function,   Δf(Hz)=2*b_csech*u/(2pi*Tp(sec)) -> Tp(ms)=5.2983*5/(pi*Δf(kHz))=8.4325/Δf(kHz)
*For the GausianHermite,   Δf(Hz)=4*1.474*2*b_ghermite/(2pi*Tp(sec)) -> Tp(ms)=4.69/Δf(kHz) ;
   Note: Fourier transform and scaling of the ghermite function give; F{(1-(at)^2)*exp{-((at)^2)}}=(1+2*y^2)*e-(y^2), y=ω/2a, half-width @ half height of Fourier transform occurs at y=1.474
 For the wurstN, Tp(ms) = (Qo/(2*pi))*Δfs/(f1^2) which defines the adiabatic sweep condition.  Both Δfs & f1 are in kHz (f1 is usually ~.6kHz for an ~1G B1 RF rotating-frame field strength)
                        = 2.005(kHz^-2)*Δfs(kHz), assuming a f1=.63kHz
Calculation of Niq, Nc+1 and Tpc:
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* Nc+1 = [[Tp(ms)/(50E-6*2048)]],  with [[,,,]] = next larger integer i.e. roundup
* Niq  = [[Tp(ms)/(50E-6*(Nc+1))]]
* Tpc(ms) = 50E-6*(Nc+1)*Niq

* One must check that for a given requested Δf(kHz) the calculated Tpc(ms) lies within the range 1*50E-6*1024=.0512 < Tpc(ms) <419.4304=4096*50E-6*2048
 i.e. Δf_min_csech = .0201 kHz
*     Δf_min_ghermite = .01118kHz
      Δfs_min_wurst = .0255kHz (assuming f1=.63kHz, smaller values of f1 will permit a lower min value of Δfs)
 and
      Δf_max_csech = 164.697kHz
*     Δf_max_ghermite = 91.6kHz
      Δfs_max_wurst = 209.19kHz (assuming f1=.63kHz, larger values of f1 will permit a larger max value of Δfs)

Summary:
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i)   Select the modulation type
ii)  Ask for the required bandwidth of the pulse = Δf(kHz)(use Δfs for the wurst pulse)
iii) Make sure it is within the min and max available for the given type of modulation pulse
iv)  Calculate Tp(ms) for the modulation type & verify it is within available limits (which should be true if condition iii) OK)
v)   Calculate Nc+1, Niq and Tpc and verify Nc+1 and Niq are within limits. Niq should be between 1024 and 2048
vi)  Calculate the I,Q pairs in 2's compliment using

For complex-sech:
 b_csech =    5.2983 I'csech(x)=[511*sech(x)*cos(u*ln(sech(x)))]  Q'sech(x)=[511*sech(x)*sin(u*ln(sech(x)))], with u=5 [...]=nearest integer
For gaussian-hermite
 b_ghermite = 2.5    I'ghermite(x)=[511*(1-x^2)*exp(-(x^2))] Q'ghermite=0
For wurstN
 b_wurstN   = 1      I’wurstN(x)=(1-(abs(sin(pi*x/2)))^N)*cos((Qo/8)*((Δfs/f1)^2)*(x^2))  Q’wurst(x)=-(1-(abs(sin(pi*x/2)))^N)*sin((Qo/8)*((Δfs/f1)^2)*(x^2)), Qo=5, for N=40 Δfs=Δf*1.3, for N=80 Δfs=Δf*1.2

for x=b_i*2*(2n-Niq-1)/(2*(Niq-1)), where n goes from 1 to Niq
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