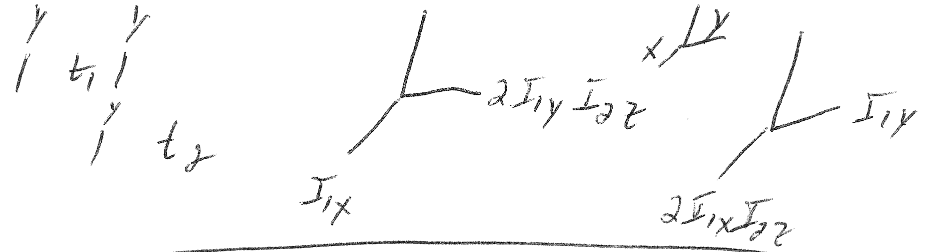
IV-b) H,H-COSY



$\rho = I_{1z} + I_{2z}$ Focus on I_{1z}

$$I_{1z} \xrightarrow{(\frac{\pi}{2})_y} I_{1x}$$

$$I_{1x} \xrightarrow[t_1]{H_J} I_{1x} C_J^1 + 2 I_{1y} I_{2z} S_J^1$$

$$I_{1x} C_J^1 \xrightarrow[t_1]{H_{cs}} C_J^1 \left[I_{1x} C_{\omega_1}^1 + I_{1y} S_{\omega_1}^1 \right] = C_J^1 C_{\omega_1}^1 I_{1x} + C_J^1 S_{\omega_1}^1 I_{1y}$$

$$2 I_{1y} I_{2z} S_J^1 \xrightarrow[t_1]{H_{cs}} 2 I_{2z} S_J^1 \left[I_{1y} C_{\omega_1}^1 - I_{1x} S_{\omega_1}^1 \right]$$

$$2 I_{1y} I_{2z} S_J^1 C_{\omega_1}^1 - 2 I_{1x} I_{2z} S_J^1 S_{\omega_1}^1$$

---

collect terms

$C_J^1 C_{\omega_1}^1 I_{1x} \xrightarrow{(\pi/2)_y} -A\, I_{1z}$ Pop

$C_J^1 S_{\omega_1}^1 I_{1y} \longrightarrow B\, I_{1y}$ evolves at ω_1

$S_J^1 C_{\omega_1}^1 2 I_{1y} I_{2z} \longrightarrow C\, 2 I_{1y} I_{2x}$ DQC, singlet

$-S_J^1 S_{\omega_1}^1 2 I_{1x} I_{2z} \longrightarrow -D\, 2 I_{1z} I_{2x}$ AP SQC

$\boxed{I_{1y} \text{ TERM - gives DIAG}}$

$$B I_{1y} \xrightarrow[t_2]{H_J} B \left[I_{1y} C_J^2 - \overset{AP}{\cancel{2 I_{1x} I_{2z}}} S_J^2 \right]$$

$$B C_J^2 I_{1y} \xrightarrow[t_2]{H_{cs}} B C_J^2 \left[I_{1y} C_{\omega_1}^2 - I_{1x} S_{\omega_1}^2 \right]$$

$tr(\rho \cdot I^+) \neq 0$

$$= \boxed{\begin{array}{l} C_J^1 S_{\omega_1}^1 C_J^2 C_{\omega_1}^2 I_{1y} \\ - C_J^1 S_{\omega_1}^1 C_J^2 S_{\omega_1}^2 I_{1x} \end{array}} \text{ — observable}$$

② $-BS_J^2\, 2I_{1x}I_{2z} \xrightarrow[t_2]{H_J} -BS_J^2\left[\overset{\nearrow AP}{2I_{1x}I_{2z}}C_J^2 + I_{1y}S_J^2\right]$

$-BS_J^2\cancel{S_2^2}\, I_{1y} \xrightarrow[t_2]{H_{CS}} -BS_J^2\left[I_{1y}C\omega_1^2 - I_{1x}S\omega_1^2\right]$

$= -BS_J^2C\omega_1^2 I_{1y} + BS_J^2S\omega_1^2 I_{1x}$

$$\boxed{\begin{aligned}&= -C_J^1 S\omega_1^1 S_J^2 C\omega_1^2 I_{1y}\\ &+ C_J^1 S\omega_1^1 S_J^2 S\omega_1^2 I_{1x}\end{aligned}}$$ — ∂SS

$-DI_{1z}I_{2x}$ term $\boxed{\text{Gives X-PKS}}$

$\xrightarrow[t_2]{H_J}$
$-D\left[2I_{1z}I_{2x}C_J^2 + I_{2y}S_J^2\right]$

$\xrightarrow[t_2]{H_{CS}}$
$~~-DC_J^2[2I_{1z}I_{2x}~~ \quad -DC_J^2 2I_{1z}I_{2x} \xrightarrow[t_2]{H_{CS}} -DC_J^2\cancel{2I_{1z}}\left[I_{2x}C\omega_2^2 + I_{2y}S\omega_2^2\right]$ AP

$-DS_J^2 I_{2y} \xrightarrow[t_2]{H_{CS}} -DS_J^2\left[I_{2y}C\omega_2^2 - I_{2x}S\omega_2^2\right]$

$= -DS_J^2C\omega_2^2 I_{2y} = -S_J^1 S\omega_1^1 S_J^2 C\omega_2^2 I_{2y}$ X PK (ω_1,ω_2)

$+DS_J^2S\omega_2^2 I_{2x} = S_J^1 S\omega_1^1 S_J^2 S\omega_2^2 I_{2x}$ X PK (ω_1,ω_2)

~~$-C_J^1 S\omega_1^1 S_J^2 C\omega_1^2 I_{1y}$~~ Diag (ω_1,ω_1)

C_J^1 ~~$S\omega_1^1 S_J^2 S\omega_1^2$~~ I_{1x} Diag (ω_1,ω_1)

From I_{1z}

③ all terms!

I_1z		I_2z
$-S_J^1 Sw_1^1 S_J^2 Cw_2^2 \; I_2y$	← XPK (w_1, w_2) →	$-S_J^1 Sw_2^1 S_J^2 Cw_1^2 \; I_1y$
$S_J^1 Sw_1^1 S_J^2 Sw_2^2 \; I_2x$	← XPK (w_1, w_2) →	$S_J^1 Sw_2^1 S_J^2 Sw_1^2 \; I_1x$
$C_J^1 Sw_1^1 C_J^2 Cw_1^2 \; I_1y$	← Diag (w_1, w_1) →	$C_J^1 Sw_2^1 C_J^2 Cw_2^2 \; I_2y$
$-C_J^1 Sw_1^1 C_J^2 Sw_1^2 \; I_1x$	← Diag (w_1, w_1) →	$-C_J^1 Sw_2^1 C_J^2 Sw_2^2 \; I_2x$

I_{z1} $\quad$ I_{z2}

$I_{x1} \rightarrow I_{x2}$

S_J terms don't change

y

$I_1z \rightarrow Sw_1^1$

$I_2z \rightarrow I_2y \; Sw_2^1$

y

y

I_1z	I_2z
$I_2y \; Sw_1^1 \; Cw_2^2$	$I_1y \; Sw_2^1 \; Cw_1^2$
$I_2x \; Sw_1^1 \; Sw_2^2$	$I_1x \; Sw_2^1 \; Sw_1^2$
$I_1y \; Sw_1^1 \; Cw_1^1$	$I_2y \; Sw_2^1 \; Cw_2^1$
$I_1x \; Sw_1^1 \; Sw_1^2$	$I_2x \; Sw_2^1 \; Sw_2^2$

$(\frac{\pi}{2})y$

$I_1z \rightarrow I_1x$

$I_2z \rightarrow I_2x$

Π

Π

I_2z

~~$-S_J^1 S_J^2 Sw_2^1 Cw_1^2 \; I_2y$~~ XPK (w_1, w_2)

~~$S_J^1 S_J^2 Sw_2^1 Sw_1^2 \; I_2x$~~ XPK (w_1, w_2)

~~$C_J^1 C_J^2 Sw_2^1 Cw_2^2 \; I_1y$~~ DIAG (w_2, w_2)

~~$-C_J^1 C_J^2 Sw_2^1 Sw_2^2 \; I_1x$~~ Diag (w_2, w_2)

④ Two Important Pts

1) t_1 modulation appears as sines or cos, non-quad. ∴ work off Res & throw away ½ sig OR phase cycle

2) Diags along T_1 mod are products c·s. Diags are doubly sine modulated, see trig identities

Diag:

$$s(\omega_1 t_1)c(\tfrac{Jt_1}{2}) =$$

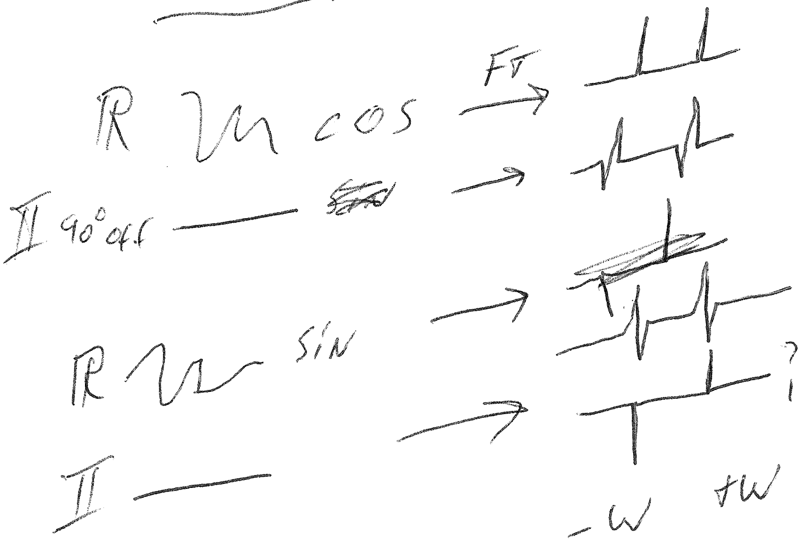
$$= \tfrac{1}{2}\left[s(\omega_1 + \tfrac{J}{2})t_1 + s(\omega_1 \overset{-}{\cancel{+}} \tfrac{J}{2})t_1\right]$$

X-PK

$$s(\omega_1 t_1)s(\tfrac{Jt_1}{2})$$

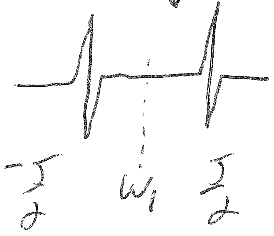
$$= \tfrac{1}{2}\left[c((\omega_1 - \tfrac{J}{2})t_1) - c((\omega_1 + \tfrac{J}{2})t_1)\right]$$

Recall



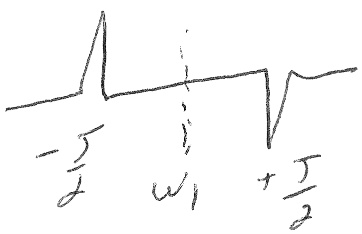
$$s(\omega_1 t_1)c(\tfrac{Jt_1}{2}) = \text{Diag}$$

$\downarrow$ FT



$$s(\omega_1 t_1)s(\tfrac{Jt_1}{2})$$

$\downarrow$ FT



#5 Trig Identities:

$$S(\alpha)C(\beta) = \frac{S(\alpha+\beta) + S(\alpha-\beta)}{2}$$

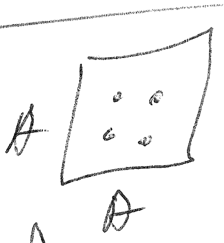
$$C(\alpha)C(\beta) = \frac{C(\alpha+\beta) + C(\alpha-\beta)}{2}$$

$$S(\alpha)S(\beta) = \frac{C(\alpha-\beta) \mp C(\alpha+\beta)}{2}$$

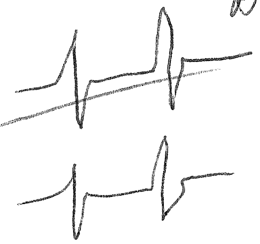
~~I_{2z}~~ $I_{2y} \longrightarrow S(\frac{Jt_1}{2})S(\omega_1 t_1) \Rightarrow C(\omega_1 - \frac{J}{2})t \mp C(\omega_1 t + \frac{Jt}{2})$

$S(\frac{Jt_2}{2})C(\omega_2 t_2)$

$\Rightarrow S(\frac{J}{2} + \omega_2) + S(\frac{J}{2} - \omega_2)$



I_{2x} = XPK
I_{1y} = Diag
} positive part of V_1

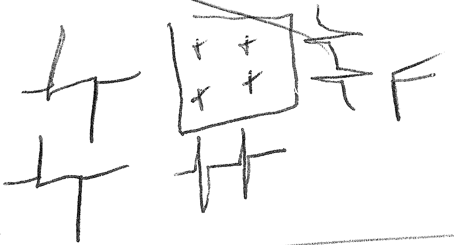


$I_{2x} = \{ S(\frac{Jt_1}{2})S(\omega_1 t_1) \rightarrow$ ~~$S(\omega_1 + \frac{J}{2}) + S(\omega - J/2) \Rightarrow$~~

$S(\frac{Jt_2}{2})S(\omega_2 t_2) \rightarrow$ ~~$S(\omega_2 + \frac{J}{2}) + S(\omega - J/2) \Rightarrow$~~

$I_{2x} \{ S_J^1 S_1^1 \rightarrow C(\omega_1 - \frac{J}{2}) - C(\omega_1 + J/2)$

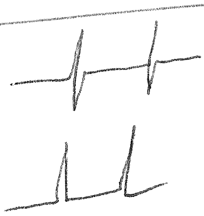
$S_J^2 S_2^2 \rightarrow C(\omega_2 - \frac{J}{2} - C(\omega_2 + J/2)$

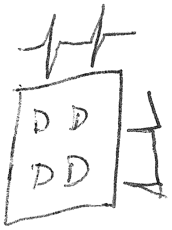


X PKS all (+)

I_{1y} $S(\omega_1 t)C(\frac{Jt_1}{2}) \rightarrow S(\omega_1 + \frac{J}{2}) + S(\omega_1 - \frac{J}{2})$

Diag $C(\omega_1 t_2)C(\frac{Jt_2}{2}) \rightarrow$ ~~$C(\omega_1 + \frac{J}{2}) + C(\omega_1 - \frac{J}{2})$~~





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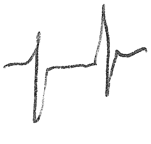


A·D = Dis

A·A = A
A·D = D
D·D = A

I_{1y} = II ?

II-3) Given a pair of I-S spins, expand on the Follow sph. ops. IN cartesian Terms

---

recall $I_x \xrightarrow{H_{cs}} I_x C(\omega t) + I_y S(\Delta\omega t)$

~~$I_x = I_+ + iI_-$~~

~~$I_y = I_+$~~

$$\boxed{\begin{array}{l} I_+ = I_x + iI_y \\ I_- = I_x - iI_y \end{array}}$$

Note these are defined not derived

$I_x = \frac{I_+ + I_-}{2}$

$I_y = \frac{I_+ - I_-}{2i}$

$$cI_x + sI_x = \frac{1}{2}\left[(I_+ + I_-)c + \cancel{I}_y\frac{(I_+ - I_y)}{i}s\right]$$

$$= \frac{1}{2}\left[I_+c + I_-c + \frac{I_+s}{i} - \frac{I_-}{i}s\right]$$

$$cI_x + sI_y = \frac{1}{2}\left[\left(I_+c + \frac{I_+s}{i}\right) + \left(I_-c - \frac{I_-}{i}s\right)\right]$$

$$= \frac{1}{2}\left[(I_+c - iI_+s) + (I_-c + iI_-s)\right]$$

$e^{ix} = c(x) + is(x)$

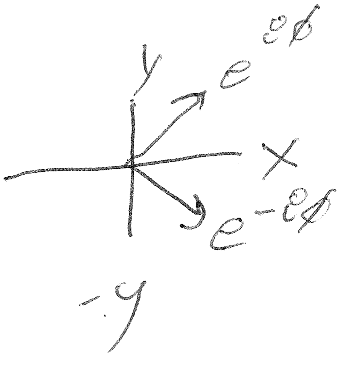
$e^{-x} = c(x) - is(x)$

$$= \frac{1}{2}\left[I_+(c - is) + I_-(c + is)\right]$$

$$\boxed{\cancel{I_\phi} = \frac{1}{2}\left[I_+e^{-i\phi} + I_-e^{i\phi}\right]} = cI_x + I_y s$$

$$\boxed{I_x c(\phi) + I_y s(\phi) = \frac{1}{2}\left[I_+e^{-i\phi} + I_-e^{i\phi}\right]}$$

2 counter Rotating Freqs



② $\{I_x, I_y, I_z, \mathbb{1}\}$ - cartesian basis set

$\{I_+, I_0, I_-, \mathbb{1}\}$ - spherical Basis set

Can write for 2-spin IS as well

$xyz \rightarrow -i\hbar$

$zyx \rightarrow +i\hbar$

recall $[M_x, M_y] = -i\hbar M_z$ $\quad [M_z, M_y] = +i\hbar M_x$

$[M_y, M_z] = -i\hbar M_x$ $\quad [M_y, M_x] = +\hbar M_z$ $\quad$ ladder ops

$[M_z, M_x] = -i\hbar M_y$ $\quad [M_x, M_z] = +i\hbar M_y$ $\quad [M^2, M_x] = 0$

$\vdots \quad = 0$

$M^2 = M_x^2 + M_y^2 + M_z^2$ $\quad \vdots \quad = 0$

$$\boxed{\begin{aligned} I_+ &\equiv I_x + iI_y \\ I_- &\equiv I_x - iI_y \\ I_0 &\equiv I_z \end{aligned}}$$

II-3 continued) $\boxed{I_+ = I_x + iI_y}$

$$\boxed{I_+S_0 = (I_x + iI_y)S_z = I_xS_z + iI_yS_z}$$

$$I_+S_- = (I_x + iI_y)(S_x - iS_y)$$

$$= I_xS_x - iI_xS_y + iI_yS_x + I_yS_y$$

$$\boxed{I_+S_- = I_xS_x + I_yS_y + i(I_xS_y + I_yS_x)}$$

$$I_+S_+ = (I_x + iI_y)(S_x + iS_y)$$

$$= I_xS_x + iI_xS_y + iI_yS_x - I_yS_y$$

$$\boxed{I_+S_+ = I_xS_x - I_yS_y + i(I_xS_y + I_yS_x)}$$

③ VI-3-00) Calculate The evol. of ops under

$$H_{CS} = -\omega_S S_z - \omega_I I_z \equiv -\omega_S S_0 - \omega_I I_0$$

$$I_+ \xrightarrow{H_{CS}} e^{-iHt/\hbar} I_+ e^{iH_{CS}t/\hbar}$$

$$I_\pm \xrightarrow{\Delta\omega I_z t} I_\pm e^{\mp i\Delta\omega t}$$

no scrambling of ops under H_{CS}!

$$I_\pm \xrightarrow{H_{CS}} I_x c + I_y s = \frac{1}{2}\left[I_+ e^{-i\phi} + I_- e^{i\phi} \right]$$

$$\therefore \boxed{I_\pm \xrightarrow{H_{CS}} I_\pm e^{\mp i\phi}}$$

$\left.\begin{matrix} S_0 = \\ I_0 = \end{matrix}\right\}$ Don't evolve

---

$I_+ S_0 = (I_x c + I_y s) S_z \Rightarrow S_z$ doesn't evolve

$\phi = ((-\Delta\omega_S - \omega_I)t)$

$$\Rightarrow I_+ S_0 \xrightarrow{H_{CS}} I_\pm S_0 e^{\mp i\phi}$$

$$\hookrightarrow I_+ S_0 e^{-i\phi} = I_+ S_0 e^{-i(-\Delta\omega_S - \Delta\omega_I)t}$$

$\Delta\omega_1 = \omega_1 - \omega_0$

$$= I_+ S_0 e^{i(\Delta\omega_S)t} e^{i\Delta\omega_I t}$$

$$I_- S_0 e^{-i(\Delta\omega_S t)} e^{i\Delta\omega_i t}$$

$\phi_I = -\Delta\omega_i t$

$\phi_S = -\Delta\omega_S t$

$$I_+ S_- \xrightarrow{H_{CS}} I_+ e^{-i\phi_I} S_- e^{+i\phi_S} =$$

$$= I_+ S_- e^{-i(+\Delta\omega_I t \cancel{+} \Delta\omega_S t)}$$

④ $I_+ S_+ = I_+ e^{-i\phi_I} S_+ e^{-i\phi_S}$

$= I_+ S_+ e^{i(\omega_S + \omega_I)t}$

$I_+ \Rightarrow$ Doesn't evolve under S_z & VV

$\phi_I = -\omega_I t$

$\phi_S = -\omega_S t$

---

iii) Same now $H_J = J I_z S_z$

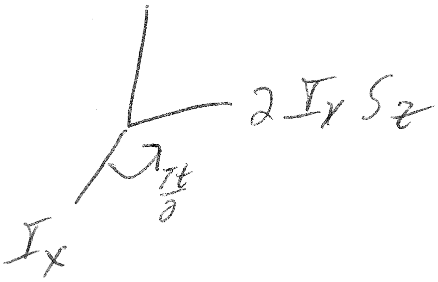
$e^{iH_J t/\hbar} I_+ e^{iH_J t/\hbar} =$

$I_\pm \xrightarrow{H_J} I_\pm c(\frac{Jt}{2}) \pm 2 I_\pm S_z s(\frac{Jt}{2})$

$$\boxed{I_\pm \xrightarrow{H_J} I_\pm c(\frac{Jt}{2}) \pm 2 I_\pm S_z s(\frac{Jt}{2})}$$

$= I_\pm c(\frac{Jt}{2}) \pm 2 I_\pm S_0 s(\frac{Jt}{2})$

before



$\rho(t) = I_x c(\frac{Jt}{2}) + 2 I_y S_z s(\frac{Jt}{2})$

$$\boxed{I_x = \frac{I_+ + I_-}{2} \quad \Big| \quad I_y = \frac{(I_- - I_+)i}{2}}$$

we phase cycle out I^-

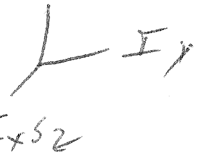
$\therefore I_x = \frac{I_+}{2}$ $\quad I_y = \frac{-i I_+}{2}$

$\rho(t) \Rightarrow \frac{I_+}{2} c(\frac{Jt}{2}) - i I_+ S_0 s(\frac{Jt}{2})$

$I_+ \xrightarrow{H_J} \Rightarrow I_+ c(\frac{Jt}{2}) - 2i I_+ S_0 s(\frac{Jt}{2})$

⑤

$$I_+S_0 \xrightarrow{H_J} I_xS_z\, c\left(\frac{Jt}{2}\right) + \frac{I_y}{2}\, s\left(\frac{Jt}{2}\right)$$



I_xS_z

$$= \frac{I_+S_0}{2}\, c\left(\frac{Jt}{2}\right) - \frac{i\,I_+}{\cancel{4}\ 2}\, s\left(\frac{Jt}{2}\right)$$

$I_+S_- = I_xS_y \xrightarrow{H_J}$ X doesn't evolve

ZQC

$I_+S_+ = I_xS_x \xrightarrow{H_J}$ X Doesn't evolve for 2-spin

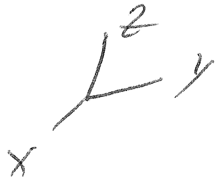
MQC

---

iii

VI-3-iiii) Appy $(\frac{\pi}{2})_x$ For OB in i) ~~&~~ a

⑥



Phase cycleout
$I_- S_-$

$$I_+ \xrightarrow[(\frac{\pi}{2})_x]{Hr} I_x + i I_y \xrightarrow{Hr} I_x \pm i I_z$$

$$I_x = \frac{I_+ + I_-}{2} \quad I_z = I_0 \Rightarrow \frac{I_+ + I_-}{2} + i I_0 = I_+ + i I_0$$

$$I_+ S_- = (I_x + iI_y)(S_x - iS_x) = I_x S_x - I_x i S_y + I_y i S_x + I_y S_y$$

$$I_+ S_- = I_x S_x + I_y S_y + i(I_y S_x - I_x S_y)$$

$$\xrightarrow{(\frac{\pi}{2})_x} I_x S_x + I_z S_z + i(I_z S_x - I_x S_z)$$

$$= I_+ S_+ + I_0 S_0 + i(I_0 S_+ - I_+ S_0)$$

$$I_+ S_0 = (I_+ + i I_y) S_z = I_x S_z + i I_y S_z \qquad I_y = -i I_+$$

$$\xrightarrow{(\frac{\pi}{2})_x} -I_x S_y \pm i I_z S_y \qquad I_x = I_+$$

$$\cancel{= +i I_+ S_+ - I_0 S_+}$$

$$= -(I_+)(-iS_+) - i(I_0)(-iS_+)$$

$$= i I_+ S_+ + i^2 I_0 S_+$$

$$\boxed{I_+ S_0 \xrightarrow{(\frac{\pi}{2})_y} = i I_+ S_+ - I_0 S_+}$$

VI-4) want to see how U(t) changes sph. basis (i.e. pulse w/ phase)

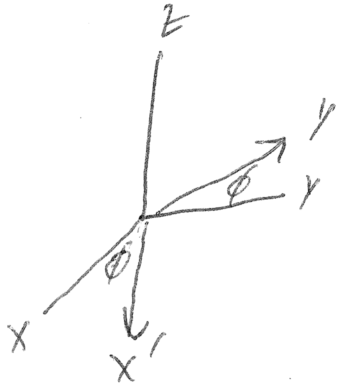
U(t) = delays, Hcs, HJ, etc

$\rho_0 \xrightarrow{U(t)} \rho_t$

$\rho_t = a\cdot\mathbb{1} + b\cdot S_0 + c\cdot S_0 + d\cdot I_+ + e\cdot I_{-}$; ...

= the effects of the ϕ shift in pulse can be seen each basis element above eg) a, b, c, d...

Note: a ϕ shift in RF is equiv to defining rotating frame



In QM this is seen as

$R = e^{-iF_z\phi}$; $F_z = I_z + S_z$ = tot ang mom in z

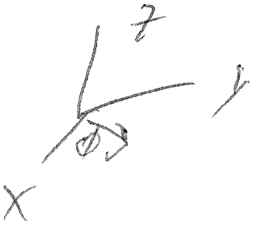
~~$I_z \xrightarrow{R_x}$~~

$I_z \xrightarrow{R_z} e^{-iH_t t/\hbar} I_0 e^{iH_t t/\hbar}$ $H_t = I_z + S_z$

$e^{-iI_z t}\, e^{iS_z t}\, I_0\, e^{iI_z t}\, e^{iS_z t} = e^{-iF_z t} I_z e^{iF_z t}$

+ we already defined unitary rotations I-14

eg) $I_x \xrightarrow{R_z} I_x C(\phi) + I_y S(\phi)$



Ⓑ :

$$I_+S_0 \xrightarrow{R} S_0 I_+ e^{-i\phi}$$

$$I_0 S_+ \xrightarrow{u_z} I_0 S_+ e^{-i\phi}$$

$$S_+ \xrightarrow{u_z} S_+ e^{-i\phi}$$

$$I_+ \xrightarrow{u_z} I_+ e^{-i\phi}$$

$$I_x = \frac{I_+ + I_-}{2}$$

$$I_y = i\frac{(I_- - I_+)}{2}$$

$$I_- \xrightarrow{\cancel{u_z}} I_x - iI_y \xrightarrow{u_z}$$

$$I_x c + I_y s$$

$$I_x \xrightarrow{u_z(\phi)} I_x c + I_y s$$

$$-i(I_y) \xrightarrow{\cancel{u_z}\, u_z(\phi)} -i(I_y c - I_x s) = -iI_y c + iI_x s$$

$$= I_x c + iI_x s = I_x e^{i\phi}$$

$$+ I_y s - iI_y c \quad + I_y(s - ic)$$

$$= \frac{I_+ + I_-}{2} e^{i\phi} + \frac{i(I_- - I_+)}{2}(s - ic)$$

$$+ \frac{(I_- - I_+)}{2}(is - i^2 c) =$$

$$+ \left(\frac{I_- - I_+}{2}\right)(c + is)$$

$$= \frac{1}{2}\left[(I_+ + I_-)e^{i\phi} + (I_- - I_+)e^{i\phi}\right.$$

$$= \frac{1}{2} e^{i\phi}\left(I_+ + I_- + I_- - I_+\right) = \frac{2I_-}{2} e^{i\phi} = \boxed{I_- \xrightarrow{u_z\phi} = I_- e^{i\phi}}$$

④ $I_- \xrightarrow{u_z(\phi)} I_- e^{i\phi}$ all SQC Follow For I_-

$I_- \xrightarrow{u_z(\phi)} I_- e^{i\phi}$

$S_- \xrightarrow{u_z} S_- e^{i\phi}$

$I_- S_0 \xrightarrow{u_z} S_0 I_- e^{i\phi}$

$I_0 S_- \xrightarrow{u_z} I_0 S_- e^{i\phi}$

remember ϕ = RF Phase change.
ie, redefined
Rot Frame

$I_+ = I_x + iI_y$ $\quad I_x = \frac{I_+ + I_-}{2}$

DQC: $I_+ S_+$

$I_- S_-$

$S_- = S_x - iS_y$ $\quad S_y = \frac{i(I_- - I_+)}{2}$

NO!

$I_+ S_+ = (I_x + iI_y)(S_x + iS_y) = I_x(S_x + iS_y) + iI_y(S_x + iS_y)$

$= I_xS_x + iI_xS_y + iI_yS_x - I_yS_y$

$= I_xS_x - I_yS_x + i(I_xS_y + I_yS_x)$

↖ rotate each ~~on~~ term

$I_xS_x \xrightarrow{u_z} (I_xC + I_yS)(S_xC + S_yS)$

$= I_xC(S_xC + S_yS) + I_yS(S_xC + S_yS)$

$= I_xS_xC^2 + CSI_xS_y + CSI_yS_x + S^2I_yS_y$

keep

	$\mathbb{1}$	S_+	S_0	S_-
$\mathbb{1}$	$\mathbb{1}$	S_+	S_0	S_-
I_+	I_+	I_+S_+	I_+S_0	I_+S_-
I_0	I_0	I_0S_+	I_0S_0	I_0S_-
I_-	I_-	I_-S_+	I_-S_0	I_-S_-

↑

The IS-spherical basis set!

	ZQC		SQC		DQC
			I_+		I_+S_+
$\mathbb{1}$	I_0	NOIS	I_-		I_-S_-
	S_0		S_+		
	I_-S_+		S_-		
	I_+S_-		I_+S_0		
slow order →	I_0S_0		I_0S_+	AP	
			I_-S_0		
			I_0S_-		

VI-4
cont

$$e^{-iF_z\phi} I_+ e^{iF_z} = e^{-iI_z\phi} e^{-iS_z\phi} I_+ e^{iS_z\phi} e^{+iI_z\phi}$$ Keep

$$= e^{-iS_z\phi} e^{iS_z\phi} \cdot e^{-iI_z\phi} I_+ e^{iI_z\phi}$$

$$= 1 \cdot I_+ e^{-i\phi}$$

$$I_+S_+ \xrightarrow{uz} e^{-iI_z\phi} e^{-iS_z\phi} I_+S_+ e^{iI_z\phi} e^{iS_z\phi}$$

$$= e^{-iI_z\phi} I_+ e^{iI_z\phi} \cdot e^{-iS_z\phi} S_+ e^{iS_z\phi}$$

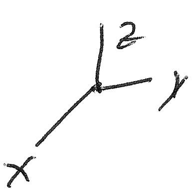
$$= I_+ e^{-i\phi} \cdot S_+ e^{-i\phi} = \boxed{I_+S_+ e^{-i2\phi}}$$

$$I_-S_- \xrightarrow{uz} e^{-iI_z\phi} e^{-iS_z\phi} I_-S_- e^{+iI_z\phi} e^{iS_z\phi}$$

$$= e^{-iI_z\phi} I_- e^{iI_z\phi} \cdot e^{-iS_z\phi} S_- e^{iS_z\phi}$$

$$= I_- e^{+i\phi} \cdot S_- e^{i\phi} = \boxed{I_-S_- e^{i2\phi}}$$

use These



* They are made consistent with NMR notes

$I_x \xrightarrow{u_x} I_x$

$\xrightarrow{u_y} I_x C(\phi) - I_z S(\phi)$

$\xrightarrow{u_z} I_x C(\phi) + I_y S(\phi)$

$I_z \xrightarrow{u_x} I_z C(\phi) - I_y S(\phi)$

$\xrightarrow{u_y} I_z C(\phi) + I_y S(\phi)$

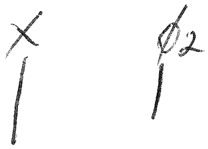
$\xrightarrow{u_z} I_z$

$I_y \xrightarrow{u_x} I_y C(\phi) + I_z S(\phi)$

$\xrightarrow{u_y} I_y$

$\xrightarrow{u_z} I_y C(\phi) - I_x S(\phi)$

VI-5



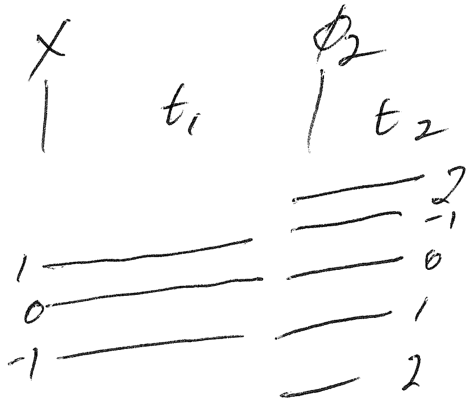
$\phi_{Rx} = -\Sigma \Delta p \Delta \phi_{Tx}$

3-coupled spins :. $M = 2N+1$ = # exp'ts needed

N = # spins

$M = 2(3)+1 = 7$ needed

:. use 8



selecting coh's @ end.

$p_f = -2, 0, 2$

$p_1 - 3, -1, 1, 3$

---

recall: $\overset{\Delta}{\pi} 2m$ $\quad \rho = I_0 C + I_+ S_5 + I_- S_5$ $\quad M=2$

0, π

$\rho(\pi) = I_0 + I_+ e^{-i\pi} + I_- e^{i\pi}$

$+ I_-$

$\rho(0) = I_0 + I_+$

$e^{i\pi} = e^{-i\pi} = -1$

$\phi_{Rx} = e^{-\pi}$

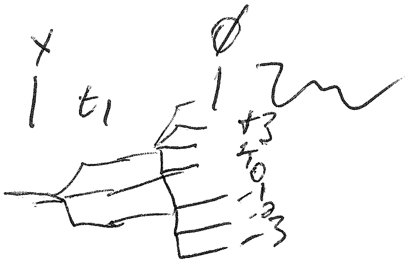
$\rho(\pi) = I_0 e^{-i\pi} + I_+ e^{-i\pi} e^{-i\pi} + I_-$

$\rho(0) = I_0 + I_+ + I_-$

(Quad Ghost Gets Thru

$0 + I_+ + I^-$

②



3 spin

Select for

$P_f = -3, -1, 1, 3$

$P_f = -2, 0, 2$

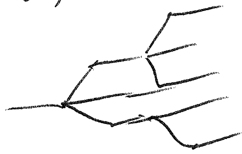
*much like for 2 spin 2 pulse
- even ODD effect.
- See Notes

Phase Circle

$$\Delta\phi_i^{\circ} = \frac{2\pi(k-1)}{M}$$

$P_i, P_i \pm k_i$

~~$P_0, P_0 \pm K_0, P_0 \pm 2K_0$~~



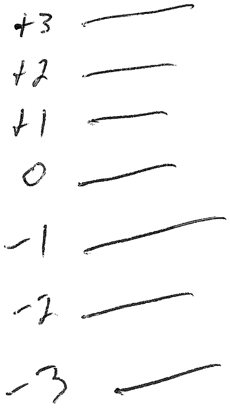
$M=2 \quad \Delta\phi_1 = 0$

$\Delta\phi_2 = \pi$

$\Delta\phi_1 \quad k=1 \quad i=1 \quad P_1 ; P_1 \pm 1, P_1 \pm 2$

$$P(0) = I_3 + I_2 + I_1 + I_0 + I_- + I_{2-} + I_{3-}$$

$$P(\pi) = I_3 e^{-3\pi} + I_2 e^{-2\pi} + I_1 e^{-\pi} + I_0 + I_- e^{+\pi} + I_{2-} e^{2\pi} + I_{3-} e^{3\pi}$$



$$\boxed{\begin{aligned}P(0) &= I_3 + I_2 + I_1 + I_0 + I_- + I_{2-} + I_{3-} \\ P(\pi) &= I_3 e^{-3\pi} + I_2 e^{-2\pi} + I_1 e^{-\pi} + I_0 + I_{-1} e^{+\pi} + I_{2-} e^{+2\pi} + I_{3-} e^{3\pi}\end{aligned}}$$

$e^{i\pi} = -1$

$e^{2\pi} = 1$

$e^{-2\pi} = +1$

Now $\phi_{Rx} = 0, \pi$

$\phi_{Rx} = 0 \Rightarrow P(\pi) = -I_3 + I_2 - I_1 + I_0 - I_{1-} + I_{2-} - I_{3-}$

$\phi_{Rx} = \pi \Rightarrow P(\pi) = I_3 e^{-2\pi} + e^{-\pi} I_2 + I_1 + I_0 e^{\pi} + I_- e^{2\pi} + I_{2-} e^{5\pi} + I_{3-} e^{4\pi}$

$= I_3 - I_2 + I_1 - I_0 + I_- - I_{2-} + I_3,$

[illegible] ③

i. $\rho(0) \qquad =$

$+ \rho_{Tx}(\pi)\, \rho_{kx}(0) = I_2 + I_0 + I_{2-}$

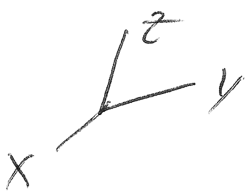
$\rho_{Tx}(0)\, \rho(0)\cdot e^{i\pi} + \rho(\pi)\, e^{i\pi} = I_3 + I_1 + I_{1-} + I_{3-}$

$P(b) \pm K\cdot M \; ; \; K = 0, 1, 2, \dots$

VI-6) $I_+ S_z \xrightarrow{(\pi/2)x}$

$I_+ = I_x + i I_y$

$S_z = S_6$



$$(I_x + i I_y) S_z = I_x S_z + i I_y S_z$$

$$\xrightarrow[(\pi/2)_x]{} -I_x S_y + - i I_z S_y$$

$$= -I_x S_y - i I_z S_y$$

$I_x = \frac{I_+ + I_-}{2}$ $I_z = I_0$

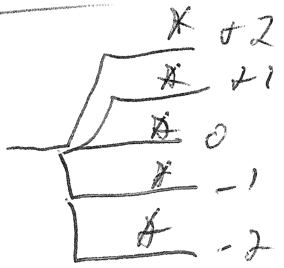
$S_y = \frac{i(I_- - I_+)}{2}$

$$= -\left(\frac{I_+ + I_-}{2}\right)\left(\frac{i(I_- - I_+)}{2}\right) - \frac{i I_0 (i(S_- - S_+))}{2}$$

$$= \frac{-i}{4}\left[I_+(I_- - I_+) + I_-(I_- - I_+)\right] - \frac{i^2}{2}(I_0 S_- - I_0 S_+)$$

$$= \frac{-i}{4}\left[\underset{ZQ}{I_+ I_-} - \underset{DQ}{I_+ I_+} + \underset{DQ}{I_- I_-} - \underset{ZQ}{I_- I_+}\right] + \frac{\underset{SQ}{I_0 S_-} - \underset{SQ}{I_0 S_+}}{2}$$

Summary $I_+ S_z \xrightarrow{\pi/2}$ 2 SQ
2 DQ
2 ZQ states!



$\cancel{A}$ = all created

VI-~~8~~) π-Pulses Don't create new cohs, just flip signs

$I_+ = I_x + I_y i$

IS $\quad I_+S_0 \xrightarrow[I \& S]{\pi_x}$

$(I_x + iI_y)S_z = I_xS_z + iI_yS_z$

$\xrightarrow[\pi_x]{} -I_xS_z - -I_yS_z i$

$= -I_xS_z + iI_yS_z$

$-I_xS_z + iI_yS_z$

$-\left(\frac{I_+ + I_-}{2}\right)(S_0) + i\left[\frac{i(I_- - I_+)}{2} S_0\right]$

$= \frac{-I_+S_0 - I_-S_0}{2} + i^2\left[\frac{(I_- - I_+)S_0}{2}\right]$

$= \frac{1}{2}S_0\left[-I_+ - I_- - I_- + I_+\right) = \frac{1}{2}S_0\left[-2I_-\right] = -I_-S_0$ ✓

$I_+S_0 \xrightarrow{\pi} -I_-S_0$

$I_xS_z \xrightarrow{\pi_x} -I_xS_z$

$+iI_yS_z \quad +i(+I_yS_z)$

$\boxed{I_+S_0 \xrightarrow{\pi_{x,I}} -I_+S_0}$

$I_xS_z \xrightarrow{\pi_I} -I_xS_z \quad = -\left(\frac{I_+ + I_-}{2}\right)S_0$

$-iI_yS_z \quad -i\left(i\left(\frac{I_- - I_+}{2}\right)S_0\right)$

$+iI_yS_z$

$= \frac{1}{2}S_0\left[-I_+ - I_- - i^2(I_- - I_+)\right]$

$= \frac{1}{2}S_0\left[-I_+ - I_- + I_- - I_+\right.$

$\frac{1}{2}S_0(-2I_+)$

$= \cancel{2} = -I_+S_0$

VI-8) $\overset{v}{|}$ $\overset{v+\phi}{|}$

Quadrature in v_1

$\phi = 0, \frac{2\pi}{3}, \frac{4\pi}{3}$ $s(t) = e^{i\omega t} e^{i\phi} s_0$

$$e^{i\phi} \cdot e^{i 2\pi/3} = (c+is)\left[c\left(\frac{2\pi}{3}\right) + is\left(\frac{2\pi}{3}\right)\right)$$

$$= (c+is)(-0.5 - 0.8i)$$

$$= c(-0.5-0.8i) + is(-0.5-0.8i)$$

$$= -0.5c - 0.8ic + -0.5is - 0.8i^2 s$$

$$= -0.5c - 0.8ic - 0.5is + 0.8s$$

$$= -0.5c$$

$$e^{i\phi}e^{i2\pi/3} = (-0.5c + 0.8s) + i(-0.8c \cancel{+0.8s} - 0.5s)$$

$$e^{i\phi}e^{4\pi/3} = (c+is)(-0.5+0.8i)$$

$$= c(-0.5+0.8i) + is(-0.5+0.8i)$$

$$= -0.5c + 0.8ic + -0.5is + 0.8i^2 s$$

$$= (-0.5c - 0.8s) + i(0.8c - 0.5s)$$

ϕ_2	ADC 1 $\mathbb{R}$	ADC 2 $\mathbb{I}$
0	c	s
$2\pi/3$	$-0.5c+0.8s$	$-0.8c-0.5s$
$4\pi/3$	$-0.5c-0.8s$	$0.8c-0.5s$

②

ϕ_2	ADC I	ADC II	B1	B2
0	C	S	A1	A2
$2\pi/3$	$-0.5C+0.8S$	$-0.8C-0.5S$	$-$ A1	$-$A2
$4\pi/3$	$-0.5C-0.8S$	$0.8C-0.5S$	$-$A1	$-$A2

2C 2S

S_x S_y

Quad det

i) $S_x + S_y i$

---

ii) $0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ case

$\phi = \phi_{Tx} - \phi_{Rx}$

$s(t) = S_0 e^{i\omega t} e^{i\phi}$

		$\mathbb{R}$	$\mathbb{I}$		
ϕ_2	$e^{i\phi}$	ADC1	ADC2	Buf1	Buf 2
0	$e^{i\phi}e^{0}$	C	iS	A1	A2
$\frac{\pi}{2}$	$e^{i\phi}e^{i\pi/2}$	$-S$	iC	A2	$-$A1
π	$e^{i\phi}e^{i\pi}$	$-C$	$-iS$	$-$A1	$-$A2
$\frac{3\pi}{3}$	$e^{i\phi}e^{3\pi/2 i}$	S	$-iC$	$-$A2	A1

$= 4C + 4S$

$$e^{i\phi}e^{i\pi/2} = C\left(\tfrac{\pi}{2}\right) + iS\left(\tfrac{\pi}{2}\right) = i\,(C + iS) = iC - S$$

$$e^{i\phi}e^{i\pi} = C(\pi) + iS(\pi) = -1\,(C + iS) = -C - iS$$

$$e^{i\phi}e^{\frac{3\pi}{2}i} = C\left(\tfrac{3\pi}{2}\right) + iS\left(\tfrac{3\pi}{2}\right) = -i\,(C + iS) = -iC + S$$

③ For echo

				$\phi_{rx} = 2\phi_2$
ϕ_2	0	$\frac{2\pi}{3}$	$\frac{4\pi}{3}$	
ϕ_{RX}	0	$\frac{4\pi}{3}$	$\frac{8\pi}{3}$	
Phase Fac	$e^{i\phi} e^{0}$	$e^{i\phi} e^{4\pi/3}$	$e^{i\phi} e^{8\pi/3}$	
R ADC1	C	$-0.5C - 0.8S$	$-0.5C + 0.8S$	
I ADC2	iS	$0.8C - 0.5S$	$-0.8C - 0.5S$	
Buff I	$A1$	$-A1 + A2$ ~~$-A1 - A2$~~	$-A2 - A1$	$3.6\ C$
Buff 2	$A2$	$-A1 - A2$	$A1 - A2$	$3.6\ S$

$c\left(\frac{\pi}{3}\right) = -0.5$

$s\left(\frac{\pi}{3}\right) = 0.8$

$c\left(\frac{8\pi}{3}\right) = -0.5$

$s\left(\frac{8\pi}{3}\right) = -0.8$

$$(C + iS)(-0.5 + 0.8i)$$
$$= C(-0.5 + 0.8i) + iS(-0.5 + 0.8i)$$
$$= -0.5C + 0.8iC - 0.5iS - 0.8S$$
$$= -0.5C - 0.8S + i(0.8C - 0.5S)$$

$(c+is)(-0.5+0.8i)$ $\underleftarrow{\phi_2 = 4\pi/3}$

$c(-0.5+0.8i)+is(-0.5+0.8i)$

$-0.5c+0.8ic-0.5is+0.8i^2s$

$-0.5c+0.8ic-0.5is-0.8s$

$=(-0.5c-0.8s)+i(0.8c-0.5s)$

$c(\frac{8\pi}{3})=-0.5$

$s(\frac{8\pi}{3})=-0.8$

$(c+is)(-0.5-0.8i)$

$=c(-0.5-0.8i)+is(-0.5-0.8i)$

$=-0.5c-0.8ic-0.5is-0.8i^2s$

$=-0.5c-0.8ic-0.5is+0.8s$

$=(-0.5c+0.8s)+i(-0.8c-0.5s)$

$$\begin{array}{r} 0.8c-0.5s \\ 0.5c+0.8s \\ \hline 1.3c+0.3 \end{array}$$

$$\begin{array}{r} 0.5c-0.8s \\ +0.8c+0.5s \\ \hline 1.3c-0.3s \end{array}$$

$$\begin{array}{r} 0.5c+0.8s \\ -0.8c+0.5s \\ \hline -0.3c+1.3s \end{array}$$

$$\begin{array}{r} -0.5c+0.8s \\ 0.8c+0.5s \\ \hline 0.3c+1.3s \end{array}$$

$s(t) = S_0 e^{i\omega t} e^{i\phi}$ $\phi = \phi_{Tx} - \phi_{rx}$

ϕ_2	ϕ_{Rx}	$e^{i\phi}$
0	0	e^{0}
$\frac{\pi}{2}$	$\pi/2$	$e^{i\phi} e^{i\pi/2}$
π	π	$e^{i\phi} e^{i\pi}$
$\frac{3\pi}{2}$	$3\pi/2$	$e^{i0} e^{i3\pi/2}$

$\phi_{rx} = -\Delta P \phi_2$

$\phi = \phi_{Tx} - \phi_{rx}$

$\phi_2 =$	0	$\pi/2$	π	$\frac{3\pi}{2}$
Phase Factor	$e^{i\phi} e^{0}$	$e^{i\phi} e^{i\pi/2}$	$e^{i\phi} e^{i\pi}$	$e^{i\phi} e^{i3\pi/2}$
$PF =$	$e^{i\phi}$	$i e^{i\phi}$	$-e^{i\phi}$	$-i e^{i\phi}$
$\mathbb{R}$	C	$-S$	$-C$	S
$\mathbb{I}$	S	C	$-S$	$-C$
ϕ_{rx}	0	$\pi/2$	π	$3\pi/2$
ϕ_{rx}	0	π	0	π

P_{Ax} $\phi_{rx} = -\Delta P \phi_2$

$P_e \Rightarrow \phi_r = 2\phi_2$

For echo,

$\phi_2 =$	0	$\frac{\pi}{2}$	π	$\frac{3\pi}{2}$
Phase Fac =	$e^{i\phi} \cdot e^{i\phi_{Rx}}$ $e^{i\phi}e^{i0}$	$e^{i\phi}e^{i\pi}$	$e^{i\phi}e^{i0}$	$e^{i\phi}e^{i\pi}$
$\phi_{Rx} = -\Delta P\phi_2$ $= 2\phi_2$	0	π	0	π
PF	$e^{i\phi}e^{0}$	$-e^{i\phi}$	$e^{i\phi}$	$-e^{i\phi}$
ADC1, R	C	−C	C	−C
ADC, I	S	−S	S	−S
B1	A1	−A1	A1	−A1
B2	A2	−A2	A2	−A2
sum	4C + 4S			

* Now Detect

$$S_-(t) = S_0\left[\underset{S_x}{c(\Delta\omega t)} - i\,\underset{S_y}{s(\Delta\omega t)}\right] = S_0 e^{-i\Delta\omega t}$$

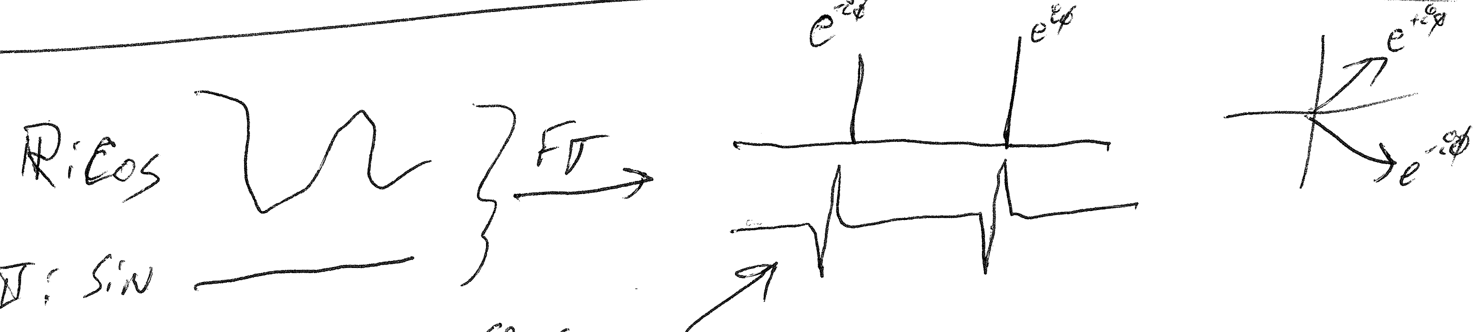
Ideally want: $s(t) = S_{Re}(t)c(\phi) - S_{Im}(t)s(\phi)$
$+ i\{ S_{Im}\, c(\phi) + S_{Re}(t)\, s(\phi)$

$$S(t) = S_0 e^{i\Delta\omega t} = S_0\left[\underset{A}{c(\Delta\omega t)} \underset{+}{+} \underset{i}{i}\, \underset{D}{s(\Delta\omega t)}\right]$$

$e^{i\phi} = c(\phi) + i s(\phi)$ $\quad\therefore\quad$ $c(\phi) = \dfrac{e^{i\phi} + e^{-i\phi}}{2}$

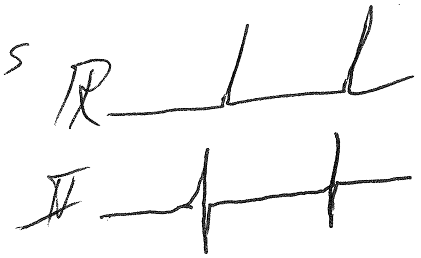
$e^{-i\phi} = c(\phi) - i s(\phi)$ $\quad\quad$ $s(\phi) = \dfrac{(-i)(e^{i\phi} - e^{-i\phi})}{2}$

Now



comes from quad shift π/2 in S_y channel

$$I_x = \frac{e^{i\phi} + e^{-i\phi}}{2} = c + is + c - is = \frac{2c}{2} = c$$



~~actual~~

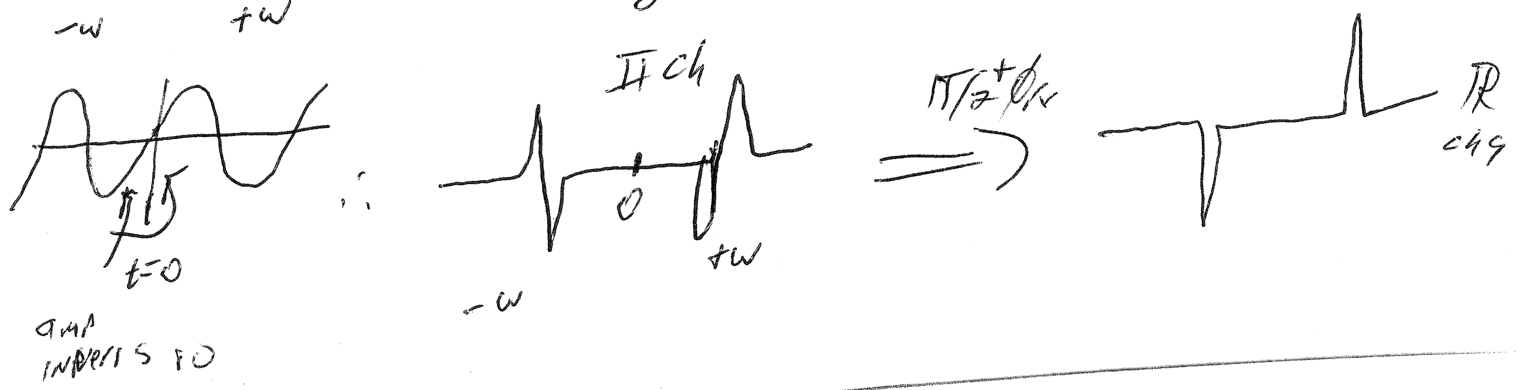
π/2 shift in othe channel

$$S(\phi) = \frac{i(e^{-i\phi} - e^{i\phi})}{2} = i\left[c - is - (c + is)\right] \qquad \phi = \phi_{tx} - \phi_{rx} + \Delta w t$$

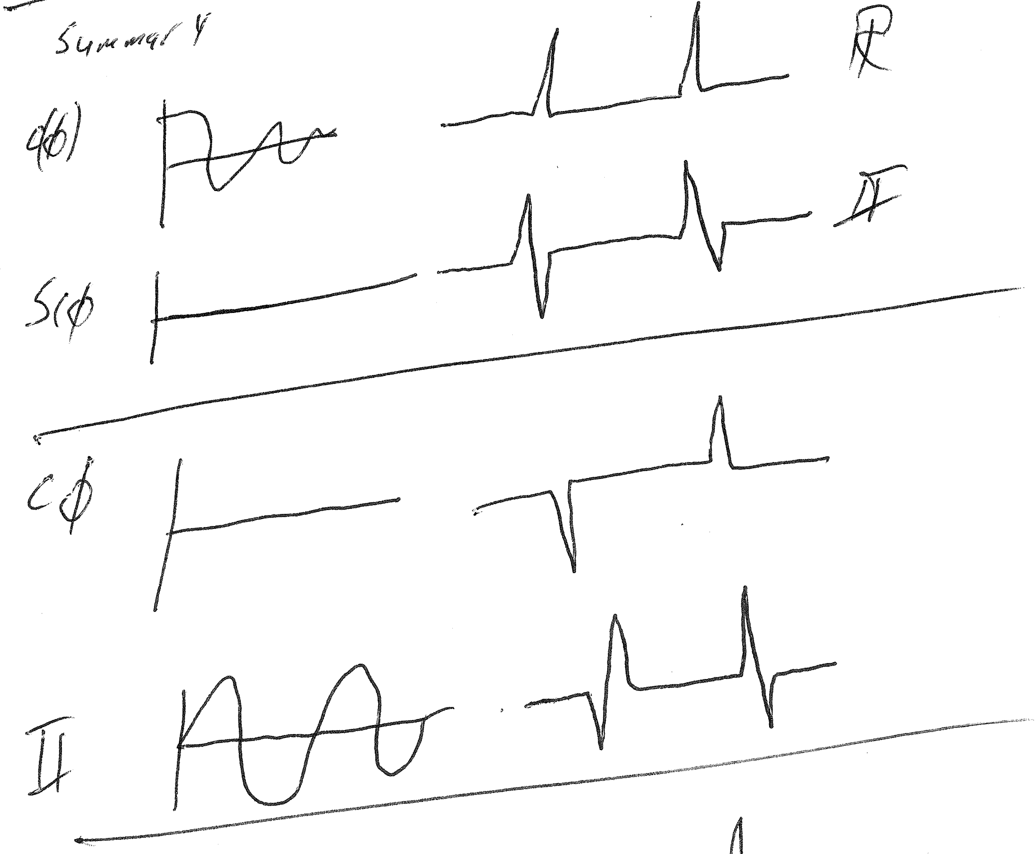
$$\Delta w = w - w_0$$

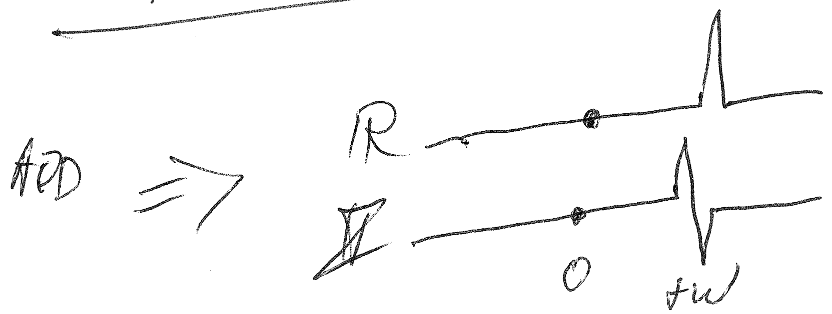
$$= i\left[c - is - c - is\right.$$

$$= \frac{i(-2is)}{2} = S(\phi)$$



Summary





$S(t) = S_0 e^{i\omega t} e^{i\phi}$ $\phi = \phi_{Tx} - \phi_{Rx}$

Keep

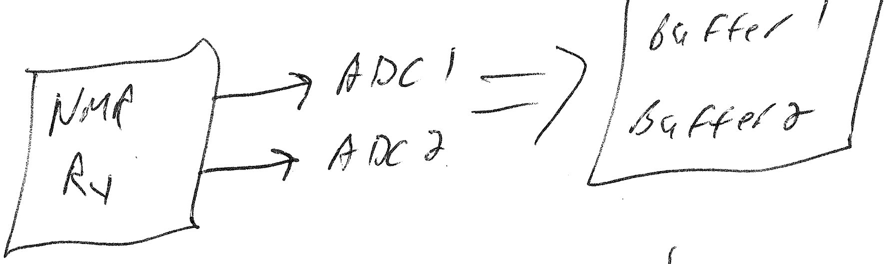
ϕ_{Tx}	$e^{i\phi}$	$\phi = \phi + \text{shift}$	Phase Factor Newe	ADC1 $\mathbb{R}$	ADC2 $\mathbb{I}$
0	$e^{i\phi} e^{i0}$	$\phi + 0$	$e^{i\phi}$	C	iS
$\pi/2$	$e^{i\phi} e^{i\pi/2}$	$\phi + \pi/2$	$ie^{i\phi}$	$-S$	iC
π	$e^{i\phi} e^{i\pi}$	$\phi + \pi$	$-e^{i\phi}$	$-C$	$-iS$
$3\pi/2$	$e^{i\phi} e^{i3\pi/2}$	$\phi + 3\pi/2$	$-ie^{i\phi}$	S	$-iC$

$c(\frac{\pi}{2}) + i s(\frac{\pi}{2}) = i$

$c\pi + i s\pi = -1$

$c(\frac{3\pi}{2}) + i s \frac{3\pi}{2} = -i$

Phase shifting ϕ_{Tx} thru software & not ϕ_{Rx}. ie ϕ_{Rx} = const in hardware.



(A1) ADC 1	(A2) ADC 2	Buffer 1	Buffer 2
C	iS	$A1$	$A2$
$-S$	iC	$A2$	$-A1$
$-C$	$-iS$	$-A1$	$-A2$
S	$-iC$	$-A2$	$+A1$
		$4C(\omega t + \phi)$	$4S(\omega t + \phi)$

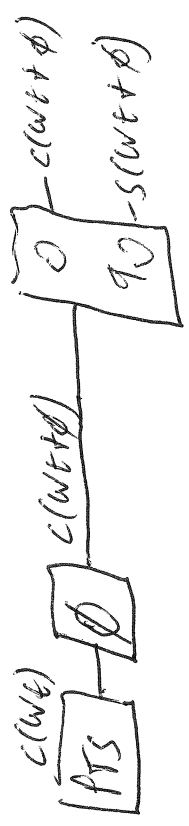
---

*Note, things are sampled w/ Dig sig Proc now (100's of MHz) -oversampled. removes Quad Ghosts & ~~[illegible]~~ shift offsets

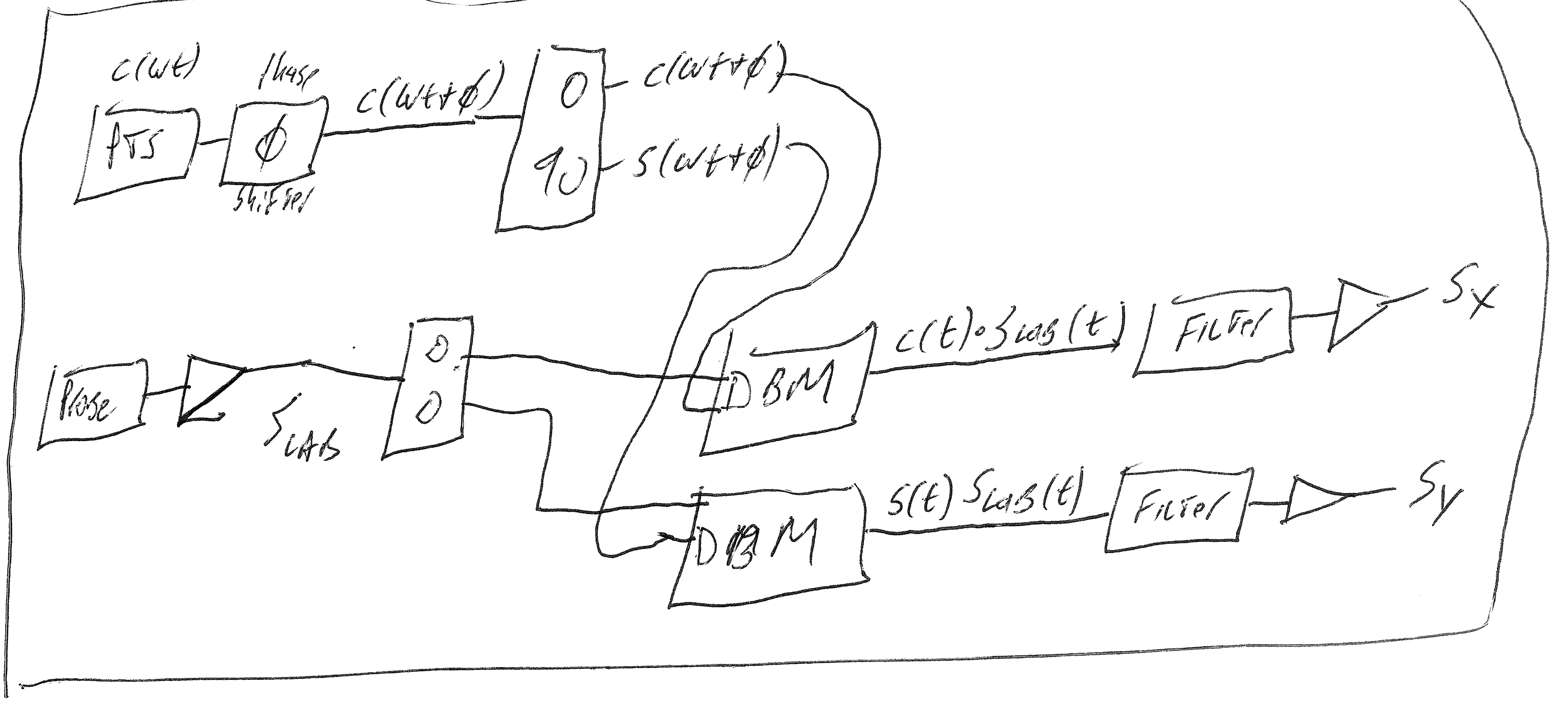
Keep

Quad det w/only one coil: ie observe S_x & S_y

* use DBM's



LF Desc



DBM - multiplies signals

$O(t) = S_1(t)\cdot S_2(t)$

DBM

S_1 = From Probe

S_2 = demodulating Sig From PTS

S_x: $c(\omega t+\phi_R)\,c(\omega_0 t+\phi_{Tx}) = c[(\omega-\omega_0)t+(\phi_R-\phi_{Tx})]$ + Fast ωs

S_y: $s(\omega t+\phi_r)\,c(\omega_0 t+\phi_{Tx}) = s[(\omega_0-\omega_0)+\phi_r-\phi_{Tx}]$ + Fast Terms

↑ Audio Filter Removes

Filter →

S_x: $c(\Delta\omega t+\phi)$

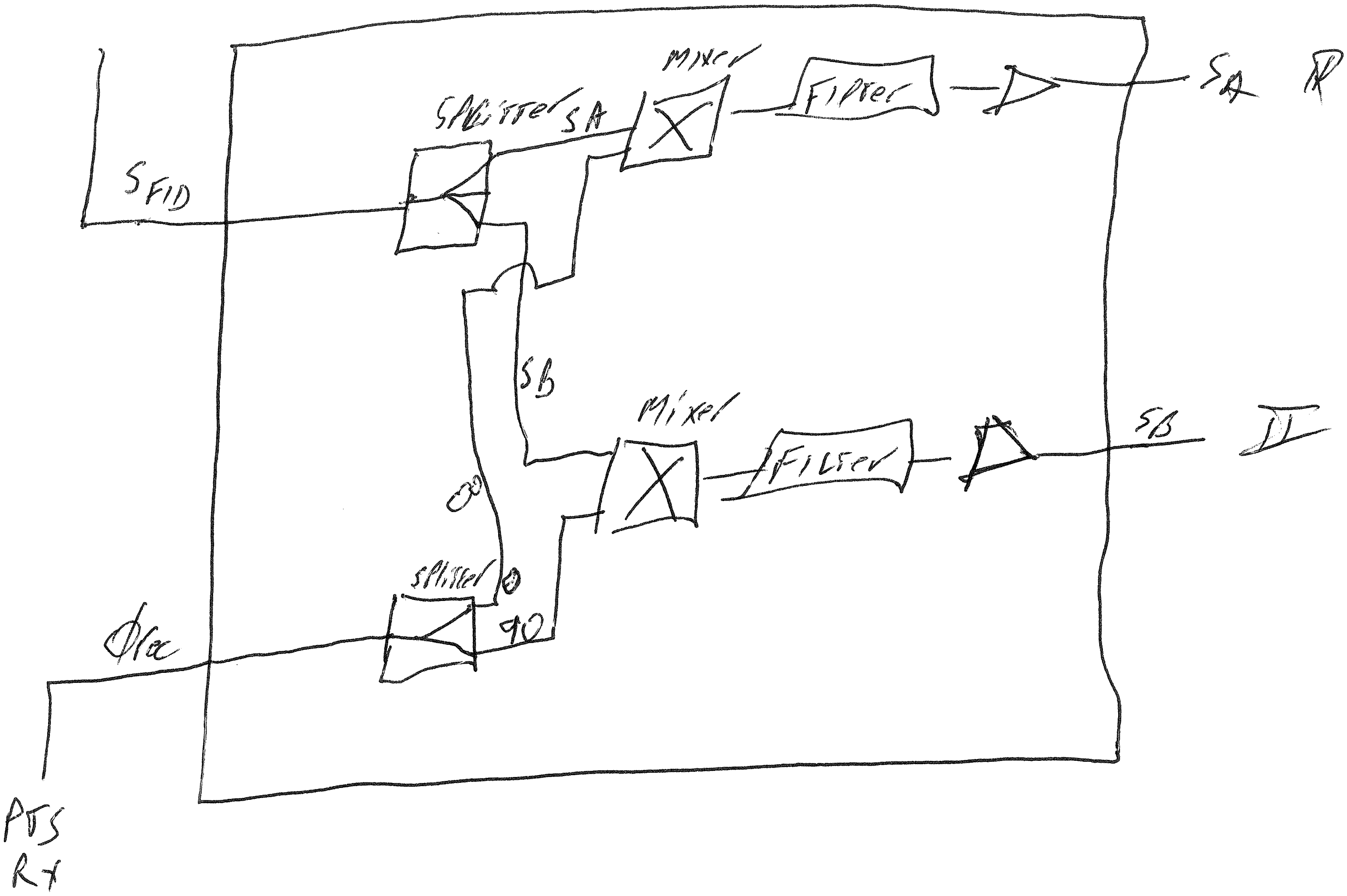
S_y: $s(\Delta\omega t+\phi)$

$\phi = \phi_{Rx}-\phi_{Tx}$

$\Delta\omega$ = rot Frame offse

Levitts Desc

Quadrature Rx



$$s(t) = S_A + i S_B$$

$$S_A(t) = \frac{i}{2} \rho_{\boxed{-}} e^{-i(\phi_{Rx} - \phi_{ref})} + \frac{i}{2} \rho_{\boxed{+}}(t) e^{i(\phi_{Rx} - \phi_{ref})}$$

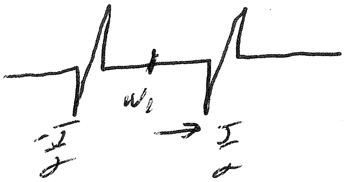
$$S_B(t) = \frac{i}{2} \rho_{\boxed{-}} e^{-i(\phi_{Rx} - \phi_{ref})} + \frac{i}{2} \rho_{\boxed{+}} e^{i(\phi_{rx} - \phi_{ref})}$$

$$s(t) = 2i \rho_{\boxed{-}} e^{-i(\phi_{rx} + \phi_{dig})}$$

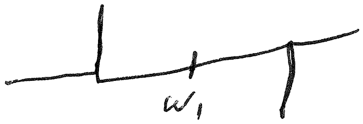
VI-9)

2D-H,H COSY before:

Diag: $s(\omega_1, t_1) c(\frac{Jt_1}{2}) = \frac{1}{2}\left[s((\omega_1 + \frac{J}{2})t) + s((\omega_1 - \frac{J}{2})t_1)\right]$

$\Rightarrow$ 

XPK: $s(\omega_1 t_1) s(\frac{Jt_1}{2}) = \frac{1}{2}\left[c((\omega_1 - \frac{J}{2})t_1) - c((\omega_1 + \frac{J}{2})t_1)\right]$

$\Rightarrow$ 

Axial PK: $c_J^1 s_{\omega_1}^1 (I_{1y} c_{\omega_1}^2 - I_{1x} s_{\omega_1}^2)$ $\quad$ I_{1y}: $+c_J^1 s_{\omega_1}^1 c_{\omega_1}^2$

$= c_J^1 s_{\omega_1}^1 c_{\omega_1}^2 I_{1y} - c_J^1 s_{\omega_1}^1 s_{\omega_1}^2 I_{1x}$ $\quad$ I_x: $-c_J^1 s_{\omega_1}^1 s_{\omega_1}^2$

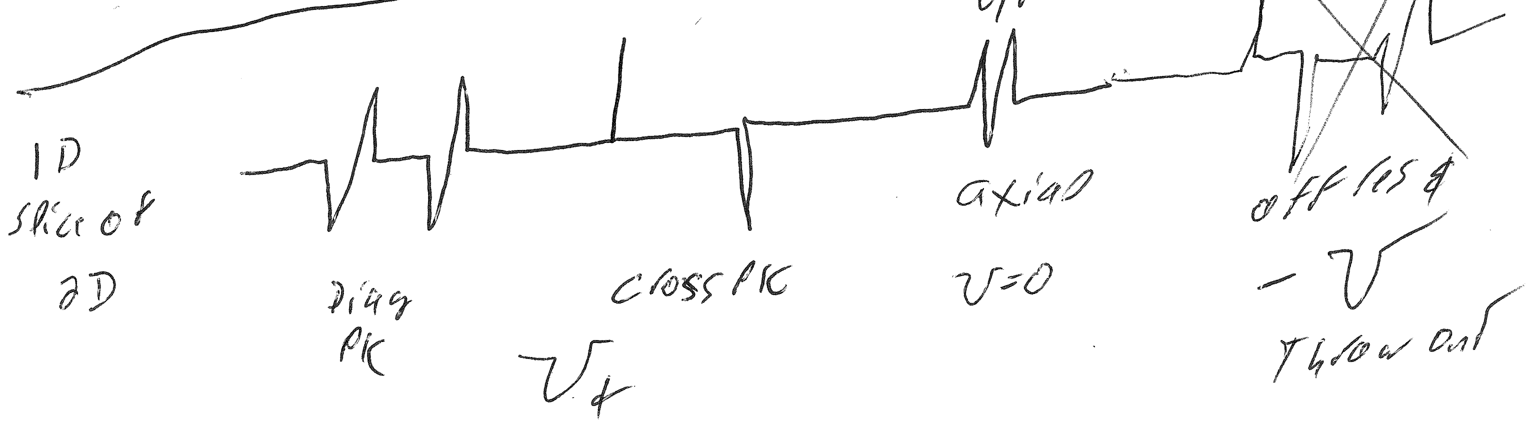
$c_J^1 [s_{\omega_1}^1 c_{\omega_1}^2 - s_{\omega_1}^1 s_{\omega_1}^2]$

$= c_J^1 [s(\omega_1 + \omega_1)t + s(\omega_1 - \omega_1)t]$

$- c_J^1 [c(\omega_1 - \omega_1)t - c(\omega_1 + \omega_1)t$

$= c_J^1 [s(2\omega_1)t + c(2\omega_1 t) + s(0) - c(0)$

$= c_J^1 [c(2\omega_1 t) + s(2\omega_1 t) - 1]$



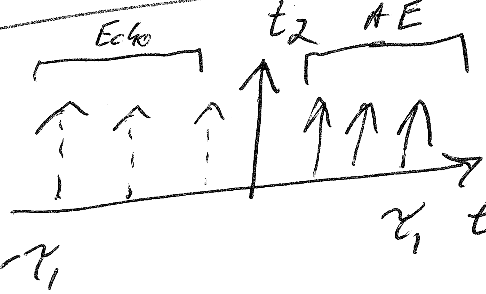
② $S(\omega_1 t_1) e^{i\omega_2 t_2}$ = Sin modulation / Amplitude modulation in non-Quad det.

$e^{i\omega_1 t_1} e^{i\omega_2 t_2}$ = Phase Modulation, Quad. detection

---

In Phase-mod spec need to take magnitude or acquire 2nd 2D data set

+aca e & ae & combine



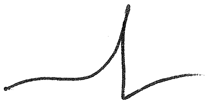
$$S(W_1, W_2) = S_0 A(W_1) e^{-i\omega_1 \tau_1} \cdot e^{i\omega_2 t_2}$$

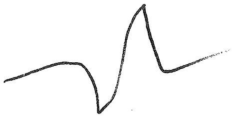
$$= S_0 A(W_1) e^{-i\omega_1 \tau_1} [A(\omega_2) + i D(\omega_2)]$$

$$S(t_1, t_2) = \iint I(\omega_1, \omega_2) e^{i\omega_1 t_1} e^{i\omega_2 t_2} dt_1 dt_2$$

$$\xrightarrow{FT} I(\omega_1, \omega_2) = S_0 [A(\omega_1) + i D(\omega_1)] \cdot [A(\omega_2) + i D(\omega_2)]$$

$$A = \frac{T_2}{1 + (\omega - \omega_i)^2 T_2^2} \qquad D = \frac{T_2^2 (W - W_i)}{1 + (W - W_i)^2 T_2^2}$$





③

$$I(w_1,w_2) = S_0\left[A(w_1)+iD(w_1)\right]\left[A(w_2)+iD(w_2)\right]$$

$$= S_0 A(w_1)\left[A(w_2)+iD(w_2)\right] + S_0 iD(w_1)\left[A(w_2)+iD(w_2)\right]$$

$$= S_0\left[A(w_1)A(w_2)+iA(w_1)D(w_2)\right] + S_0\left[iD(w_1)A(w_2) + i^2 D(w_1)D(w_2)\right]$$

$$- D(w_1)D(w_2)$$

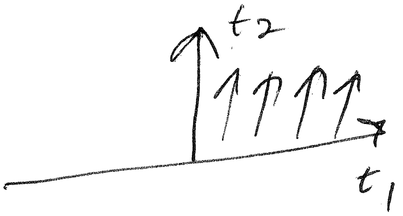
$$= S_0\left[A(w_1)A(w_2) + i\left[A(w_1)D(w_2)+D(w_1)A(w_2)\right]\right]$$

$$\boxed{= S_0\left[\underbrace{A(w_1)A(w_2)}_{\text{Pure Absorp}} - \underbrace{D(w_1)D(w_2)}_{\text{Pure Disp}} + i\left[\underbrace{(A(w_1)D(w_2)+D(w_1)A(w_2))}_{\text{Mixed}}\right]\right]}$$

To get purely absorptive pks need $D(w_1)$ or $D(w_2) = 0$

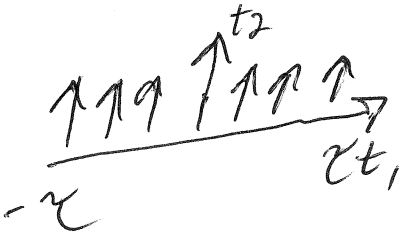
need $\int_{-t}^{t} s(w_i t_1) = 0$

& since a sine func,



conventional

$D(w_2), D(w_1) \neq 0$



$D(w_2) \neq 0$

$D(w_1) = 0$

$$I(w_1,w_2) = S_0\left[A_1A_2 - 0\right) + i\left[A_1D_2 + 0\right)$$

$$= S_0\left[A_1A_2 + i\left[A_1D_2\right)\right.$$

㉑ acquiring sigs w/ ±t

t ~~echo~~ echo's in t_2 not so great, waste sharp lines

2-independent expts

Phase-modulated

$$S_{echo} = \iint I(\omega_1,\omega_2)\, e^{-i\omega_1 t}\, e^{i\omega_2 t_2}\, d\omega_1 d\omega_2$$

$$S_{ae} = \iint I(\omega_1,\omega_2)\, e^{i\omega_1 t}\, e^{i\omega_2 t_2}\, d\omega_1 d\omega_2$$

Amp-modulations

$$S_{c(t_1,t_2)} = \iint I(\omega_1,\omega_2)\, c(\omega_1 t_1)\, e^{i\omega_2 t_2}\, d\omega_1 d\omega_2$$

$$S_{s(t_1,t_2)} = \iint I(\omega_1\omega_2)\, s(\omega_1 t_1)\, e^{i\omega_2 t_2}\, d\omega_1 d\omega_2$$

Phase-modulation e/ae & FT along υ_2

E

$$e^{-i\omega_1 t_1} e^{i\omega_2 t_2} \Big\downarrow \text{FT}$$

$$e^{-i\omega_1 t}[A(\omega_2)+iD(\omega_2))$$

ae

$$e^{i\omega_1 t_1} e^{i\omega_2 t_2} \Big\downarrow \text{FT}$$

$$e^{i\omega_1 t}[A(\omega_2)+iD(\omega_2)]$$

See over

① $c(\phi) = e^{i\phi} + e^{-i\phi}$

$\boxed{\text{E/AE ADDITION}}$

VI-9)

$\underline{E}$

$e^{-iv_1 t_1} e^{iv_2 t_2}$

$\downarrow FT(2)$

$e^{-iv_1 t_1}[A_2 + iD_2]$

$= [C_1' ~~+~~ -iS_1'][A_2 + iD_2] = X$

$\underline{AE}$

$e^{iv_1 t_1} e^{iv_2 t_2}$

$\downarrow FT(2)$

$e^{iv_1 t_1}[A_2 + iD_2]$

$Y = [C_1' + iS_1'][A_2 + iD_2]$

$X + Y = [C_1' - iS_1'][A_2 + iD_2)$

$+ [C_1' + iS_1')(A_2 + iD_2)$

$= 2C_1'[A_2 + iD_2)$

$-X + Y = [C_1' + iS_1'][A_2 + iD_2]$

$- (C_1' - iS_1')[A_2 + iD_2]$

$= 2iS_1'[A_2 + iD_2]$

$2C_1'(A_2 + iD_2) + 2iS_1'(A_2 + iD_2)$

$= 2[C_1' + iS_1'][A_2 + iD_2) = 2e^{iv_1 t_1}(A_2 + iD_2]$

$\downarrow FT_1$

$2[A_1' + iD_1][A_2 + iD_2)$

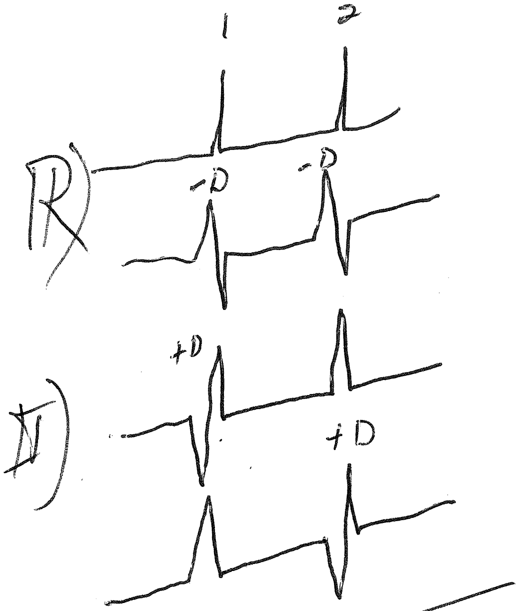
$= 2[A_1[A_2 + iD_2] + iD_1(A_2 + iD_2]]$

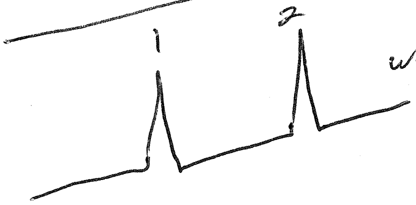
$= 2[\underline{A_1 A_2} + iA_1 D_2 + \underline{iD_1 A_2} - D_1 D_2)$

$= A_1 A_2 + iD_1 A_2 + [iA_1 D_2] - D_1 D_2$

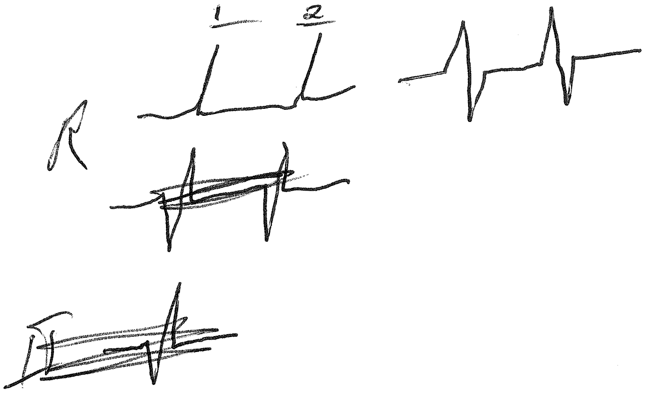
②

$2 e^{i v_1 t_1} [A_+ + i D_+]$





works!

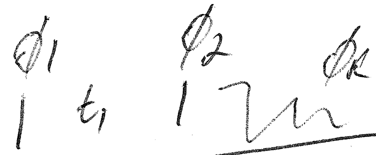


VI-10)

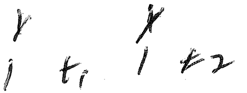
1) Need Quad in T1

2) Phase-Sens

Keep



Recall



$P_0 = I_{1z} + I_{2z}$

I_{1z} terms $\qquad$ I_{2z}

$I_{x1} : S_1^1 C_J^1 C_J^2 S_1^2 \leftarrow \text{Diag} \rightarrow I_{x2} : S_2^1 C_J^1 C_J^2 S_2^2$

$I_{y2} : S_2^1 C_J^1 C_J^2 C_2^2$

$I_{y1} : S_1^1 C_J^1 C_J^2 C_1^2$

$I_{x2} : S_1^1 S_J^1 S_J^2 S_2^2 \leftarrow \text{X Pks} \rightarrow I_{x1} : S_2^2 S_J^1 S_J^2 S_1^2$

$I_{y2} : S_1^1 S_J^1 S_J^2 C_2^2$ ✓ $\qquad I_{y1} : S_2^1 S_J^1 C_J^2 C_1^2$

$CS = \frac{S(\alpha+\beta) + S(\alpha-\beta)}{2}$ = odd $\qquad$ ~~SS = C(α+β) +~~ $SS = \frac{C(\alpha-\beta) - C(\alpha+\beta)}{2}$ = even

---

S & C modulation, ∴ Non-Quad!

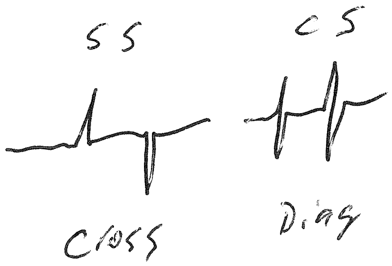
1) Note t1 is terms of

Throw out 1/2 sig

& could work off pks &

S·S modulated, ∴ See ~~A~~ B

2) Note cross pks are Absorptive ~~Pea~~ pks. However, Diag is S·C

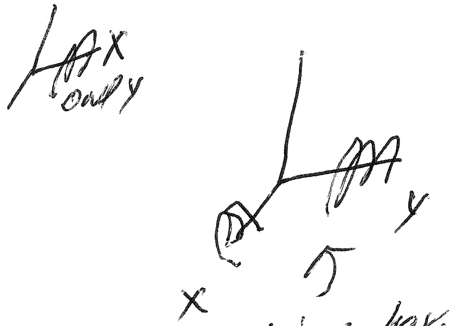


∴ can't record fully absorptive for both cr & Diag

②

Amplitude Modul: NON-Quad. : $S(\omega_1 t_1)\, e^{i\omega_2 t_2}$

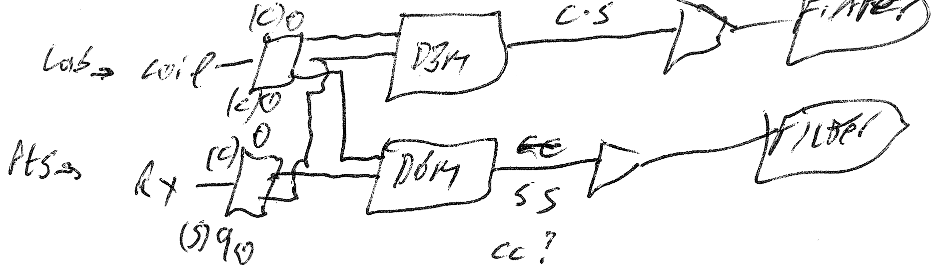
: $c(\omega_1 t_1)\, e^{i\omega_2 t_2}$

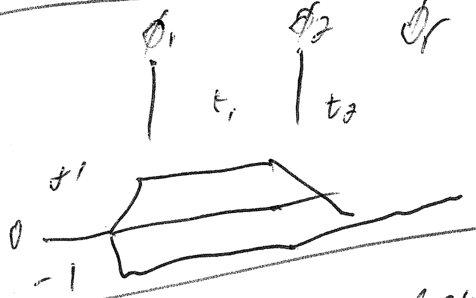


Phase modulated : Quad Det'n : $e^{i\omega_1 t_1}\, e^{i\omega_2 t_2}$

like having 2-coil detect'n, IN Quad: ie see x & Y

Quad requires DBM's & phase split by $\frac{\pi}{2}$





Quad 2N+1 To select cohs

4 steps, N = spin pairs = 1 [illegible]

* Need to select partic coh for quad

* Need to select e & Ae sel for Abs in 2D

Need

exps 2

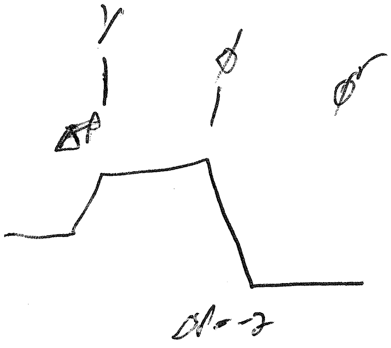
exp 1

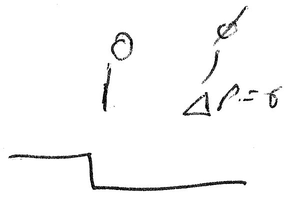
B) $Q_{rx} = -\Sigma \Delta P_x \phi_x$

+1 $\underline{P_P}$ $P_A = P_P e^{-i\phi_2}$

0 $\underline{P_{AX}}$ P_{AX}

-1 $\underline{P_N}$ $P_N = P_N e^{-i\phi_2}$





$\phi_r = 0$

$\phi_r = -(-2)\phi_2$

$= 2\phi_2$

ϕ_2	ϕ_{rx}
0	0
1	2
2	0
3	2

⇒ e

& Quad int.

ϕ_2	ϕ_r
0	0
1	0
2	0
3	0

Just Need 4 scans for E & AE each

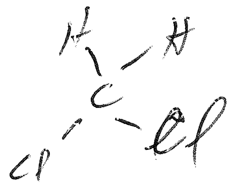
* Sometimes better to

ϕ_1	ϕ_2	ϕ_r
0	0	0
0	1	2
0	2	0
0	3	2
π	0	2
π	1	0
π	2	2
π	3	6

to remove pulse imperfection in ϕ_1

VI-11) $CHCl_3$ CH_2Cl_2 COSY pks

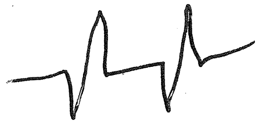
↗ No pks



$\leftarrow {}^2J = 0?$

but nothing btw $CHCl_3$ & CH_2Cl_2

VI-12) DQF-COSY

recall cosy Diag:  is Dispersive

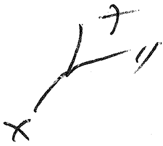
(S_1^1, S_1^2) $S(\omega_1, \omega_1)$

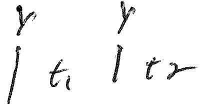
$I_{x1}: S_1^1 C_j^1 C_j^2 S_1^2$ (S_1^1, C_1^2) $S(\omega, t_1) C(\omega, t_0)$

$I_x^2 = S_1^1 C_j^1 C_j^2 C_1^2$

∴ but SC modulated pk $\Rightarrow S(\;)$ 

* Diag sigs cancel out
Due to Disp char & sign change
* lots of overlap esp w/weak sig



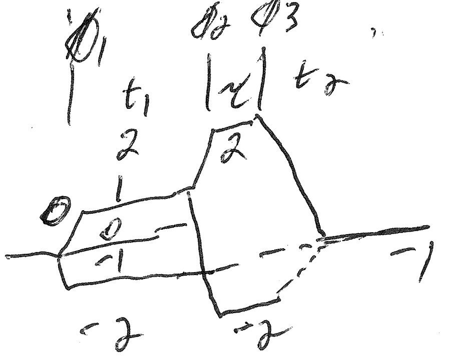


$I_{z1} \xrightarrow{\overset{y}{|}} I_{x1} \xrightarrow{t_1} I_{y1} \xrightarrow{\overset{y}{|}} I_{y1} \xrightarrow{t_2}$ diag

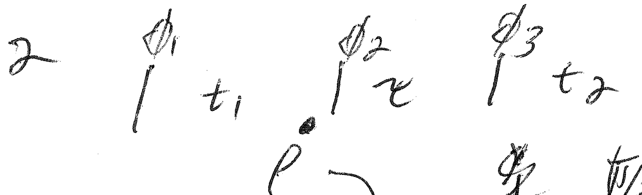
$\xrightarrow{t_2}$ cross peak

$I_{z1} \xrightarrow{\overset{y}{|}} I_{x1} \xrightarrow{t_1} 2I_{x1}I_{z2} \xrightarrow{\overset{y}{|}} -2I_{z1}I_{y1}$

* Trick is to filter out SQ IP which just gen Diag anyway



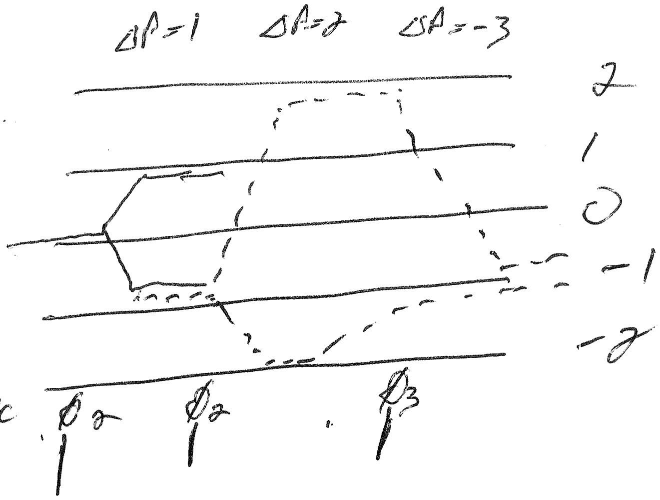
τ is short, just enough for φ3 phase shift ~~off~~



~~φ~~ $(\pi/2)_y$

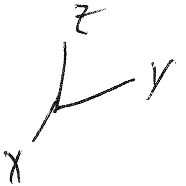
Note at ρ:

I_{1x}	I_{z1}
I_{1y}	I_y
$2I_{1y}I_{2z}$	$I_{1y}I_{2x}$ mqc
$2I_{1x}\,2I_z$	$-2I_{1z}I_{2x}$



echo: Δp=1 Δp=1 Δp=-3
φ1 φ2 φ3

Ae: Δp=-1 Δp=-1 Δp=+1
φ1 φ2 φ3



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again H,H-COSY $I_{z1} \xrightarrow{t_1} I_{y1} \xrightarrow{(\frac{\pi}{2})_y} I_{y1} \longrightarrow$ diag

$+2_{x1}I_{z2} \longrightarrow -2I_{z1}I_{x2} \longrightarrow$ cross

---

MQC-COSY

retain MQ tel $I_{z1} \xrightarrow[(\pi/2)_y]{\phi_1} I_{x1} \xrightarrow{t_1} 2I_{y1}I_{z2} \xrightarrow{(\frac{\pi}{2})_y} \boxed{2I_{y1}I_{x1}}$

$2I_{1y}I_{2x} \Rightarrow \quad I_+ = I_x + iI_y \quad \therefore \quad I_x = \frac{I_+ + I_-}{2} \quad I_y = \frac{(I_- - I_+)i}{2}$

$I_- = I_x - iI_y$

$$\therefore 2I_{1y}I_{2x} = 2i\left[\frac{(I_{1-} - I_{1+})}{2} \cdot \frac{I_{2+} + I_{2-}}{2}\right] = \frac{i}{2}\left[I_{1-}(I_{2+} + I_{2-}) - I_{1+}(I_{2+} + I_{2-})\right]$$

③ $2I_{1y}I_{2x} = \frac{i}{2}\left[I_{1-}I_{2+} + I_{1-}I_{2-} - I_{1+}I_{2+} - I_{1+}I_{2-}\right.$ keep

$$= \frac{i}{2}\left[\underset{ZQC\ (\emptyset\ \text{out})}{(I_{1-}I_{2+} - I_{1+}I_{2-})} + \underset{DQC\ (\text{keep})}{\underbrace{(I_{1-}I_{2-} - I_{1+}I_{2+}}}\right)$$

$$\frac{i}{2}\left(I_{1-}I_{2-} - I_{1+}I_{2+} = \right)$$

$$= (I_{a1} - iI_{B1})(I_{a2} - iI_{B2}) - (I_{a1} + iI_{B1})(I_{a2} + iI_{B2})$$

$$= I_{a1}(I_{a2} - iI_{B2}) = \cancel{I_{a1}I_{a2}} - \underline{I_{a1}I_{B2}\,i}$$

$$-iI_{B1}(I_{a2} - iI_{B2}) = \underline{-iI_{B1}I_{a2}} + \cancel{i^2 I_{B1}I_{B2}}$$

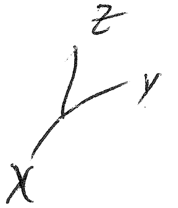
$$-I_{a1}(I_{a2} + iI_{B2}) = \cancel{-I_{a1}I_{a2}} - \underline{iI_{a1}I_{B2}}$$

$$-iI_{B1}(I_{a2} + iI_{B2}) = \cancel{-I_{a2}I_{B1}\,i} - \cancel{i^2 I_{B1}I_{B2}}$$

$$\underline{-I_{B1}I_{a2}\,i}$$

$\Big\} \times \frac{i}{2}$

$$\left(-2I_{a1}B_2\,i - 2iI_{B1}I_{a2}\right)\frac{i}{2}$$



$$I_{x1}I_{y2} + I_{y1}I_{x2}$$

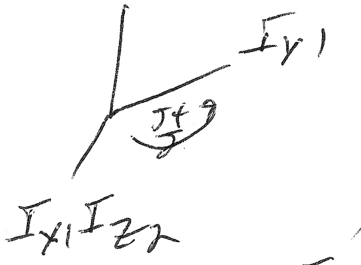
$$\Big\downarrow (\pi/2)_x$$

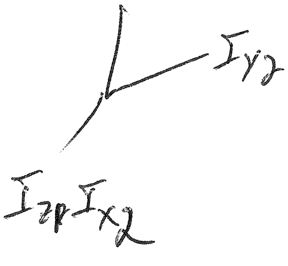
$$+ I_{x1}I_{z2} + I_{z1}I_{x2}$$

$$s\left(\tfrac{Jt}{2}\right) I_{y1} \Big\downarrow J \quad I_{y2}\, s\left(\tfrac{Jt}{2}\right)$$

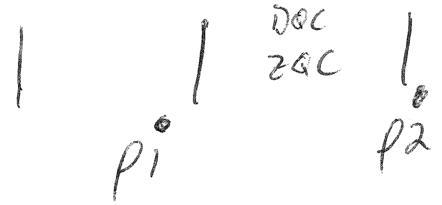
$$c(\cancel{I_{x1}I_{z2}}) \qquad c(\cancel{I_{z1}I_{x2}})$$

$$+ s(\cancel{I_{y1}}) \qquad + s(\cancel{I_{y2}})$$





④



$\rho 1: -C_J' C_1' I_{1x} \qquad \xrightarrow{(\pi/2)y} \qquad -A\, I_{1z}$ — (Pop Drop)

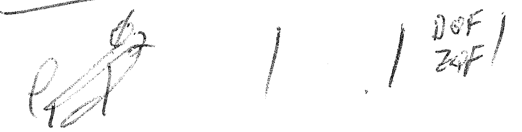
$C_J' S_1' I_{1y} \qquad\qquad B\, I_{1y}$ — (evolves as $\omega_1 \rightarrow$ Diag)

$S_J' C_1' 2 I_{1y} I_{2z} \qquad\qquad C\, 2I_{1y}I_{2x}$ ~~DO~~ (DQC - Drop)

$-S_J' S_1' 2 I_{1x} I_{2z} \qquad\qquad -D\, 2I_{1z}I_{2x}$ (evolves as $\omega_2 \rightarrow$ X-Pk)

Now w/2nd Pulse above b/w DQC & ZQC, I_{1y} Not coupled is Filtered out

---

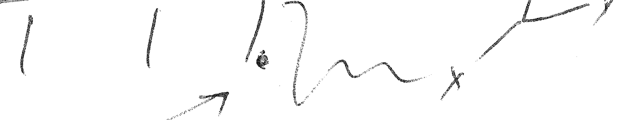


$-D2I_{1z}I_{2x} \xrightarrow{(\pi/2)x} -D2I_{1y}I_{2x}$

$\boxed{\text{See Pg 3}}$

$$-D I_{1y} I_{2x} = -D2\left[\frac{i}{2}\left[\underbrace{I_{1-}I_{2+} - I_{1+}I_{2-}}_{\text{ZQC - 0 - OUT}}\right) + \left(\underbrace{I_{1-}I_{2-} - I_{1+}I_{2+}}_{\text{DQC (Kept)}}\right)\right]$$

$$= \frac{-D}{2}\left[2I_{x1}I_{y2} + 2I_{y1}I_{x2}\right]$$



$-\frac{D}{2}2I_{x1}I_{y2} \xrightarrow{(\pi/2)x} -D2I_{x1}I_{z2}$

$+$

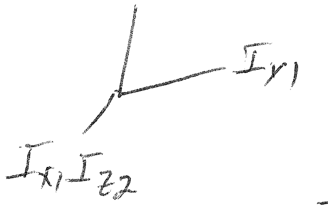
$-\frac{D}{2}2I_{y1}I_{x2} \qquad -\frac{D}{2}2I_{z1}I_{x2}$

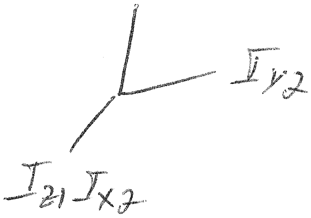
These Terms exactly like

$-\frac{D}{2}2I_{1z}I_{2x}$ From Prob VI-6

⑤

$\xrightarrow[t_2]{H_{CS}} \xrightarrow[t_2]{H_J}$





$\left(\frac{-D}{2}\right) 2I_{z1}I_{x2} \longrightarrow \overset{\nearrow AP}{\cancel{2I_{z1}I_{x2}}}\, C_J^2 + I_{y2} S_J^2$

$I_{y2} S_J^2 \xrightarrow[t_2]{H_{CS}} S_J^2 \left[I_{y2} C_2^2 - I_{x2} S_2^2 \right]$

$\left(\frac{-D}{2}\right) 2I_{x1}I_{z2} \xrightarrow[t_2]{H_J} \overset{\nearrow AP}{\cancel{2I_{x1}I_{z2}}}\, S_J^2 + 2 I_{y1} S_J^2$

$S_J^2 I_{y1} \xrightarrow[t_2]{H_{CS}} S_J^2 \left[I_{y1} C_1^2 - I_{x1} S_1^2 \right]$

---

collect Terms

$-D = -S_J^1 S_1^1$

$$\left.\begin{array}{l} I_{x1}: S_J^1 S_1^1 S_J^2 S_1^2 \\ I_{y1}: S_J^1 S_1^1 S_J^2 C_1^2 \end{array}\right\rangle \text{DIAG}$$

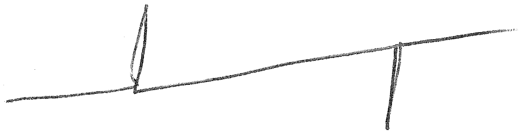
$I_x \Rightarrow \mathbb{R}$

$I_y \Rightarrow \mathbb{I}$

$$\left.\begin{array}{l} I_{x2}: S_J^1 S_1 S_J^2 S_2^2 \\ I_{y2}: \underbrace{S_J^1 S_1}\, S_J^2 C_2^2 \end{array}\right\rangle \text{X-PKS}$$

$S(t) = I_x(t) + i I_y(t)$

t_1-modulated $S \cdot S$ For all! $\longrightarrow C(w_1 - \frac{J}{2})t_1 - C(w_1 + \frac{J}{2})t_2$



$t_1 = C$ mod For Diag & XPKS

⑥

$\frac{-D}{2}\; 2 I_{z1} I_{x2} \xrightarrow{\text{Hcs}} 2 I_{z1}(I_{x2} C_2^2 + I_{y2} S_2^2)$ Phased out ?

$= 2 I_{z1} I_{x2} C_2^2 + 2 I_{z1} I_{y2} S_2^2$

$C_2^2 \Big[2 I_{z1} I_{x2} \xrightarrow{J} C_2^2 C_J^2\, 2 I_{z1} I_{x2} + C_2^2 S_J^2 I_y^2 \Big)$

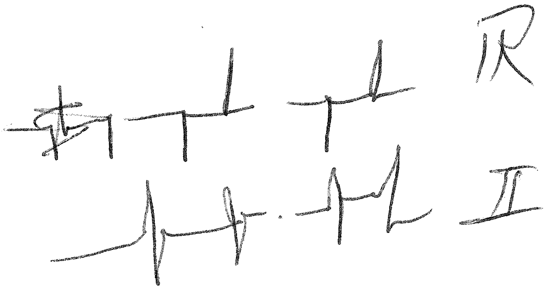
$S_2^2 \Big[2 I_{z1}^1 I_{y2} C_2^2 + - I_{x2} S_2^2 \Big)$

$2 I_{z1} I_{x2}\; C_2^2 C_J^2$ $2 I_{z1} I_{y2}\; S_2^2 C_J^2$

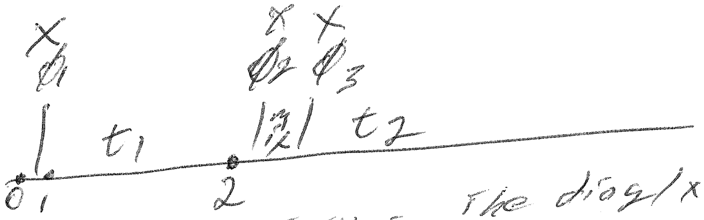
$I_{y2}\; C_2^2 S_J^2$ $- I_{x2}\; S_2^2 S_J^2$

again I_{x2}: $S_J^1 S_1^1 S_2^2 S_J^2$

I_{y2}: $S_J^1 S_1^1 C_2^2 S_J^2$



IV-12) DQF-COSY



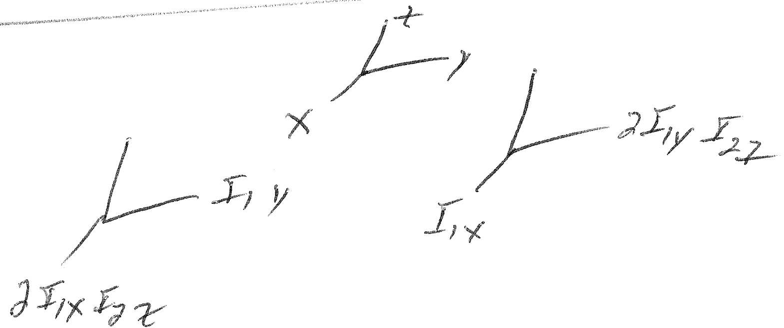
i) write the Transfer Func That characterizes the diag/x pk

Let $\phi_3 = x$

$\phi_1, \phi_2 \Rightarrow I_{1+}I_{2+} - I_{1-}I_{2-}$ (DQF Filtered

---

$\rho_0 = I_{1z} + I_{2z}$ (Focus on I_{1z})



$I_{1z} \xrightarrow{(\frac{\pi}{2})x} -I_{1y}$

$-I_{1y} \xrightarrow[H_J]{t_1} -[I_{1y}C_J' - 2I_{1x}I_{2z}S_J']$

$\xrightarrow[H_{CS}]{t_1} -C_J'\left[I_{1y}C_1' - I_{1x}S_1'\right] = -C_J'C_1'I_{1y} + C_J'S_1'I_{1x}$

$2I_{1x}I_{2z}S_J' \xrightarrow[H_{CS}]{t_1} 2I_{2z}S_J'\left[I_{1x}C_1' + I_{1y}S_1'\right]$

ρ_2: collecti

$+I_{1y}: -C_J'C_1$

$I_{1x}: C_J'S_1$

$2I_{1x}I_{2z}: S_J'C_1$

$2I_{1y}I_{2z}: S_J'S_1'$

(ρ_2)

$(\frac{\pi}{2})_{\phi_2=0}$ $I_{1z}: -C_J'S_1'$ (Pop) ~~(-Diag)~~

$I_{1x}: C_J'S_1'$

$-2I_{1x}I_{2y}: S_J'C_1'$ MQC-survies

$-2I_{1z}I_{2y}: S_J'S_1'$

(ρ_3)

* Here is where DQF differs

* Select out

Ⓠ $S^1_J C^1_J$: $-2 I_{1x} I_{2y}$ MQC $I_{1x} = \frac{I_{1+} + I_{1-}}{2}$ $I_{1y} = \frac{i(I_{1-} - I_{1+})}{2}$

$$\frac{-2i}{4}(I_{1+} + I_{1-})(I_{2-} - I_{2+})$$

$$= -i\left[I_{1+}(I_{2-} - I_{2+}) + I_{1-}(I_{2-} - I_{2+}) \right.$$

$$= -i\left[I_{1+}I_{2-} - I_{1+}I_{2+} + I_{1-}I_{2-} - I_{1-}I_{2+} \right.$$

$$= -i\left[\underbrace{(I_{1+}I_{2-} - I_{1-}I_{2+})}_{ZQC} + \underbrace{(I_{1-}I_{2-} - I_{1+}I_{2+})}_{DQC} \right]$$

$$= i\left[I_{1+}I_{2+} - I_{1-}I_{2-} \right]$$

$$i\left[(I_{1x} + iI_{1y})(I_{2x} + iI_{2y}) - (I_{1x} - iI_{1y})(I_{2x} - iI_{2y}) \right]$$

$$= i\left[I_{1x}(I_{2x} + iI_{2y}) \cancel{i} \right. = \cancel{iI_{1x}I_{2x}} - I_{1x}I_{2y}$$

$$+ iI_{1y}(I_{2x} + iI_{2y}) = -I_{1y}I_{2x} - \cancel{iI_{1y}I_{2y}}$$

$$- I_{1x}(I_{2x} - iI_{2y}) = -i\cancel{I_{1x}I_{2x}} - I_{1x}I_{2y}$$

$$- iI_{1y}(I_{2x} - iI_{2y}) = \cancel{I_{1y}I_{2x}} - iI_{1y}I_{2y}$$

$$\Rightarrow \boxed{-I_{1x}I_{2y} - I_{1y}I_{2x}} = i\left[I_{1+}I_{2+} - I_{1-}I_{2-} \right]$$

③

$-I_{1x}I_{2y} \xrightarrow{(\frac{\pi}{2})_X} -I_{1x}I_{2z} : C_i^1 S_J^1$ (evolves @ ω_1 Diag

$-I_{1y}I_{2x}$ $\qquad -I_{2z}I_{2x} : C_i^1 S_J^1$ (" " @ ω_2 XPk)

---

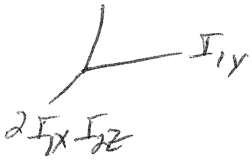
2 important pts:

1) Both terms above modulated the same in t_1
- ∴ we can phase the same → A

* remember before Diag & XPk modulated DiF in t_1 (C·S & S·S)

* now DQF is S·C

2) I_zI_x etc above appear along same (x) axis I_xI_z *



$-2I_{1x}I_{2z} \xrightarrow[t_2]{H_J} -2I_{1x}I_{2z}C_J^2 - I_{1y}S_J^2$

$-2I_{1x}I_{2z}C_J^2 \xrightarrow[t_2]{H_{cs}} -2(I_{1x}C_i^2 + I_{1y}S_i^2)I_{2z}C_J^2$

$= I_{1x}I_{2z} : -2C_i^2C_J^2 \; C_i^1S_J^1$

$I_{1y}I_{2z} : -2 \; S_i^2C_J^2 \; C_i^1S_J^1$

$-C_J^2 I_{1y} \xrightarrow[t_2]{H_{cs}} -S_J^2[I_{1y}C_i^2 - I_{1x}S_i^2)$

$I_{1y} : C_i^1S_J^1 \; S_J^2C_i^2$ ⟩ Diag

$I_{1x} : C_i^1S_J^1 \; S_J^2S_i^2$

④

$$-2I_{1z}I_{2x} \xrightarrow[t_2]{H_J} -2I_{1z}I_{2x}C_J^2 - I_{2y}S_J^2$$

$$-2I_{1z}C_J^2\left[I_{2x}C_2^2 + I_{2y}S_2^2\right]$$

$$-S_J^2\left[I_{2y}C_2^2 - I_{2x}S_2^2\right]$$

---

collect	Diag	XPKS
NOT OBSERVED	$2I_{1x}I_{2z}: -C_1S_J^1C_1^2C_J^2$	$2I_{1z}I_{2x}: -C_1^1S_J^1C_J^2C_2^2$
	$2I_{1y}I_{2z}: -C_1^1S_J^1S_1^2C_J^2$	$2I_{1z}I_{2y}: -C_1^1S_J^1C_J^2S_2^2$
	$I_{1y}: -C_1^1S_J^1C_1^2S_J^2$	$I_{2y}: -C_1^1S_J^1S_J^2C_2^2$
	$I_{1x}: +C_1S_J^1S_1^2S_J^2$	$I_{2x}: +C_1^1S_J^1S_J^2S_2^2$

LF: only in phase terms obs!

$$C \cdot S = \frac{S(\alpha+\beta) + S(\alpha-\beta)}{2}$$

$$S(\alpha)S(\beta) - \frac{1}{2}\left[C(\alpha-\beta) - C(\alpha+\beta)\right]$$

$$S_0\,S(\omega t) \xrightarrow{\sin FT} S_0\,A(\omega)$$

$$\xrightarrow{\cos FT} S_0\,D(\omega)$$

$$e^{i\omega t} \xrightarrow{FT} A(\omega) + iD(\omega)$$

$$S_0\,C(\omega t) \xrightarrow{\sin FT} S_0\,D(\omega)$$

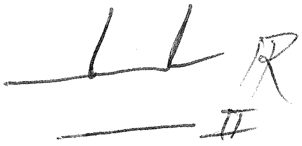
$$\xrightarrow{\cos FT} S_0\,A(\omega)$$

⑤

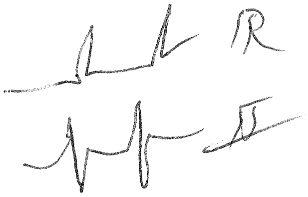
$$I_{2x} = S_J^2 S_\Omega^2 = c(w - \tfrac{J}{2}) - c(w + \tfrac{J}{2})$$

$$I_{2y} = S_J^2 C_w^2 = S(w + \tfrac{J}{2}) + S(w - J/2)$$

~~Sin FT~~ use $\xrightarrow[\text{in } t_1]{\text{sin FT}}$

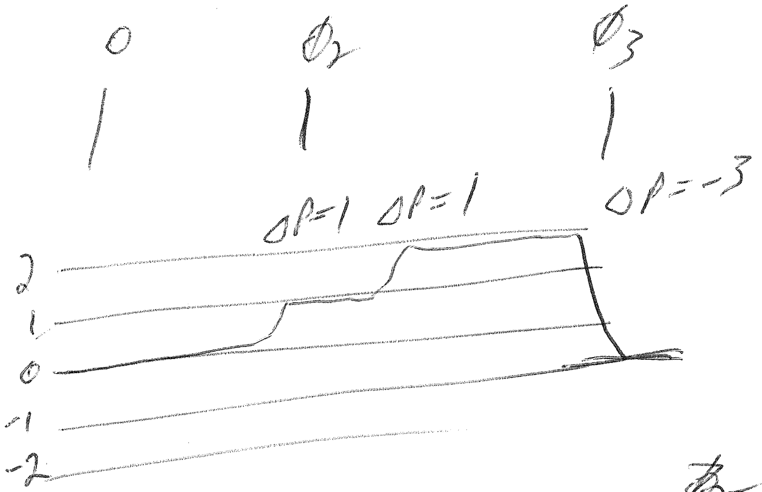


$\xrightarrow[\text{in } t_2]{\text{FT}}$



VI-12) $\phi_1 = 0$ $\phi_2, \phi_3 = 0, 1, 2, 3$

iii)



$$\phi_{Rx} = -\sum \Delta P \phi = -1 - 1 + 3 = \cancel{\phi_3}$$

$$= -\phi_1 - \phi_2 + 3\phi_3 = -\phi_2 + 3\phi_3$$

ϕ_1	0000	0000	0000	0000
ϕ_2	0000	0111	2222	3333
ϕ_3	0123	0123	0123	0123
ϕ_R	0321	3210	2103	1032

VI-12) (iii)   3-SPIN I_1 I_2 I_3

J_{12} J_{13} J_{23} $\neq 0$

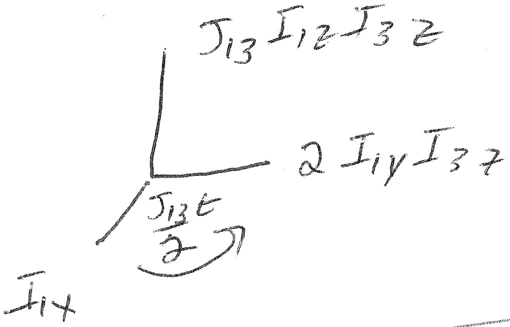
* calc Tx Funcs yielding XPK @ (ν_2, ν_3) in a DQF-COSY

* schematize multiplet

$$2 I_{1x} I_{2z} \xrightarrow{J_{13} I_{3z} I_{1z}} 2 e^{-i J_{13} I_{1z} I_{3z} t} I_{1x} e^{+i J_{13} I_{1z} I_{3z} t} I_{2z}$$

$$\rightarrow 2\left[I_{1x} c\left(\frac{J_{13} t}{2}\right) + 2 I_{1y} I_{3z} s\left(\frac{J_{13} t}{2}\right)\right) I_{2z}$$

$$2 I_{1x} I_{2z} c\left(\frac{J_{13} t}{2}\right) + 4 I_{1y} I_{3z} I_{2z} s\left(\frac{J_{13}}{t}\right)\Big)$$



Stay same as 2-spin

$$2 I_{1x} I_{2z} \xrightarrow{J_{23} I_{2z} I_{3z} t} 2\left[e^{-i J_{23} I_{2z} I_{3z} t} I_{1x} e^{i J_{23} I_{2z} I_{3z} t}\right) I_{2z}$$

$$= 2 I_{1x} I_{2z}$$ (NO J_{12} or J_{13} ~~coup~~ here)

$$2 I_{1x} I_{2y} \xrightarrow{J_{12} I_{1z} I_{2z}} 2 I_{1x} I_{2y}$$

But!   watch!

$$2 I_{1x} I_{2y} \xrightarrow{J_{13} I_{1z} I_{3z} t} \Rightarrow$$

$$2 I_{1x} I_{2z} c\left(\frac{J_{13} t}{2}\right) + 4 \ldots$$

②

$$I_{2z} \xrightarrow{(\frac{\pi}{2})_y} I_{2x} \xrightarrow[I_{2z}I_{3z}]{J_{23}\,t_1} I_{2x}\,C\left(\frac{J_{23}t_1}{2}\right) + 2I_{2y}I_{3z}\,S\left(\frac{J_{23}t_1}{2}\right)$$

I_{2x} Part

$$I_{2x}\,C'_{J_{23}} \xrightarrow{J_{13}\,I_{1z}I_{3z}} I_{2x}\,C'_{J_{23}}$$

$$I_{2x}\,C'_{J_{23}} \xrightarrow{J_{12}\,I_{1z}I_{2z}} C'_{J_{23}}\left[I_{2x}\,C'_{J_{12}} + 2I_{1z}I_{2x}\,S'_{J_{12}}\right]$$

$$= C'_{J_{23}}C'_{J_{12}}I_{2x} + C'_{J_{23}}S'_{J_{12}}\,2I_{1z}I_{2x}$$

$$2I_{2y}I_{3z}\,S'_{J_{23}} \xrightarrow{J_{13}\,I_{1z}\cancel{I_{3z}}\,t_1} 2I_{2y}I_{3z}\,S'_{J_{23}}$$

$$2I_{2y}I_{3z}\,S'_{J_{23}} \xrightarrow{J_{12}\,I_{1z}I_{2z}} 2I_{3z}\,S'_{J_{23}}\left[I_{2y}\,C\left(\frac{J_{12}t_1}{2}\right) - 2I_{2x}I_{1z}\,S\left(\frac{J_{12}t_1}{2}\right)\right]$$

$$= \boxed{2I_{2y}I_{3z}\,S'_{J_{23}}\,C'_{J_{12}}} - 4I_{1z}\cancel{I_{2x}}I_{3z}\,S'_{J_{23}}\,S'_{J_{12}}$$

$$2I_{2y}I_{3z}\,S'_{J_{23}}C'_{J_{12}} \xrightarrow[t_1]{H_{CS}} 2I_{3z}\,S'_{J_{23}}C'_{J_{12}}\left[I_{2y}\,C(w_2t_1) - I_{2x}\,S(w_2t_1)\right]$$

y y y

$$\Rightarrow \boxed{2I_{2y}I_{3z} : S'_{J_{23}}\,C'_{J_{12}}\,C'_{w_2}}$$

$$2I_{2x}I_{3z} : -S'_{J_{23}}\,C'_{J_{12}}\,S'_{w_2}$$

③

$$2I_{2y}I_{3z} \xrightarrow{(\frac{\pi}{2})y} 2I_{2y}I_{3x}$$ MQC

$$2I_{2x}I_{3z} \xrightarrow{(\frac{\pi}{2})y} 2I_{2z}I_{3x}$$ SQC ϕ-out

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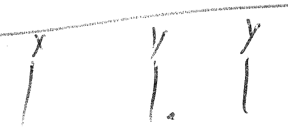


$$2I_{2y}I_{3x} = \underbrace{\frac{i}{2}(I_{2-}I_{3+} - I_{2+}I_{3-})}_{ZQC} + \underbrace{\frac{i}{2}(-I_{2+}I_{3+} - I_{2-}I_{3-})}_{DQC-}$$

$$\frac{i}{2}(I_{2+}I_{3+} - I_{2-}I_{3-}) = \frac{1}{2}(2I_{2x}I_{3y} + 2I_{2y}I_{3x})$$

$$2I_{2x}I_{3y} \xrightarrow{(\frac{\pi}{2})y} -2I_{2z}I_{3y} : S^1_{J23}C^1_{J12}C^1_{\omega_2} \rightarrow (\omega_3 - XPK)$$

$$2I_{2y}I_{3x} \xrightarrow{(\frac{\pi}{2})y} -2I_{2y}I_{3z} : S^1_{J23}C^1_{J12}C^1_{\omega_2}$$ (evolves @ ω_2 now $_{\text{Diag}}$)

* T_1 modulate S_JC_J for both!

$$(-)2I_{2z}I_{3y} \xrightarrow{J_{12}t_2} 2I_{2z}I_{3y}$$

$$(-)2I_{2z}I_{3y} \xrightarrow{J_{13}I_{1z}I_{3z}t_2} 2I_{2z}[I_{3y}C^2_{J13} - 2I_{1z}I_{3x}S^2_{J13})$$

$$\Rightarrow 2I_{2z}I_{3y}C^2_{J13}$$

$$-4I_{1z}\cancel{I_{2z}}I_{3x}S^2_{J13}$$

① $(-)\,2I_{2z}I_{3y}\,C^{2}_{J13} \xrightarrow{J_{23}I_{2z}I_{3z}t_2} \boxed{C^{2}_{J13}}\left[2I_{2z}I_{3y}\,C^{2}_{J23} - \boxed{I_{3x}\,S^{2}_{J23}}\right]$

$(-)\ -I_{3x}:\left(C^{2}_{J13}\,S^{2}_{J23}\,S^{1}_{J23}\,C^{1}_{J12}\,C^{1}_{\omega 2}\right)=A$

$+\ A\,I_{3x} \xrightarrow[t_2]{H_{cs}} A\left[I_{3x}C^{2}_{3} + I_{3y}S^{2}_{3}\right)$

$\therefore\ I_{3x}:\ C^{2}_{\underline{J13}}\,S^{2}_{J23}\,S^{1}_{J23}\,C^{1}_{J12}\left[C^{1}_{\omega 2}\,C^{2}_{\omega 3}\right]$ ✓

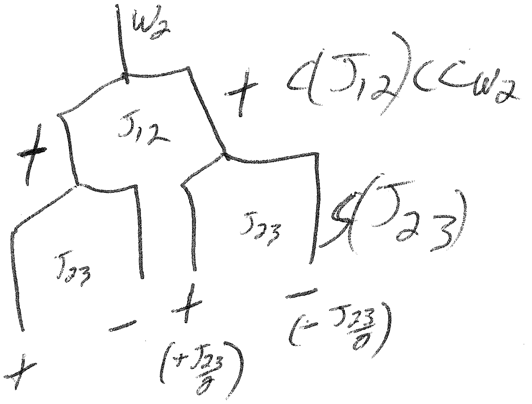
$I_{3y}:\ C^{2}_{\underline{J13}}\,S^{2}_{J23}\,S^{1}_{J23}\,C^{1}_{J12}\left[C^{1}_{\omega 2}\,S^{2}_{\omega 3}\right)$

$I_{3x}: t_1:\ S^{1}_{J23}\,C^{1}_{J12}\,C^{1}_{\omega 2}$	$I_{3y}: t_1:\ S^{1}_{J23}\,C^{1}_{J12}\,C^{1}_{\omega 2}$
$I_{3x}: t_2:\ S^{2}_{J23}\,C^{2}_{J13}\,C^{2}_{\omega 3}$	$I_{3y}: t_2:\ S^{2}_{J23}\,C^{2}_{J13}\,S^{2}_{\omega 3}$

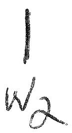
Focus on Real $\mathbb{R}: I_{3x} \Longrightarrow S\cdot C\cdot C$ = odd · even · even
= odd   Sine funcs

⑤ $S^1_{J23}\ C^1_{J12}\ C_{w2}\ \vdots\ I_{3x}\ \vdots\ t_1 \longrightarrow$

~~s~~FFT
(sine)



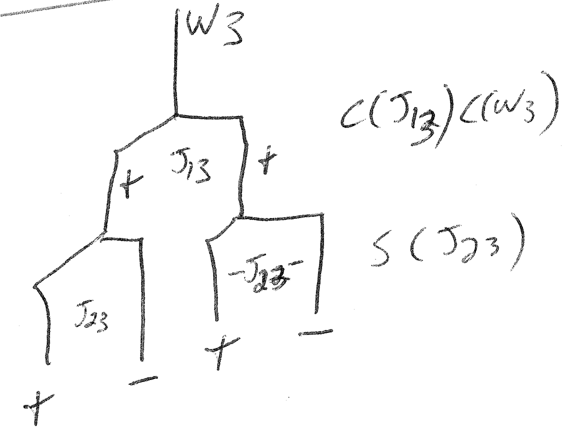
$$C(a)C(b) = \frac{C(a+b) + C(a-b)}{2}$$

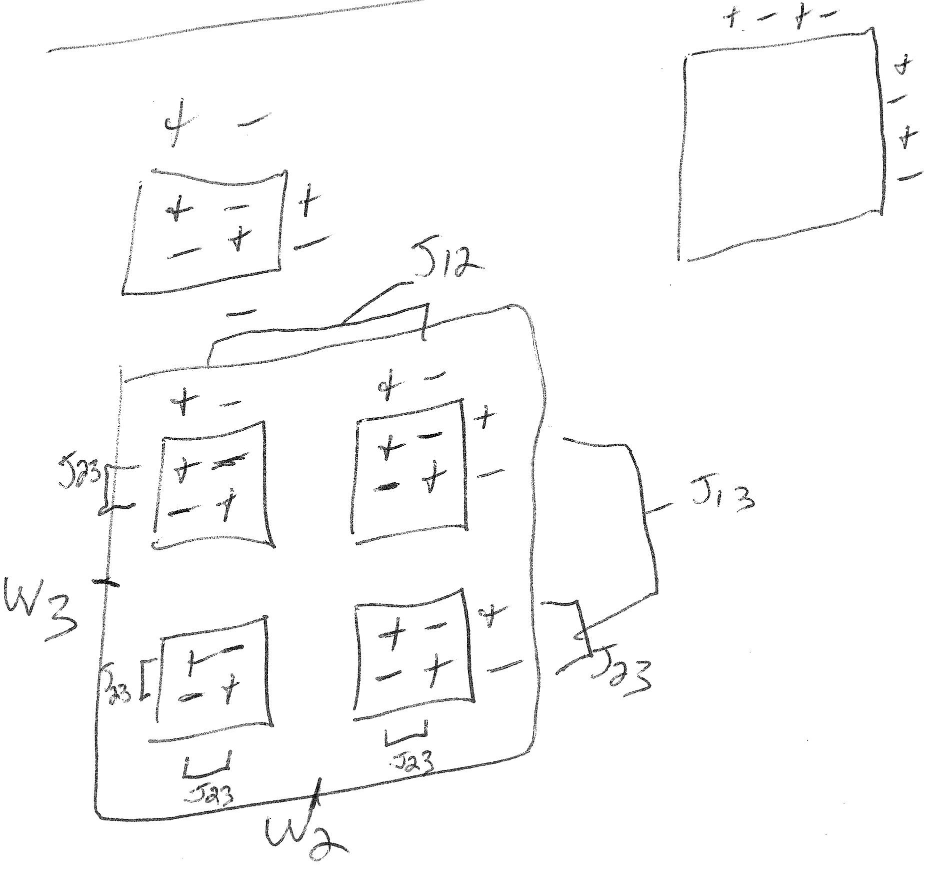


$I_{3x}\ \vdots\ t_2\ \vdots\ S^2_{J23}\ C^2_{J13}\ C^2_{w_3}.$

+ same as in T1

sine FFT →

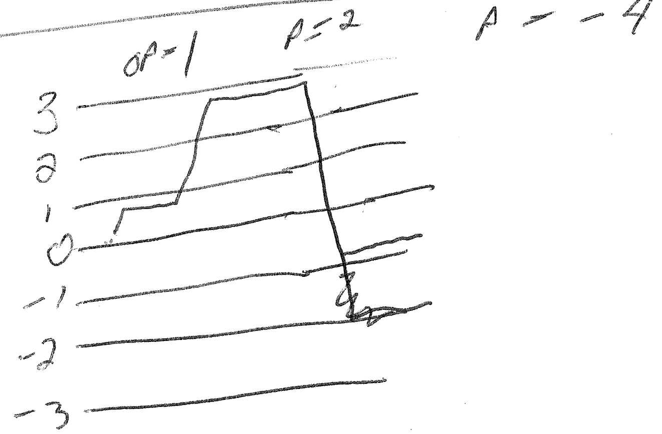




VI-13 TQF-COSY

i) Demonstrate that the last RF pulse in TQF COSY has to be:

$0, \frac{\pi}{3}, \frac{2\pi}{3}, \pi, \frac{4\pi}{3}, \frac{5\pi}{3}$



$$I_x \xrightarrow{\omega t I_z} I_x C(\omega t) + I_y S(\omega t)$$

$$= \frac{I_+}{2} e^{-i\omega t} + \frac{I_- e^{i\omega t}}{2}$$

ϕ-out

PPE $\rho_t(\phi=0) = \sum_{p=-3}^{3} \sigma_p \Rightarrow \boxed{\rho_t(\phi) = \sum_{p=-3}^{3} \sigma_p e^{-ip\phi}}$

↳ Dens mat after RF ϕ shift

$\sigma_0 = a \cdot \mathbb{I} + b I_0 + c I_0 S_0 \ldots$

$\sigma_1 = g I_+ + h I_+ S_0 + \ldots$

$\sigma_2 = k \, I_{2+} \overset{I_{1+}}{} + l \, I_{2+} S_{0+}$

$\sigma_3 = x I_{3+} \overset{I_{2+}\,I_{1+}}{+} y I_{3+} S_0 + I_0 S_{3+} \overset{S_{2+}S_{1+}}{+} \ldots$ $I_{1+} I_{2+} I_{3}$,

$= x I_{1+} I_{2+} I_{3+} + \mathbb{I}_{\ldots}$

$\rho_{\pm 2}$ here # of ϕ

See ② for steps needed

N = # of coupled spins

Need to acquire:

$M = 2N+1 = \#$ expts

Think ~~$M = 2\left(\frac{N}{2}\right)+1$~~

Then we can select any coh

$$\sigma_p = \sum_{k=1}^{M} S(\phi_k)\, e^{ip\phi_k},$$

$$\phi_k = \frac{2\pi(k-1)}{N} \qquad k = ~~\ldots~~ 1, 2, 3 \ldots$$

②

$$\ell(\phi=0) = I_0 e^{0\phi} + I_+ e^{-i\phi} + I_- e^{i\phi}$$

$$= I_0 + I_+ + I_-$$

$$\boxed{G_P = G_P e^{-iP\phi}}$$

$$\ell(\phi=\pi) = I_0 e^{0} + I_+ e^{-i\pi} + I_- e^{i\pi}$$

$e^{i\pi} =$ [illegible] $i\,s(\pi)$

$= -1$

$e^{-i\pi} = -1$

$$\ell(\pi) = I_0 - I_+ - I_-$$

$\therefore\ \ell_0 + \ell_\pi = 2I_0$

$\ell_0 - \ell_\pi = 2(I_+ + I_-)$

Need one more ϕ step to remove I_+ or I_- Quad

To block ! cohs use:

Block 2-cohs need 3 expts

∴ Summary

cohs block	# expts, M
0	1
1	2
2	3
3	4
4	5
5	6

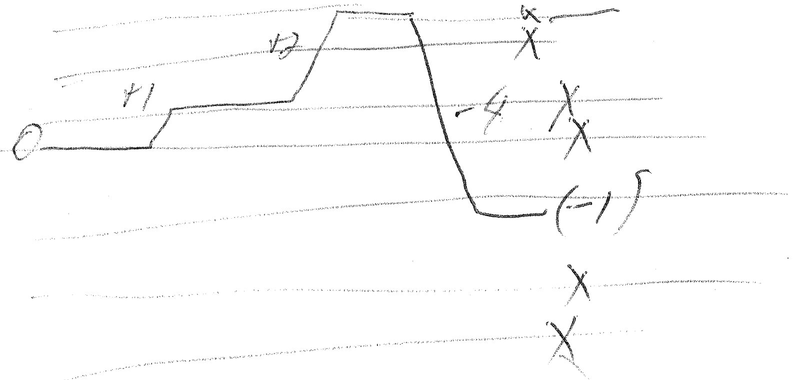
M = # expts

$$\phi_k = \frac{2\pi(k-1)}{M}$$

where $k = 1, 2 \ldots M$

③

i)



block 6-cols

∴ 7 expts

N = # of spins

$\phi_K = \cancel{2\pi(k\ldots)} \frac{2\pi(k-1)}{m}$ $m = 7$

$m = 2N+1$

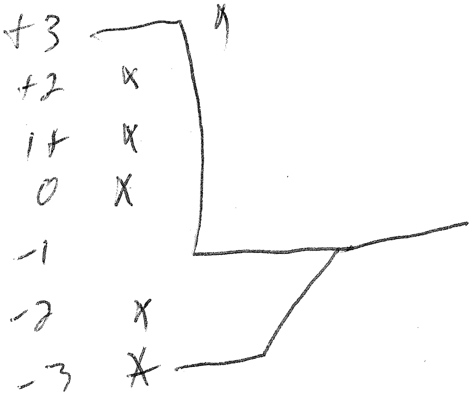
$m = 7$

$\phi_1 = \frac{2\pi(1-1)}{7} =$

$K = 1..7$

$N = 3$

$$\sum_{k=1}^{m} \frac{2\pi(k-1)}{m} = \frac{2\pi(k-1)}{7}$$



$\phi_1 = 0$

$\phi_2 = \frac{2\pi}{7}$

$\phi_3 = \frac{4\pi}{7}$

$\phi_4 = \frac{6\pi}{7}$

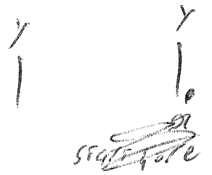
$\phi_5 = \frac{8\pi}{7}$

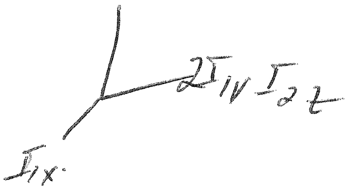
$\phi_6 = \frac{10\pi}{7}$

$\phi_7 = \frac{12\pi}{7}$

④

ii) The Tx Funcs For TOC Diag/Xpks





$\rho_0 = I_{1z} + I_{2z} + I_{3z}$ $\quad J_{12}, J_{13}, J_{23} \neq 0$

Focus on I_{1z}

J_{12}

$I_{1z} \xrightarrow{(\pi/2)_y} = I_{1x} \xrightarrow{J_{12} I_{1z} I_{2z} t_1} I_{1x} C^{1}_{J12} + 2 I_{1y} I_{2z} S^{1}_{J12}$

J_{13}

$I_{1x} C_{J12} \xrightarrow{J_{13} I_{1z} I_{3z}} C^{1}_{J12} \left[I_{1x} C^{1}_{J13} + 2 I_{1y} I_{3z} S^{1}_{J13} \right]$

$2 I_{1y} S_{J12} I_{2z} \xrightarrow{J_{13} I_{1z} I_{3z}} 2 S^{1}_{J12} I_{2z} \left[I_{1y} C^{1}_{J13} - 2 I_{1x} I_{3z} S^{1}_{J13} \right]$

J_{23}

$C^{1}_{J12} C^{1}_{J13} : I_{1x} \xrightarrow{J_{23} I_{2z} I_{3z}}$ No evol

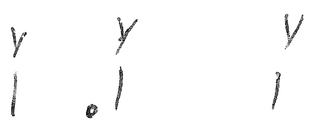
$C^{1}_{J12} S^{1}_{J13} \, 2 I_{1y} I_{3z} \xrightarrow{J_{23} I_{2z} I_{3z}}$ X

$S^{1}_{J12} C^{1}_{J13} \, 2 I_{1y} I_{2z} \longrightarrow$ X

$\boxed{- S_{J12} S^{1}_{J13} : 4 I_{1x} I_{2z} I_{3z}} \longrightarrow$ X For mqc seq

---

$- S^{1}_{J12} S^{1}_{J13} : 4 I_{2z} I_{3z} \left(I_{1x} C^{1}_{\omega_1} + I_{1y} S^{1}_{\omega_1} \right)$



$\Rightarrow - S^{1}_{J12} S^{1}_{J13} C^{1}_{\omega_1} : 4 I_{1x} I_{2z} I_{3z}$

$\boxed{- S^{1}_{J12} S^{1}_{J13} S^{1}_{\omega_1} : 4 I_{1y} I_{2z} I_{3z}}$

⑤

$S_{J12}S'_{J13}C_{\omega_1}: 4I_{1x}I_{2z}I_{3z} \xrightarrow{(\pi/2)y} 4I_zI_{2x}I_{3x}$ (DQC $-\phi$, out

$\boxed{-S_{J12}S_{J13}S_{\omega_1}: 4I_{1y}I_{2z}I_{3z}} \xrightarrow{(\frac{\pi}{2})y} \boxed{4I_{1y}I_{2x}I_{3x}}$ MQC

$I_{1x} = \frac{1}{2}(I_{1+}+I_{1-})$

$I_{1+} = I_{1x} + iI_{1y}$

$I_{1-} = I_{1x} - iI_{1y}$

$I_{1y} = \frac{i}{2}(I_{1-}-I_{1+})$

$4\frac{1}{2}\cancel{(I_{1+}+I_{1-})*\frac{1}{2}(}$ $\quad \frac{i4}{2}(I_{1-}-I_{1+})\left(\frac{I_{2+}+I_{2-}}{2}\right)\left(\frac{I_{3+}+I_{3-}}{2}\right)$

$\frac{i}{2}\left[I_{1-}(I_{2+}+I_{2-}) - I_{1+}(I_{2+}+I_{2-})\right](I_{3+}+I_{3-})$

$\frac{i}{2}\left[I_{1-}I_{2+} + I_{1-}I_{2-} - I_{1+}I_{2+} - I_{1+}I_{2-}\right)(I_{3+}+I_{3-})$

$= \frac{i}{2}\Big(I_{1-}I_{2+}I_{3+} + I_{1-}I_{2-}I_{3+} - I_{1+}I_{2+}I_{3+} - I_{1+}I_{2-}I_{3+}$

$\quad I_{1-}I_{2+}I_{3-} + I_{1-}I_{2-}I_{3-} - I_{1+}I_{2+}I_{3-} - I_{1+}I_{2-}I_{3-}$

$= \frac{i}{2}\left[I_{1-}I_{2-}I_{3-} - I_{1+}I_{2+}I_{3+}\right) + \text{ZQC} + \text{DQC}$

$I_{1-}I_{2-}I_{3-} = (I_{1x}-iI_{1y})(I_{2x}-iI_{2y})(I_{3x}-iI_{3y})$

$= \left[I_{1x}(I_{2x}-iI_{2y}) - iI_{1y}(I_{2x}-iI_{2y})\right](I_{3x}-iI_{3y})$

$= (I_{1x}I_{2x} - iI_{1x}I_{2y} - iI_{1y}I_{2x} + i^2 I_{1y}I_{2y})(I_{3x}-iI_{3y})$

$=$

⑥ $I_{1x}I_{2x}I_{3x} - iI_{1x}I_{2y}I_{3x} - iI_{1y}I_{2x}I_{3x} + i^2 I_{1y}I_{2y}I_{3x}$

$- I_{1x}I_{2x}iI_{3y} + i^2 I_{1x}I_{2y}I_{3y} + i^2 I_{1y}I_{2x}I_{3y} - i^3 I_{1y}I_{2y}I_{3y}$

$iI_{1x}I_{2x}I_{3x} - i^2 I_{1x}I_{2y}I_{3x} - i^2 I_{1y}I_{2x}I_{3x} + i^3 I_{1y}I_{2y}I_{3x}$

$-i^2 I_{1x}I_{2x}I_{3y} + i^3 I_{1x}I_{2y}I_{3y} + i^3 I_{1y}I_{2x}I_{3y} - i^4 I_{1y}I_{2y}I_{3y}$

$iI_{1x}I_{2x}I_{3x} + I_{1x}I_{2y}I_{3x} + I_{1y}I_{2x}I_{3x} - iI_{1y}I_{2y}I_{3x}$

$+ I_{1x}I_{2x}I_{3y} - iI_{1x}I_{2y}I_{3y} - iI_{1y}I_{2x}I_{3y} - I_{1y}I_{2y}I_{3y}$

$= I_{1-}I_{2-}I_{3-}$

$\frac{i}{2}(I_{1+}I_{2+}I_{3+}) = (I_{1x}+iI_{1y})(I_{2x}+iI_{2y})(I_{3x}+iI_{3y})$

$= (I_{1x}(I_{2x}+iI_{2y}) + iI_{1y}(I_{2x}+iI_{2x}))(I_{3x}+iI_{3y})$

$= \frac{i}{2}[I_{1x}I_{2x} + iI_{1x}I_{2y} + iI_{1y}I_{2x} + i^2 I_{1y}I_{2y} \quad (I_{3x}+iI_{3y})$

$= \frac{i}{2} / \ I_{1x}I_{2x}I_{3x} + iI_{1x}I_{2y}I_{3x} + iI_{1y}I_{2x}I_{3x} + i^2 I_{1y}I_{2y}I_{3x}$

$iI_{1x}I_{2x}I_{3y} + i^2 I_{1x}I_{2y}I_{3y} + i^2 I_{1y}I_{2x}I_{3y} + i^3 I_{1y}I_{2y}I_{3y}$

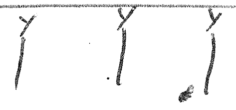
$= iI_{1x}I_{2x}I_{3x} + i^2 I_{1x}I_{2y}I_{3x} + i^2 I_{1y}I_{2x}I_{3x} + i^3 I_{1y}I_{2y}I_{3x}$

$i^2 I_{1x}I_{2x}I_{3y} + i^3 I_{1x}I_{2y}I_{3y} + i^3 I_{1y}I_{2x}I_{3y} + i^4 I_{1y}I_{2y}I_{3y}$

⑦ $I_{1-} I_{2-} I_{3-} - I_{1+} I_{2+} I_{3+}$

$$i I_{1x} \cancel{I_{2x} I_{3x}} + I_{1x} I_{2y} I_{3x} + I_{1y} I_{2x} I_{3x} - i I_{1y} \cancel{I_{2y} I_{3x}}$$
$$+ I_{1x} I_{2x} I_{3y} - i I_{1x} \cancel{I_{2y} I_{3y}} - i I_{1y} \cancel{I_{2x} I_{3y}} - I_{1y} I_{2y} I_{3y}$$

$$-i I_{1x} \cancel{I_{2x}} I_{3x} + I_{1x} I_{2y} I_{3x} + I_{1y} I_{2x} I_{3x} + i I_{1y} \cancel{I_{2y} I_{3x}} - I_{1y} I_{2y} I_{3y}$$
$$+ I_{1x} I_{2x} I_{3y} + i I_{1x} \cancel{I_{2y}} I_{3y} + i I_{1y} \cancel{I_{2x}} I_{3y}$$



$$\frac{1}{2}\left(2 I_{1x} I_{2y} I_{3x} + 2 I_{1y} I_{2x} I_{3x} + 2 I_{1x} I_{2x} I_{3y} - 2 I_{1y} I_{2y} I_{3y}\right)$$

$$= \frac{i}{2}\left(I_{1-} I_{2-} I_{3-} - I_{1+} I_{2+} I_{3+}\right)$$

Recall $I_{1z} \rightarrow I_{1x}$

8 $I_{1x} I_{2y} I_{3x} \xrightarrow{(\pi/2)_y} I_{1z} I_{2y} I_{3z}$ $(\omega_2$, XPK)

$I_{1y} I_{2x} I_{3x} \longrightarrow I_{1y} I_{2z} I_{3z}$ (evolves @ ω_1), DIAG

$I_{1x} I_{2x} I_{3y} \rightarrow I_{1z} I_{2z} I_{3y}$ $(\omega_3$, XPK)

$I_{1y} I_{2y} I_{3y} \longrightarrow I_{1y} I_{2y} I_{3y}$ — MQC, not obs..

Also. $\boxed{-S'_{J12} S'_{J13} S'_{\omega 1}} - t_1$ for all Above

8)

$$\frac{1}{8}\Big[2I_{1y}I_{2z}I_{3z} \xrightarrow{J_{12}I_{1z}I_{2z}t_2} I_{3z}\left[2I_{1y}I_{2z}C^2_{J12} - I_{1x}S^2_{J12}\right]$$

$$= 2I_{1y}I_{2z}\cancel{I_{3z}}C^2_{J12} -$$

? Wrong

$$- I_{1x}S^2_{J12}$$

$$-I_{1x}S^2_{J12} \xrightarrow{J_{13}t_2} -\left[I_{1x}C^2_{J13} + 2\overset{AP}{I_{1y}I_{3z}}S^2_{J13}\right]S^2_{J12}$$

J_{23} → No evol here

$$-I_{1x}C^2_{J13}S^2_{J12} \xrightarrow[t_2]{H_{CS}} -\left[I_{1x}C\omega^2_1 + I_{1y}S\omega^2_1\right]C^2_{J13}S^2_{J12}$$

$$I_{1x}: (-S^2_{J12}C^2_{J13}C\omega^2_1)(-S^1_{J12}S^1_{J13}S\omega^1_1)$$

DIAG

$$I_{1y}: (-S^2_{J12}C^2_{J13}\cancel{S}\,C\omega^2_1)(-S^1_{J12}S^1_{J13}S\omega^1_1)$$

$$\frac{1}{8}\left[2I_{1z}I_{2y}I_{3z} \xrightarrow[t_2]{J_{12}} I_{3z}\left[2I_{1z}I_{2y}C^2_{J12} - I_{1x}S^2_{J12}\right]\right.$$

$-$

⑨ $2I_{1z}I_{2y}I_{3z} \xrightarrow[t_2]{J_{12}} I_{3z}\left[2I_{1z}I_{2y}c^2_{J12} - I_{2x}s^2_{J12}\right]$

$-s^2_{J12}: I_{2x}I_{3z} \xrightarrow{J_{13}} X$

$c^2_{J12}: 2I_{1z}I_{2y}I_{3z} \rightarrow X$

$-s^2_{J12}\, I_{2x}I_{3z} \xrightarrow[t_2]{J_{23}} -\frac{1}{2} s^2_{J12}\left[2I_{2x}I_{3z}\, c^2_{J23} + I_{2y}\, s^2_{J23}\right]$

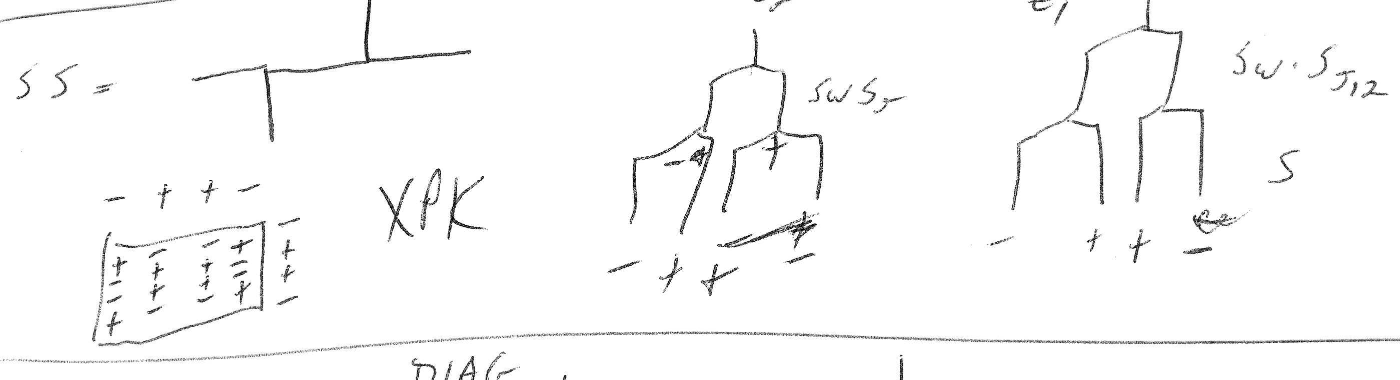
$= -\frac{1}{2}\left[s^2_{J12}\, c^2_{J23}\, 2\overset{AP}{\cancel{I_{2x}I_{3z}}} + s^2_{J12}\, s^2_{J23}\, I_{2y}\right]$

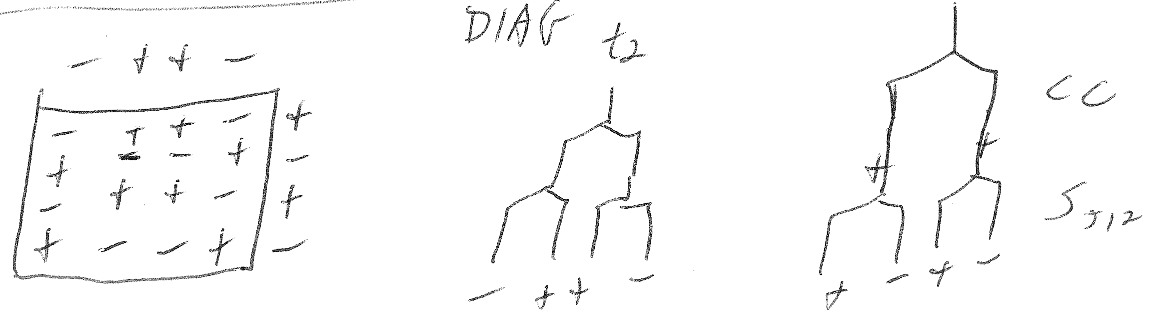
$-\frac{1}{2} s^2_{J12}\, s^2_{J23}\left[I_{2y}\, c_{\omega_2}^2 - I_{2x}\, s_{\omega_2}^2\right]$

$I_{2x}: -s_{\omega_2}^2\, s^2_{J12}\, s^2_{J23} * (-s^1_{J12}\, s^1_{J13}\, s_{\omega_1}^1)$

$I_{2y}: c_{\omega_2}^2\, s^2_{J12}\, s^2_{J23}\, (-s^1_{J12}\, s^1_{J13}\, s_{\omega_1}^1)$

~~Di~~ XPK W_{12}





10) $\omega_{1,3}$ - x/k $\qquad \overset{x}{|} \quad | \quad \overset{y}{|}$

$$2I_{1z}I_{2z}I_{3y} \xrightarrow{J_{13}I_{1z}I_{3z}t_2} I_{2z}\left[\cancel{2I_{1z}I_{3y}}^{AP} C^2_{J13} + I_{3x} S^2_{J13}\right]$$

$$I_{2z}I_{3x} S^2_{J13} \xrightarrow{J_{23}} \frac{1}{2} S^2_{J13}\left[\cancel{2I_{2z}I_{3x}}^{AP} C^2_{J23} + \boxed{I_{3y} S^2_{J23}}\right]$$

$$\xrightarrow{J_{12}} \times$$

$$\frac{1}{2} S^2_{J13} S^2_{J23} I_{3y} \xrightarrow{H_{cs}t_2} \frac{1}{2} S^2_{J13} S^2_{J23}\left[I_{3y} C(\omega_3 t_2) - I_{3x} S(\omega_3 t_2)\right]$$

I_{3y}: $+\frac{1}{2} S^2_{J13} S^2_{J23} C^2_{\omega_3} (-S^1_{J12} S^1_{J13} S^1_{\omega_1})$

ω_{13} - x/k

I_{3x}: $\left(-\frac{1}{2}\right) S^2_{J13} S^2_{J23} S^2_{\omega_3} (-S^1_{J12} S^1_{J13} S^1_{\omega_1})$

---

⑪ DIAG AK

$$\left(\frac{1}{2}\right) 2 I_{1y} I_{2z} I_{3z} \xrightarrow{J_{12} I_{1z} I_{2z} t_2} \frac{I_{3z}}{2} \left[\overset{X}{\cancel{2 I_{1y} I_{2z}}} C^{2}_{J12} - I_{1y} S^{2}_{J12} \right]$$

$$-\left(\frac{1}{2}\right) I_{1y} I_{3z} S^{2}_{J12} \xrightarrow{J_{13}} \left(\frac{-1}{4}\right) \left[2 I_{1y} I_{3z} C^{2}_{J13} - I_{1x} S^{2}_{J13} \right] S^{2}_{J12}$$

$$= \left(\frac{+1}{4}\right) S^{2}_{J12} S^{2}_{J13} I_{1x}$$

$$\frac{1}{4} S^{2}_{J12} S^{2}_{J13} I_{1x} \xrightarrow{H_{cs} t_2} \frac{1}{4} S^{2}_{J12} S^{2}_{J13} \left[I_{1x} C(\omega_1 t_2) + I_{1y} S(\omega_1 t_2) \right]$$

$$I_{1x} : \left(\frac{1}{4}\right) S^{2}_{J12} S^{2}_{J13} C^{2}_{\omega_1} : \left(- S^{1}_{J12} S^{1}_{J13} S^{1}_{\omega_1} \right)$$

$$I_{1y} : \left(\frac{1}{4}\right) S^{2}_{J12} S^{2}_{J13} S^{2}_{\omega_1} : \left(- S^{1}_{J12} S^{1}_{J13} S^{1}_{\omega_1} \right)$$

Diag ω_{11}

⑫ Summary

I_{1x}: $\left(\frac{1}{4}\right) S_{J12}^1 S_{J13}^1 S_{w1}^1 : S_{J12}^2 S_{J13}^2 C_{w1}^2$ DIAG (w_1^1, w_1^2)

I_{1y}: $\left(\frac{1}{4}\right) S_{J12}^1 S_{J13}^1 S_{w1}^1 : S_{J12}^2 S_{J13}^2 S_{w1}^2$

I_{1x}: $\left(\frac{1}{4}\right) S_{J12}^1 S_{J13}^1 S_{w1}^1 : S_{J12}^2 S_{J23}^2 S_{w2}^2$ XPK (w_1^1, w_2^2)

I_{1y}; $\left(\frac{1}{4}\right) S_{J12}^1 S_{J13}^1 S_{w1}^1 : S_{J12}^2 S_{J23}^2 C_{w2}^2$

I_{1x}: $\left(\frac{1}{4}\right) S_{J12}^1 S_{J13}^1 S_{w1}^1 \; S_{J13}^2 S_{J23}^2 S_{w3}^2$ XPK $(w_1^1 w_3^2)$

I_{1y}: $\left(\frac{1}{4}\right) S_{J12}^1 S_{J13}^1 S_{w1}^1 \; S_{J13}^2 S_{J23}^2 C_{w3}^2$

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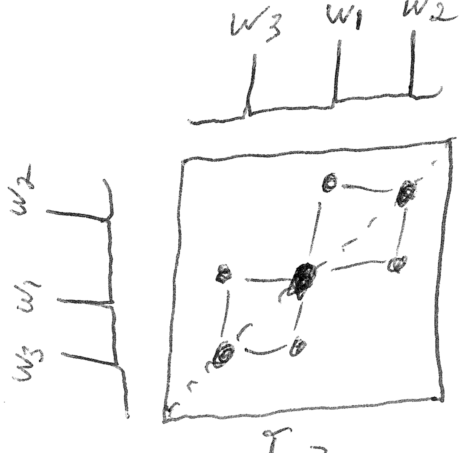
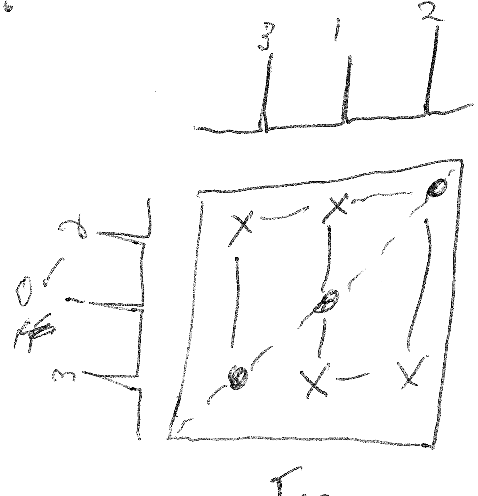
* This is just I_{1z}. Need I_{2z} & I_{3z} as well



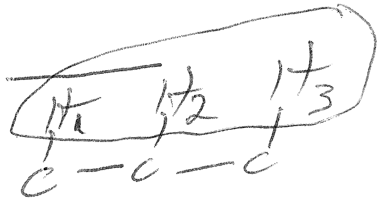
I_1z

w-out J



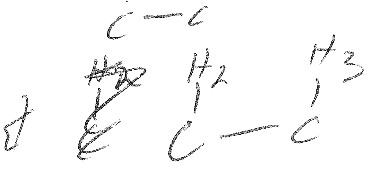
I_{2z}

& I_{3z}



* all seen at once.

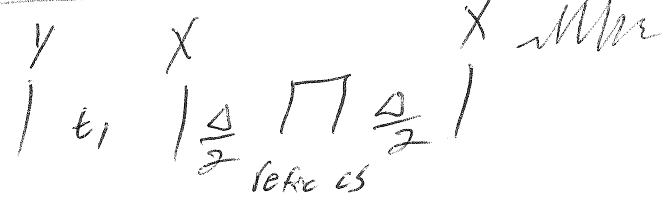
NOT

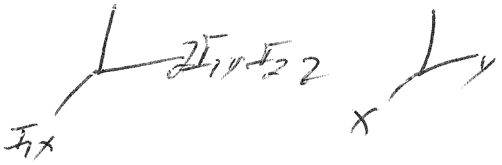


* Shows 3-spin connectivities via 3 J

II-14) relayed cosy I_{1z} I_{2z} I_{3z} $J_{12} = J_{23} \neq 0$

$J_{13} = 0$





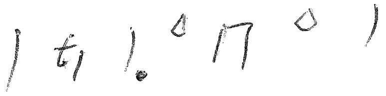
$I_{1z} \xrightarrow{H_r(y)} I_{1x} \xrightarrow{J_{12} I_{1z} I_{2z}} C'_{J12} I_{1x} + S'_{J12}\, 2I_{1y}I_{2z}$

$C'_{J12} I_{1x} \xrightarrow{J_{23} I_{2z} I_{3z}}$ X $J_{13} \rightarrow$ X

$+ S'_{J12}\, 2I_{1y}I_{2z} \longrightarrow$ X

$C'_{J12} I_{1x} \xrightarrow{H_{cs}} C'_{J12} (I_{1x} C'_1 + I_{1y} S'_1)$

$S'_{J12}\, 2I_{1y}I_{2z} \xrightarrow{H_{cs}\, t_1} S_{J12}\, 2I_{2z} (I_{1y} C'_1 - I_{1x} S'_1)$



$C'_{J12} C'_1 I_{1x} \xrightarrow{(\frac{\pi}{2})_x} I_{1x}$

$C'_{J12} S'_1 I_{1y} \longrightarrow I_{1z}$ (AOP) $\rightarrow$ (DIAG)

$S'_{J12} C'_1\, 2I_{1y}I_{2z} \longrightarrow 2\cancel{I_{1z}} I_{2x}$

$-S'_{J12} S_1\, 2I_{1x}I_{2z} \longrightarrow 2I_{1x}I_{2y}$ (MQ - 0, OUT)

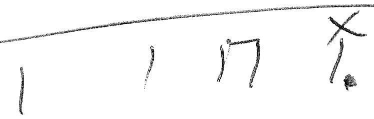
②

$I_{1x} \xrightarrow{J I_{1z} I_{2z} 2\Delta} I_{1x} C_{J12}^{\Delta} + 2 I_{1y} I_{2z} S_{J12}^{\Delta} \xrightarrow[CS]{J_{23}} X$

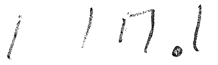
$2 I_{1z} I_{2x} \xrightarrow{J_{12} I_{1z} I_{2z}} 2 I_{1z} I_{2x} C_{J12}^{\Delta} - I_{2y} S_{J12}^{\Delta}$

$C_{J12}^{\Delta}\ 2 I_{1z} I_{2x} \xrightarrow{J_{23} I_{2z} I_{3z} \Delta} C_{J12}^{\Delta} \left(2 I_{1z} I_{2x} C_{J23}^{\Delta} - S_{J23}^{\Delta} I_{3y} \right)$

$- S_{J12}^{\Delta} I_{2y} \xrightarrow{J_{23}} - S_{J12}^{\Delta} \left(I_{2y} C_{J23}^{\Delta} - 2 I_{2z} I_{3x} S_{J23}^{\Delta} \right)$



collect: Δ



$C_{J12}^{\Delta} I_{1x}$

$-S_{J12}^{\Delta} I_{2y}$

$C_{J12}^{\Delta} C_{J23}^{\Delta}\ 2 I_{1z} I_{2x}$ $(2 I_{1z} I_{2x})$

$-C_{J12}^{\Delta} S_{J23}^{\Delta} I_{3y}$ (I_{3y})

$-S_{J12}^{\Delta} C_{J23}^{\Delta} I_{2y}$

$S_{J12}^{\Delta} S_{J23}^{\Delta}\ 2 I_{2z} I_{3x}$

~~$C_{J12} I_{1x}$~~

~~$-S_{J12} I_{2z}$~~

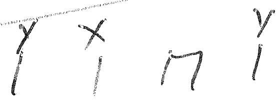
~~$C_{J12}^{\Delta} C_{J23}^{\Delta}\ 2 I_{1y} I_{2x}$~~

~~$-S_{J12}^{\Delta} S_{J23}^{\Delta}\ I_{2z}$~~

~~I_{2z}~~

~~$2 I_{1y} I_{3x}$~~

$\left(\frac{y}{2}\right)_x$ - not right



$I_{1x} \xrightarrow{y} I_{1z}$

$I_{2y} \rightarrow I_{2y}$

$2 I_{1z} I_{2x} \xrightarrow{y} 2 I_{1x} I_{3z}$

$I_{3y} \longrightarrow I_{3y}$

$I_{2y} \longrightarrow I_{2y}$

$2 I_{2z} I_{3x} \rightarrow 2 I_{2x} I_{3z}$

③ $\overset{y}{|}$ $\overset{x}{|}$ M $\overset{y}{|}_{\circ}$ remember $J_{13} = 0$

I_{1z} pop } from I_{1y} I_1 I_{1z} here is stored.

I_{2y}

from I_zI_x

$2 I_{1x} I_{2z}$

I_{3y}

I_{2y}

$2 I_{2x} I_{3z}$

$| \quad | \quad M \quad |_{\circ}$

$S^{1}_{J12}\, C^{1}_{1}\, C^{\Delta}_{J12}\, S^{\Delta}_{J23} : I_{3y}$ (IP obs t2)

$S^{1}_{J12}\, C^{1}_{1}\, S^{0}_{J12}\, C^{\Delta}_{J23} : I_{2y}$ (survives) XPK ($\omega_1 - \omega_2$)

~~$S^{1}_{J12}\, C^{1}_{1}\, C^{\Delta}_{J12}$ I_{1x}~~

$S^{1}_{J12}\, C_{1}^{1}\, C^{\Delta}_{J12}\, C^{\Delta}_{J23} : 2 I_{1z} I_{2x}$ (stays AP t_2)

$S^{1}_{J12}\, C^{1}_{1}\, S^{\Delta}_{J12}\, S^{\Delta}_{J23} : 2 I_{2z} I_{3x}$ (~~stays AP in t_2~~) (evolves into obs in t2)

~~$2 I_{2z} I_{3x} \xrightarrow{J_{12}} \times$~~

~~$\xrightarrow{J_{23}} \times$~~

~~$\xrightarrow{J_{13} = 0} \times$~~

~~$2 I_{1z} I_{3x} \xrightarrow{H_{CS}} 2 I_{1z} (I_{3x}^{c} + I_{3}^{s})$ but AP~~

$2 I_{1z} I_{2x} \xrightarrow{J_{12}} 2 I_{1z} I_{2x}\, C^{2}_{J12} + I_{2y}\, S^{2}_{J12}$

$C^{2}_{J12}\, 2 I_{1z} I_{2x} \xrightarrow{J_{23}} 2 I_{1z} (I_{2x}\, C^{2}_{J23} + 2 I_{2y} I_{3z}\, S^{2}_{J23})$ AP AP AP

④ $I_{2y} \xrightarrow{J_{12}\; t_2} I_{2y}\, C_{J12}^{2} - 2 I_{1z} I_{2x}\, S_{J12}^{2}$

$C_{J12}^{2}\, I_{2y} \xrightarrow{J_{23}} C_{J12}^{2} \left(I_{2y}\, C_{J23}^{2} - 2 I_{2x} I_{3z} S_{J23}^{2} \right)$

$- S_{J12}^{2}\, 2 I_{1z} I_{2x} \xrightarrow{J_{23}} S_{J12}^{2}\, 2 I_{1z} \left[I_{2x}\, C_{J23}^{2} - 2 I_{2y} I_{3z}\, S_{J23}^{2} \right)$

$C_{J12}^{2}\, C_{J23}^{2}\, I_{2y} \xrightarrow{H_{cs}} \boxed{C_{J12}^{2}\, C_{J23}^{2} \left[I_{2y}\, C_{2}^{2} - I_{2x}\, S_{2}^{2} \right)}$ — obs

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$I_{2y} : \rightarrow \quad S_{J12}^{1}\, C_1^{1}\, S_{J12}^{\Delta}\, C_{J23}^{\Delta} : C_{J12}^{2}\, C_{J23}^{2}\, C_{2}^{2}\, I_{2y}$ $\quad \omega_1 - \omega_2$

$\quad S_{J12}^{1}\, C_1^{1}\, S_{J12}^{\Delta}\, C_{J23}^{\Delta} : C_{J12}^{2}\, C_{J23}^{2}\, S_{2}^{2}\, I_{2x}$ $\quad$ XAK

$I_{3y} \xrightarrow{J_{12}} X \quad \xrightarrow{J_{23}} I_{3y}\, C_{J23}^{2} - 2 \overset{\nearrow AP}{I_{2z} I_{3x}}\, S_{J23}^{2}$

$\quad \xrightarrow{J_{13}} X$

$C_{J23}^{2}\, I_{3y} \xrightarrow{H_{cs}} C_{J23}^{2} \left[I_{3y}\, C_{3}^{2} - I_{3x}\, S_{3}^{2} \right)$ $\quad$ obs ✓ $(\omega_1 - \omega_3$

$I_{3y} \rightarrow \quad S_{J12}^{1}\, C_1^{1}\, C_{J12}^{\Delta}\, S_{J23}^{\Delta} : C_{J23}^{2}\, C_{3}^{2}\, I_{3y}$

$\quad S_{J12}^{1}\, C_1^{1}\, C_{J12}^{\Delta}\, S_{J23}^{\Delta} : C_{J23}^{2}\, S_{3}^{2}\, I_{3x}$ $\quad \rangle \quad \boxed{\begin{array}{c} \omega_1 - \omega_3 \\ \text{XAK} \end{array}}$

⑤ 1 1 Π 6

$$C^{1}_{J12}\, S^{1}_{1}\, I_{1Z} \xrightarrow{\overset{y}{|}} I_{1X}$$

(was stored in play)

$$I_{1X} \xrightarrow{J_{12}} \boxed{I_{1X}\, C^{2}_{J12}} + 2\, I_{1Y} I_{2Z}\, S^{2}_{J12}$$

$$I_{1X}\, C_{J12} \xrightarrow{J_{23}} C_{J12}\, [I_{1X}] \quad X$$

$$S_{J12}\, 2 I_{1Y} I_{2Z} \xrightarrow{J_{23}} S_{J12}\, 2\, I_{1Y} I_{2Z} \quad X$$

$$C^{2}_{J12}\, I_{1X} \xrightarrow{H_{CS}} C^{2}_{J12}\, [I_{1X}\, C^{2}_{1} + I_{1Y}\, S^{2}_{1}]$$

DIAG: $\quad C^{1}_{J12}\, S^{1}_{1}\, C^{2}_{J12}\, C^{2}_{1} : I_{1X}$ $\qquad (\omega_1 - \omega_1)$ Diag

From I_{1Z} $\quad C^{1}_{J12}\, S^{1}_{1}\, C^{2}_{J12}\, S^{2}_{1} : I_{1Y}$

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⑥ 11 M 1.

$$2I_{2z}I_{3x} \xrightarrow{J_{12}} X$$

$$\xrightarrow{J_{23}} \overset{A}{\cancel{2I_{2z}I_{3x}}} C^2_{J23} - I_{3y} S^2_{J23}$$

$$S^2_{J23} I_{3y} \xrightarrow{H_{CS}} S^2_{J23}\left[I_{3y} C^2_{w_3} - I_{3x} S^2_3\right]$$

$$S^{\Delta}_{J12} S^{\Delta}_{J23}\; S^1_{J12} C^1_1 : S^2_{J23} C^2_{w_3}\; I_{3y}$$

$$-S^{\Delta}_{J12} S^{\Delta}_{J22}\; S^1_{J12} C^1_1 ; S^2_{J23} S^2_3 ; I_{3x}$$

another XP~~K~~

$w_1 - w_3$

From AP evolves to observable w/ t_2

Summary

DIAG: $C^1_{J12} S^1_1 C^2_{J12} C^2_1 : I_{1x}$

$C^1_{J12} S^1_1 C^2_{J12} S^2_1 ; I_{1y}$

XPK w_1, w_2

$S^1_{J12} C^1_1 S^{\Delta}_{J12} C^{\Delta}_{J23} : C^2_{J12} C^2_{J23} C^2_2 : I_{2y}$

$S^1_{J12} C^1_1 S^{\Delta}_{J12} C^{\Delta}_{J23} : C^2_{J12} C^2_{J23} S^2_2 : I_{2x}$

XPK w_1, w_3 From IP

$S^1_{J12} C^1_1 C^{\Delta}_{J12} S^{\Delta}_{J23} ; C^2_{J23} C^2_3 : I_{3y}$

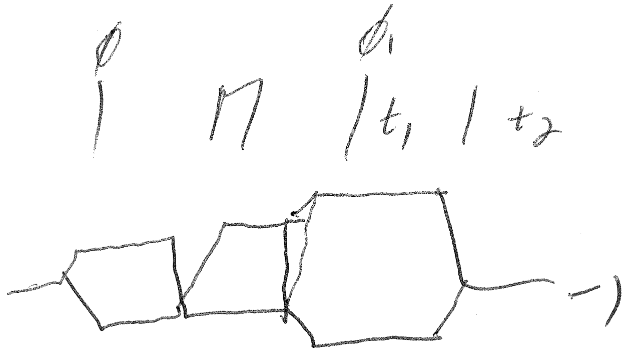
$S^1_{J12} C^1_1 C^{\Delta}_{J12} S^{\Delta}_{J23} : C^2_{J23} S^2_3 : I_{3x}$

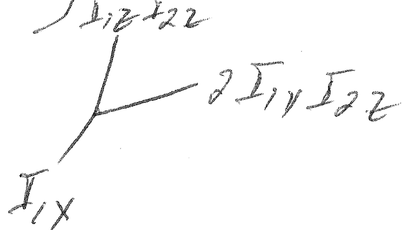
XPK w_1, w_3 From AP

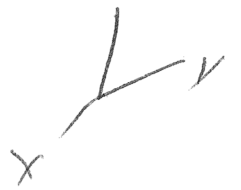
$S^1_{J12} C^1_1 S^{\Delta}_{J12} S^{\Delta}_{J23} : S^2_{J23} C^2_3 : I_{3y}$

$S^1_{J12} C^1_1 S^{\Delta}_{J12} S^{\Delta}_{J23} : S^2_{J23} S^2_3 : I_{3x}$

II-15) $J_{1z} + I_{2z} \longrightarrow I_{1x} + I_{2x}$







2D-inadequate

$I_{1\cancel{x}} \xrightarrow{J_{12}} I_{1x} C_{J_{12}}^{1} + 2 I_{1y} I_{2z} S_{J_{12}}^{1}$

| M .| |

$S_J^{\Delta} 2 I_{1y} I_{2z} \xrightarrow{\overset{y}{|}} 2 I_{1y} I_{2x}$

$I_+ = I_x + i I_y$

$I_- = I_x - i I_y$

$I_x = \frac{I_+ + I_-}{2} \quad I_y = \frac{i(I_- - I_+)}{2}$

$I_+ - I_- = 2 i I_y$

$\frac{I_+ - I_-}{2i} = I_y$

$\frac{i(I_- - I_+)}{2} = I_y$

~~$\frac{2}{4}\left[I_{1+} \left[(I_{1-} - I_{1+})(I_{2+} + i I_{2-}) i \right]\right.$~~

$2\left[i \left(\frac{I_{1-} - I_{1+}}{2}\right)\left(\frac{I_{2+} + I_{2-}}{2}\right)\right]$

$-\frac{i}{2}\left[(I_{1-} - I_{1+})(I_{2+} + I_{2-}) \right.$

$= \frac{i}{2}\left[I_{1-}(I_{2+} + I_{2-}) - I_{1+}(I_{2+} + I_{2-}) \right]$

$= \frac{i}{2}\left[I_{1-} I_{2+} + I_{1-} I_{2-} - I_{1+} I_{2+} - I_{1+} I_{2-} \right]$

$= \frac{i}{2}\left[\overset{DQC}{(I_{1-} I_{2-} - I_{1+} I_{2+})} + \overset{ZQC}{(I_{1-} I_{2+} - I_{1+} I_{2-})} \right.$

$= \frac{i}{2}(I_{1-} I_{2-} - I_{1+} I_{2+}) \rightarrow$ ϕ-IN

④ ~~$\frac{i}{2}$~~ $I_{1-}I_{2-} = (I_{1x} - iI_{1y})(I_{2x} - iI_{2y})$

$= I_{1x}(I_{2x} - iI_{2y}) - iI_{1y}(I_{2x} - iI_{2y})$

$= I_{1x}I_{2x} - iI_{1x}I_{2y} - iI_{1y}I_{2x} + i^2 I_{1y}I_{2y}$

$= I_{1x}I_{2x} - I_{1y}I_{2y} - i(I_{1x}I_{2y} + I_{1y}I_{2x})$

$I_{1+}I_{2+} = (I_{1x} + iI_{1y})(I_{2x} + iI_{2y})$

$= I_{1x}(I_{2x} + iI_{2y}) + iI_{1y}(I_{2x} + iI_{2y})$

$= I_{1x}I_{2x} + iI_{1x}I_{2y} + iI_{1y}I_{2x} - I_{1y}I_{2y}$

$= I_{1x}I_{2x} - I_{1y}I_{2y} + i(I_{1x}I_{2y} + I_{1y}I_{2x})$

$\frac{i}{2}(I_{1-}I_{2-} - I_{1+}I_{2+}) =$

$\frac{i}{2}[\ I_{1x}I_{2x} - I_{1y}I_{2y} - i(I_{1x}I_{2y} + I_{1y}I_{2x})$

$- (I_{1x}I_{2x} - I_{1y}I_{2y} + i(I_{1x}I_{2y} + I_{1y}I_{2x})$

[illegible]

$= \frac{i}{2}[\ -2i(I_{1x}I_{2y} + I_{1y}I_{2x})$

$= \boxed{I_{1x}I_{2y} + I_{1y}I_{2x} = \frac{i}{2}(I_{1-}I_{2-} - I_{1+}I_{2+})}$

③ 

$S_J^{\Delta} I_{1x} I_{2y} \xrightarrow[H_J]{t_1} X$ MQ - NO J-coup evol F $I_{1z}\ I_{2z}$

$S_J^{\Delta} I_{1x} I_{2y} \xrightarrow[t_1]{H_{CS}} S_J^{\Delta} \left(I_{1x} (\overset{A}{C\omega_1'}) + I_{1y} (\overset{B}{S\omega_1'}) \right) \left(I_{2y} \overset{C}{C\omega_2'} \cancel{+} - I_{2x} \overset{D}{S\omega_2'} \right)$

~~$= I_{1x} C\omega_1' (I_{2y} S\omega_2' - I_{2x} S\omega_2') + I_{1y} S\omega_1' ($~~

$= (I_{1x} A + I_{1y} B)(I_{2y} C - I_{2x} D)$

$= I_{1x} A (I_{2y} C - I_{2x} D) + I_{1y} B (I_{2y} C - I_{2x} D)$ $I_{1x} I_{2y}$ Part ↙

$= AC\, I_{1x} I_{2y} - AD\, I_{1x} I_{2x} + BC\, I_{1y} I_{2y} - BD\, I_{1y} I_{2x}$

$I_{1y} I_{2x} \xrightarrow[t_1]{H_{CS}} (I_{1y} \overset{A}{C_1'} - I_{1x} \overset{B}{S_1'})(I_{2x} \overset{C}{C_2'} + I_{2y} \overset{D}{S_2'})$

$I_{2x} I_{1y}$ Part

$= I_{1y} A (I_{2x} C + I_{2y} D) - I_{1x} B (I_{2x} C + I_{2y} D)$

$= AC\, I_{1y} I_{2x} + AD\, I_{1y} I_{2y} - BC\, I_{1x} I_{2x} - BD\, I_{1x} I_{2y}$

NOW ADD $I_{1x} I_{2y} + I_{1y} I_{2x} =$

$AC\, I_{1x} I_{2y} - AD\, I_{1x} I_{2x} + BC\, I_{1y} I_{2y} - BD\, I_{1y} I_{2x}$

$+ \quad AC\, I_{1y} I_{2x} + AD\, I_{1y} I_{2y} - BC\, I_{1x} I_{2x} - BD\, I_{1x} I_{2y}$

$\cancel{=}$

④ ~~A~~ $AC = c_1' c_2' = [c(w_1 + w_2) + c(w_1 - w_2)] / 2$

$AD = c_1' s_2' = [s(w_1 + w_2) + s(w_1 - w_2)] / 2$

$BC = s_1' c_2' = [s(w_1 + w_2) + s(w_1 - w_2)] / 2$

$BD = s_1' s_2' = [c(w_1 - w_2) - c(w_1 + w_2)] / 2$

$AC [I_{1x} I_{2y} + I_{1y} I_{2x}) \xrightarrow{90x} I_{1x} I_{2z} + I_{2z} I_{2x}$

$AD [I_{1y} I_{2y} - I_{1x} I_{2x}] \longrightarrow I_{1z} I_{2z} - I_{1x} I_{2x}$ (NOP & MQ)

$BC [I_{1y} I_{2y} - I_{1x} I_{2x}] \longrightarrow I_{1z} I_{2z} - I_{1x} I_{2x}$ (NOP & MQ)

$BD [- I_{1y} I_{2x} - I_{1x} I_{2y}] \longrightarrow - I_{1z} I_{2x} - I_{1x} I_{2z}$

$| M | t_1$.

survives

$\Rightarrow AC [I_{1x} I_{2z} + I_{1z} I_{2x}]$

$- BD [I_{1z} I_{2x} + I_{1x} I_{2z}]$

$= AC\, I_{1x} I_{2z} + AC\, I_{1z} I_{2x} - BD\, I_{1z} I_{2x} - BD\, I_{1x} I_{2z}$

$= I_{1x} I_{2z} [AC - BD] + I_{1z} I_{2x} [AC - BD]$

$AC - BD = [c(w_1 + w_2) + c(w_1 - w_2)] / 2$

$- [c(w_1 - w_2) - c(w_1 + w_2)] / 2$

$= c(w_1 + w_2) t_1$

⑤ 1 Π 1 1.

collect

$$\frac{S_J^\Delta}{2} c[(\omega_1+\omega_2)t_1]\left[I_{1x}I_{2z} + I_{1z}I_{2x}\right]$$

$$I_{1x}I_{2z} \xrightarrow[t_2]{H_J} \frac{1}{2}[2I_{1x}I_{2z}] \xrightarrow[t_2]{H_J} \frac{1}{2}\left[\overset{MA}{\cancel{2I_{1x}I_{2z}}}C_J^2 + I_{1y}S_J^2\right]$$

(Diag)

$$\frac{1}{2} I_{1y} S_J^2 \xrightarrow[t_2]{H_{cs}} \frac{1}{2} S_J^2 \left[I_{1y}C_1^2 - I_{1x}S_1^2\right]$$

$$I_{1z}I_{2x} \xrightarrow{H_J^2} \frac{1}{2}\left[\overset{MA}{\cancel{2I_{1z}I_{2x}}}C_J^2 + I_{2y}S_J^2\right)$$

$$\frac{S_J^2}{2} I_{2y} \xrightarrow[t_2]{H_{cs}} \frac{S_J^2}{2}\left[I_{2y}C_2^2 - I_{2x}S_2^2\right]$$

$$\boxed{1 \frac{\Delta}{2}\, \Pi\, \frac{\Delta}{2}\, 1\, t_1\, 1\, t_2}$$

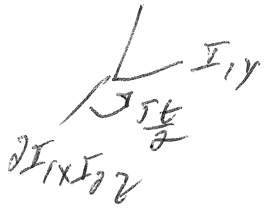
collect

$$\frac{S_J^\Delta}{2} c[(\omega_1+\omega_2)t_1] \cdot \frac{S_J^2}{2}\, \begin{matrix} C_1^2 \; I_{1y} \\ S_1^2 \; I_{1x} \end{matrix}$$

$$\begin{tikzcd}
\frac{1}{4} S_J^\Delta C^1_{(1+2)} S_J^2 C_1^2 : I_{1y} \arrow[d, leftrightarrow] \\
-\frac{1}{4} S_J^\Delta C^1_{(1+2)} S_J^2 S_1^2 : I_{1x}
\end{tikzcd}
\qquad
\begin{tikzcd}
\frac{1}{4} S_J^\Delta C^1_{(1+2)} S_J^2 C_2^2 : I_{2y} \arrow[d, leftrightarrow] \\
-\frac{1}{4} S_J^\Delta C^1_{(1+2)} S_J^2 S_2^2 : I_{2x}
\end{tikzcd}$$

⑥

$S(\frac{Jt}{2}) = S(\frac{J\Delta}{2})$

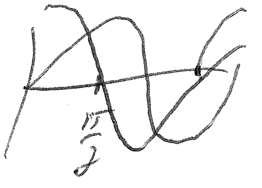


$\boxed{\frac{J}{2}\cdot\Delta}$

$\Delta = \frac{1}{2J} \Rightarrow \frac{J}{2}\cdot\frac{1}{2J} = \frac{1}{4}$

$C(\frac{2\pi}{4}) = 0$

$S(\frac{2\pi}{4}) = 1$



$| \frac{\delta}{2}\ \Pi\ \frac{1}{4J_{cc}} | t_1 | t_2$

Let $S_J^\Delta = 1$ $\Delta = \frac{1}{2J_{cc}}$

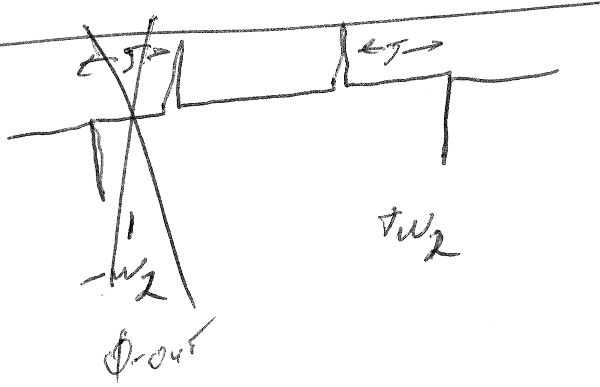
$C_{1+2}^1 S_J^2 C_1^2 : I_{1y}$

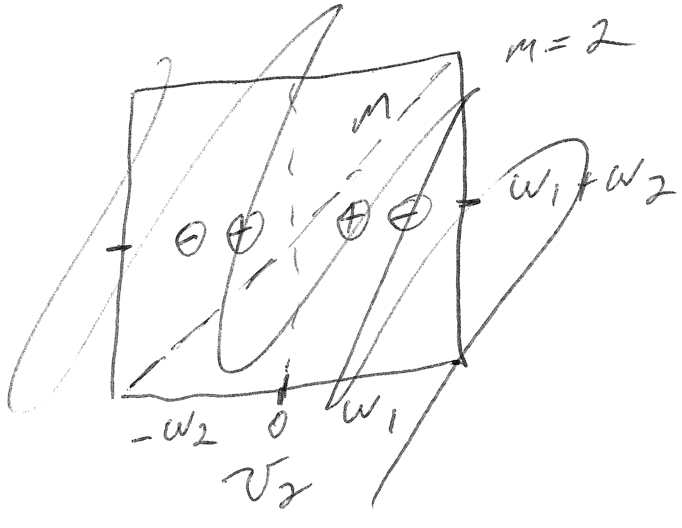
$- C_{1+2}^1 S_J^2 S_1^2 : I_{1x}$

$C_{1+2}^1 S_J^2 C_2^2 : I_{2y}$ II

$- C_{1+2}^1 S_J^2 S_2^2 : I_{2x}$ R

$S(\omega_2 t_2) S(\frac{J t_2}{2}) \xrightarrow{FT}$





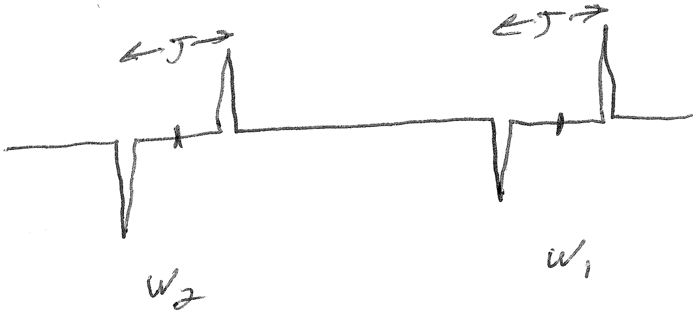
⑦ I) $C^{1}_{(1+2)} S^{2}_{J} C^{2}_{1}$ I_{1y} $C^{1}_{(1+2)} S^{2}_{J} C^{2}_{2}$: I_{2y}

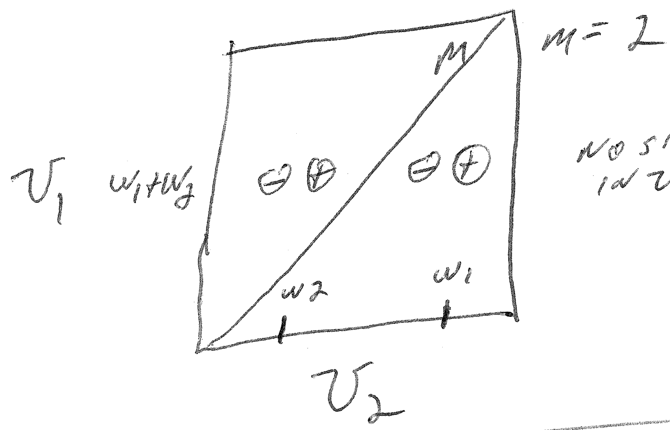
R) $C^{1}_{(1+2)} S^{2}_{J} S^{2}_{1}$ I_{1x} $C_{(1+2)} S^{2}_{J} S^{2}_{2}$: I_{2x}

Plugged This in SIM ↙

& ~~I_{2x}~~

IN $V_2 \Longrightarrow$





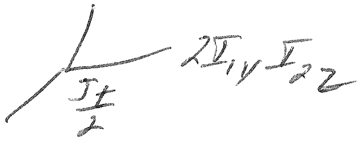
NO SHIFT IN V_1

$^{13}C_1 - {}^{13}C_2$

(w_1) (w_2)

$S/N = \frac{1}{10{,}000}$ Normal 1D ^{13}C

II-15) ii) optimum Δ for inad

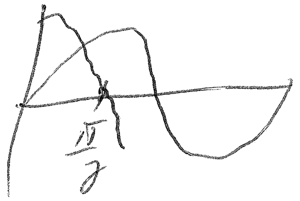


S_J^{Δ} $\quad | \frac{\Delta}{2} \Pi \frac{\Delta}{2} |$

$\sin\left(\frac{Jt}{2}\right) \Rightarrow \sin\left(\frac{J\Delta}{2}\right)$ $\quad \frac{J}{2} \cdot \Delta \quad \Delta = \frac{1}{2J} \Rightarrow \frac{J}{2} \cdot \frac{1}{2J} = \frac{1}{4}$

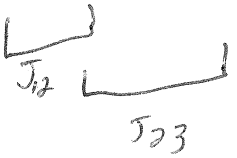
$\boxed{\sin\left(\frac{2\pi}{4}\right) = 1}$ $\quad c(\pi/2) = 0$

$\Delta = \frac{1}{2J_{cc}}$



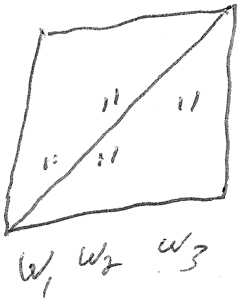
$\omega_1 \neq \omega_2 \neq \omega_3$

iii) $\overset{\omega_1}{I_1} - \overset{\omega_2}{I_2} - \overset{\omega_3}{I_3}$

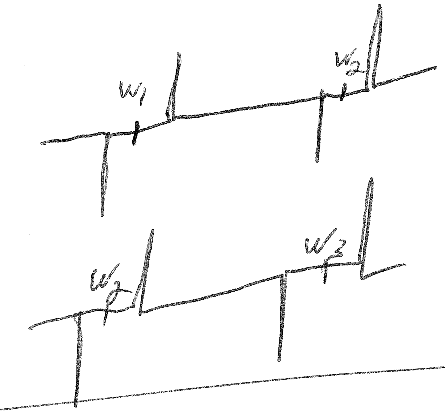


$J_{13} = 0$

$J_{12} = J_{23}$



lineshapes



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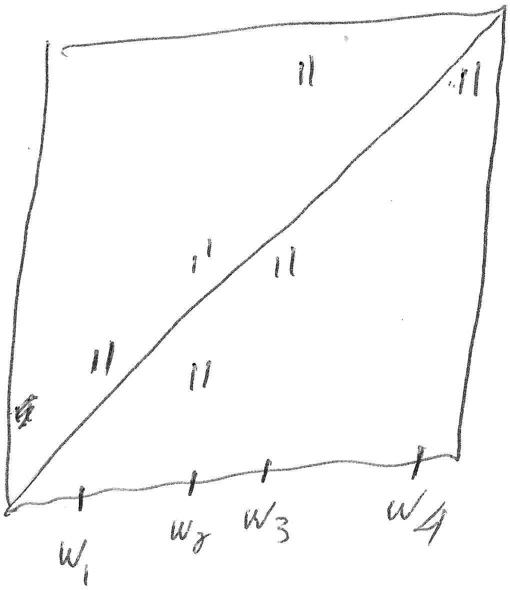
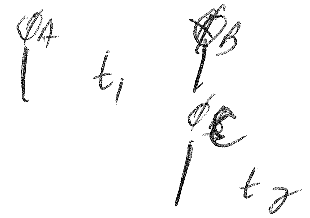
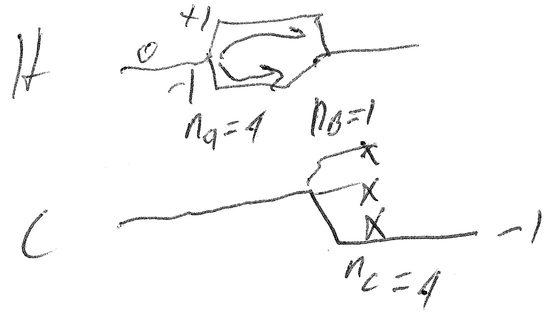
iv) $C_1 - C_2 - C_3 - C_3$



VI-17)
e)





$$n = n_a \cdot n_B \cdot n_C$$
$$= 4 * 1 * 4$$

$$\phi_A = \frac{2\pi}{n_a} \cdot m = \frac{\pi}{2} \cdot m$$

$$\phi_B = 0$$

$$\phi_C = \frac{2\pi}{n_C} \cdot fl\left(\frac{m}{n_a}\right)$$
$$= \frac{\pi}{2} fl\left(\frac{m}{4}\right)$$

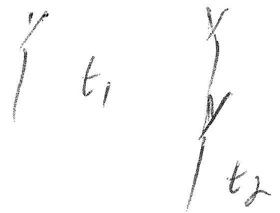
m	ϕ_A	ϕ_B	ϕ_C	ϕ_{Rx}	Echo ϕ_{DIG}	AF ϕ_{DIG}
0	0	0	0	0	0	0
1	1	0	0	0	3	1
2	2	0	0	0	2	2
3	3	0	0	0	1	3
4	0	0	1	0	1	1
5	1	0	1	0	0	2
6	2	0	1	0	3	3
7	3	0	1	0	2	0
8	0	0	2	0	2	2
9	1	0	2	0	1	3
10	2	0	2	0	0	0
11	3	0	2	0	3	1
12	0	0	3	0	3	3
13	1	0	3	0	2	0
14	2	0	3	0	1	1
15	3	0	3	0	0	2

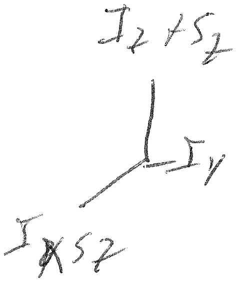
32 exPtS
t_1-Quad
& ABSORPTION
LS

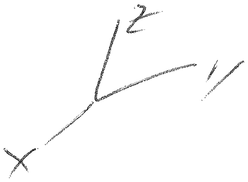
$\phi_{path,echo} = \phi_A - \phi_C + \phi_{Dig}$ ∴ $\phi_{Dig} = -\phi_A + \phi_C$

$\phi_{path,AF} = -\phi_A - \phi_C + \phi_{Dig}$ $\phi_{Dig} = \phi_A + \phi_C$

IV-17)
ii)





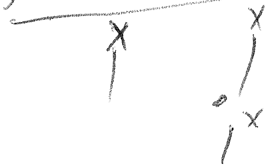


5

$I_z + S_z \xrightarrow{90 I_x} I_x \xrightarrow[I_z S_z t_1]{H_J} I_x C_J^1 + 2 I_y S_z S_J^1$

$I_x C_J^1 \xrightarrow{H_{CS}} (I_x C_{\omega I}^1 + I_y S_{\omega I}^1) C_J^1$

$S_J^1 2 I_y S_z \xrightarrow{H_{CS}} 2 S_z (I_y C_{\omega I}^1 - I_x S_{\omega I}^1) S_J^1$



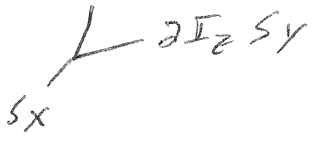
$\cancel{C_J^1 I_x}$
$\cancel{S_J^1 I_y S_z}$

$C_J^1 C_{\omega I}^1 I_x \xrightarrow{\cancel{H_R} I,S} I_x$ (evolves as ω_I) Φ-out

$C_J^1 S_{\omega I}^1 I_y \longrightarrow I_z$ PoP Φ-out

$S_J^1 C_{\omega I}^1 2 I_y S_z \longrightarrow 2 I_z S_y$ AP (keep)

$- S_J^1 S_{\omega I}^1 2 I_x S_z \longrightarrow 2 I_x S_y$ MQ - Φout



$S_J^1 C_{\omega I}^1 2 I_z S_y \xrightarrow[t_2]{H_J} \cancel{2 I_z S_y S_J^2 - S_y}$

AP

$2 I_z S_y C_J^2 - S_y S_J^2$

$\cancel{-I_y S_J^2 \xrightarrow{H_c}}$ $\quad - S_y S_J^2 \xrightarrow[t_2]{H_{CS}} -S_J^2 [S_y C_{\omega S}^2 - S_x S_{\omega S}^2]$

② collect

t_1

$S_J^1 C_{\omega I}^1 \; 2I_yS_z$

t_2

$-S_J^2 C_{\omega S}^2 S_y$ I

$+S_J^2 S_{\omega S}^2 S_x$ R

$2I_yS_z$ $\quad I_+ = I_x + iI_y$;; $I_y = \frac{i(I_- - I_+)}{2}$

$I_- = I_x - iI_y$

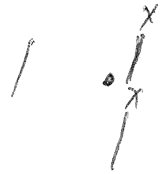
$\frac{2i}{2}(I_-S_z - I_+S_z)$ ← need to Ph-cycle for I_+ & I_- separately

---

echo: t_1

$-i(I_+S_z) = -i(I_x + iI_y)S_z$

$(-iI_x - i^2I_y)S_z = -iI_xS_z + I_yS_z$



$-iI_xS_z \xrightarrow{H_r} -iI_xS_y$

$I_yS_z \xrightarrow{H_r} \boxed{I_zS_y}$

∴ $\frac{1}{2}[2I_zS_y] \xrightarrow[H_{cs}]{H_J}$

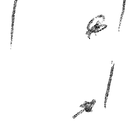
$\frac{1}{2}$ sig now ↗

AE: t_1

$\frac{2i}{2}I_-S_z = i((I_x - iI_y)S_z) = i$ ~~$I_xS_z + I_x$~~

$= i(I_xS_z - iI_yS_z) = iI_xS_z + I_yS_z$

$iI_xS_z \xrightarrow{H_r} I_xS_y$ MQ



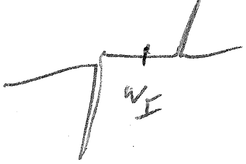
$\xrightarrow{H_r}$ $I_yS_z \rightarrow I_zS_y \xrightarrow[H_{cs}]{H_J}$ IP sig

③

t_1

$S_J^1 C_{WI}^1 : 2I_yS_z$

AP- Doublet

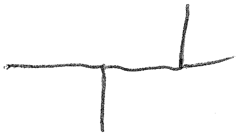


~~Still~~ No Diag now but WI, WS instead

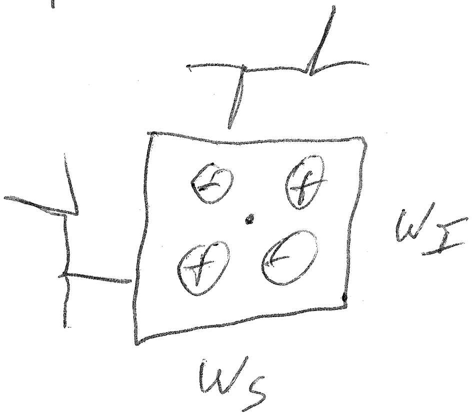
t_2

$S_J^2 S_{WS}^2 : S_x$

$-S_J^2 C_{WS}^2 : S_y$

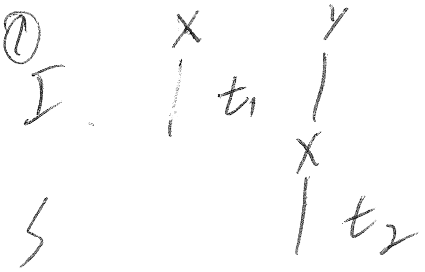


AP two

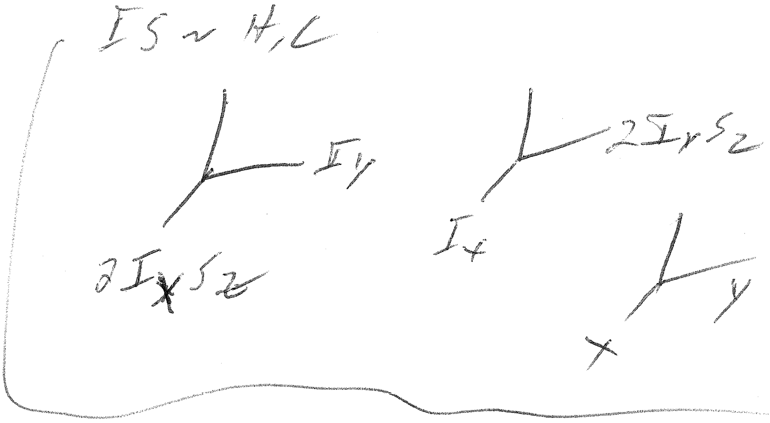


~~actually sim~~

①



$\boxed{H,C-COSY}$



Rot

$I_z \xrightarrow{H_r} -I_y$

CS

$-I_y \xrightarrow{H_{cs}} -\left[I_y c(w_1t) - I_x s(w_1t)\right.$

$= -I_y c(w_1t) + I_x s(w_1t)$

J-coup

$-c(w_1t)I_y \rightarrow -c(w_1t)\left[I_y c(\frac{Jt_1}{2}) + 2I_xS_z s(\frac{Jt_1}{2})\right.$

$-c(w_1t)I_y \xrightarrow{H_J} = -c(w_1t)c(\frac{Jt_1}{2})I_y + c(w_1t)s(\frac{Jt_1}{2})2I_xS_z$

$I_x s(w_1t) \xrightarrow{H_J} s(w_1t)\left[I_x c(\frac{Jt_1}{2}) + 2I_yS_z s(\frac{Jt_1}{2})\right.$

$= s(w_1t)c(\frac{Jt_1}{2})I_x + s(w_1t)s(\frac{Jt_1}{2})2I_yS_z$

---

collect terms & pulse

$-c(w_1t)c(\frac{Jt_1}{2})I_y \xrightarrow{(\frac{\pi}{2})_{y,I,S}} I_y$ (Precessed @ w_1 during t_2; ignore)

$c(w_1t)s(\frac{Jt_1}{2})2I_xS_z \longrightarrow -2I_zS_x$ [*use this, evolves into observable)

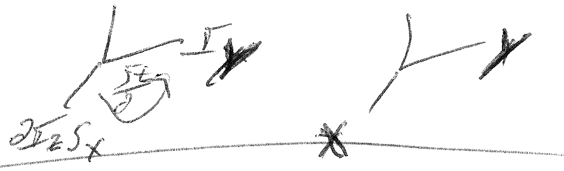
$s(w_1t)c(\frac{Jt_1}{2})I_x \longrightarrow -I_z$ (Population)

$s(w_1t)s(\frac{Jt_1}{2})2I_yS_z \longrightarrow 2I_xS_x$ (singlet + DQC)

also 2-spin DQC - NO H_J evol.!

② $\underbrace{\left[c(w_1t_1)s\left(\frac{Jt_1}{2}\right)\right]}_{A}2I_zS_x$

$[H_J, H_{cs}]=0$



$A\,2I_zS_x \xrightarrow{H_J} A\left[c\left(\frac{Jt_2}{2}\right)2I_zS_x + s\left(\frac{Jt_2}{2}\right)S_y\right]$

$A\,c\left(\frac{Jt_2}{2}\right)2I_zS_x \xrightarrow{H_{cs}} A\,c\left(\frac{Jt_2}{2}\right)2I_z\left[S_x\,c(w_2t_2)+S_y\,s(w_2t_2)\right]$

$=$ all AP! $\rho(\cdot I^+)=0$

$A\,s\left(\frac{Jt_2}{2}\right)\left[S_y\,s(w_2t_2)-S_x\,c(w_2t_2)\right]) = \rho$

$= A\,s\left(\frac{Jt_2}{2}\right)s(w_2t_2)S_y = c(w_1t_1)s\left(\frac{Jt_1}{2}\right)s(w_2t_2)s\left(\frac{Jt_2}{2}\right)S_y$

$-A\,s\left(\frac{Jt_2}{2}\right)c(w_2t_2)S_x = \boxed{-c(w_1t_1)s\left(\frac{Jt_1}{2}\right)c(w_2t_2)s\left(\frac{Jt_2}{2}\right)S_x}$ — Keep & Detect

---

DETECT ON $_{1st}\,S(w_2)$

Was OK → e^{-iw_2t} ~~$= S_x\,c(w_2t_2) - i\,S_y\,s(w_2t_2)$~~

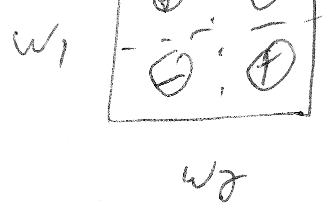
~~actually e^{-iw_2t} $c(w_1t_1$~~ $\rfloor$ ~~$s\left(\frac{Jt_1}{2}\right)s\left(\frac{Jt_2}{2}\right)$~~

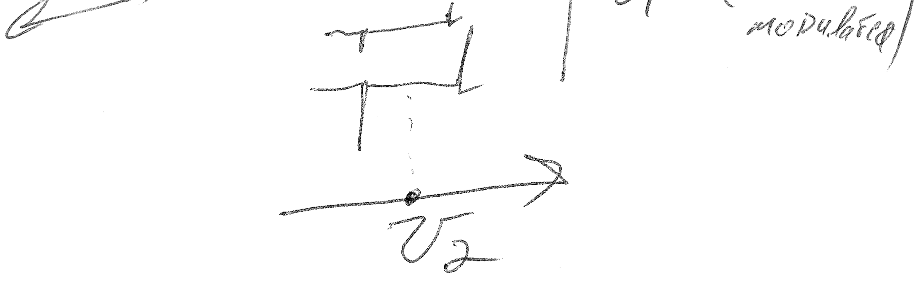
$s(t_2) \propto Tr(\rho\cdot I_{S^+}) = c(w_1t_1)s\left(\frac{Jt_1}{2}\right)s\left(\frac{Jt_2}{2}\right)e^{-iw_2t_2}$

$\Downarrow$ FT

throwout 1/2 sig bc no quaddetect.
coil along Sx ~~but~~ NOT Sy

a.p. Doublet centered @ w2

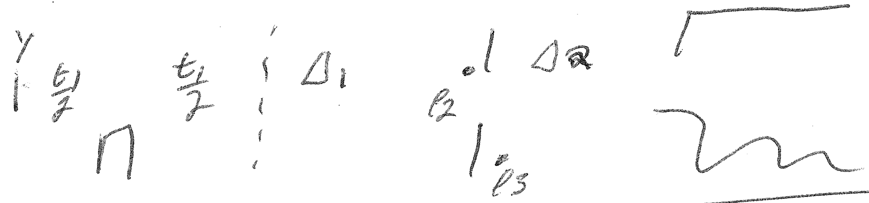




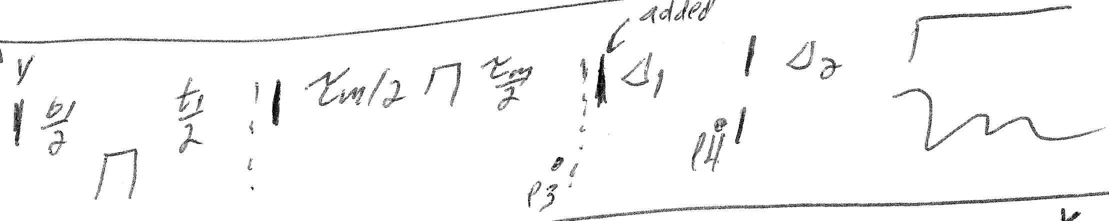
AP Doublets in each Dimension

Keep

V-18



INEPT-COS



relayed H,X-COSY

Relay H,H

1) explain how modified seq works

INEPT cosy; IS: $I_z + S_z \xrightarrow{90_x^I} I_x c_{\omega_I}^1 + I_y s_{\omega_I}^1$

$\Delta = \frac{1}{2J}$

$c_{\omega_I}^1 I_x \xrightarrow{J I_z S_z} I_x c_J^{\Delta 1} + 2 I_y S_z s_J^{\Delta}$

$2 I_y S_z \xrightarrow{cs} 2 S_z (I_y c_{\omega_I}^{\Delta 1} - I_x s_{\omega_I}^{\Delta 1})$

t_1

$I_x c_{\omega_I}^1$

$\rho_2 = 2 I_y S_z ; c_{\omega_I}^{\Delta 1} \cancel{c_{\omega_I}^1}$

$-2 I_x S_z ; s_{\omega_I}^{\Delta 1} \cancel{c_{\omega_I}^1}$

$\rho_3 \xrightarrow{90_x^I} 2 I_y S_z \xrightarrow{90_x^I} 2 I_z S_z \xrightarrow{90_x^S} -2 I_z S_{\cancel{x}y} c_{\omega_I}^{\Delta 1}$ keep

$+2 I_x S_y s_{\omega_I}^{\Delta 1}$ MQC ϕ-ou

$-2 I_x S_z \longrightarrow -2 I_x S_z \longrightarrow$

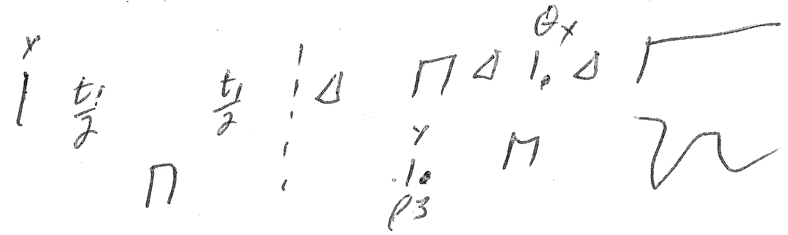
$-2 I_z S_y c_{\omega_I}^{\Delta 1} \xrightarrow{J I_z S_z} [-2 I_z S_y c_J^{\Delta 1} + S_x s_J^{\Delta 1}) c_{\omega_I}^{\Delta 1}$

$S_x c_{\omega_I}^{\Delta 1} \xrightarrow{c} [c_{\omega_S}^2 S_x + s_{\omega_S}^2 S_y) c_{\omega_I}^{\Delta 1} ; t_2$

$I_x c_{\omega_I}^1 ; t_1$

*has ω_I evol ω_I^{Δ} in t_2 that's hard to phase out

①



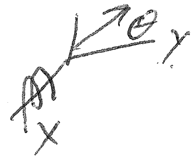
DePT-COSY

I S) $I_z \rightarrow I_x \xrightarrow{H_{cs}} I_x C\omega_I^1 + I_y S\omega_I^1$

$C\omega_I^1$) $I_x \xrightarrow{J I_z S_z} I_x C_J^\Delta + 2 I_y S_z S_J^\Delta$

$2 I_y S_z \xrightarrow{(\frac{\pi}{2})_y^S} 2 I_y S_x$ (P_3)

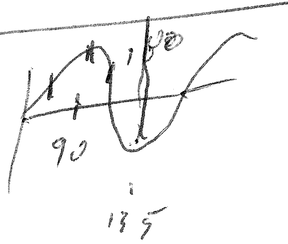
$2 I_y S_x \xrightarrow{J I_z S_z} y$ $2 I_y S_x$



$I_y C\theta + I_z S\theta)$

θ_x

$2(I_y C\theta + I_z S\theta) S_x$



θ	Sθ
45	$1/\sqrt{2}$
90	1
135	$1/\sqrt{2}$

$\theta = 90$ $2 I_z S_x \xrightarrow{J I_z S_z} 2 I_z S_x C_J^\Delta + S_y S_J^\Delta$

$S_y \xrightarrow{H_{cs}} S_y C\omega_S^2 - S_x S\omega_S^2$

$C\omega_I^1 : I_x$

ω_1

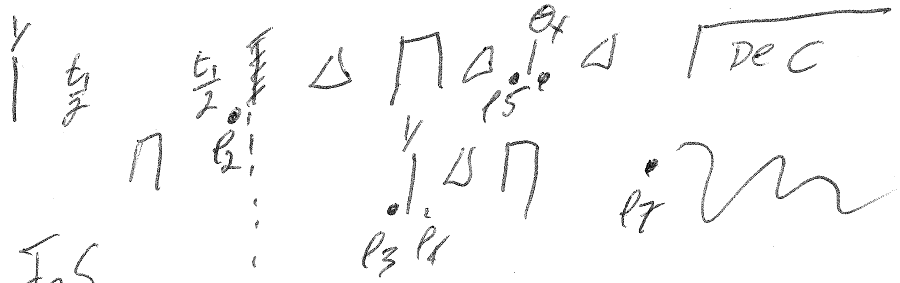
amp mod

$S_x : - S\omega_S^2$

$S_y : C\omega_S^2$

① DEPT-COSY

Keep



I_2S

I_2S; $I_{1z}+I_{2z} \xrightarrow{H_{R,Y}} I_{1x}+I_{2x} \xrightarrow{H_{CS}} (I_{1x}+I_{2x})C_{\omega_I}'$ ρ_2

$+ (I_{1y}+I_{2y})S_{\omega_I}'$

~~I~~

$I = I_{1z}+I_{2z}$

C_{ω_I}' | $I_{1x} \xrightarrow[\Delta]{J I_{2z} S_z} X \xrightarrow[\Delta]{J I_{1z} S_z} I_{1x} C_J^\Delta + 2 I_{1y} S_z S_J^\Delta$

$I_{2x} \xrightarrow{J I_{2z} S_z} I_{2x} C_J^\Delta + 2 I_{2y} S_z S_J^\Delta \xrightarrow[\Delta]{J I_{1z} S_z} X$

$I_{1y} \xrightarrow[\Delta]{J I_{1z} S_z} I_{1y} C_J^\Delta - 2 I_{1x} S_z S_J^\Delta$

$I_{2y} \xrightarrow[\Delta]{J I_{2z} S_z} I_{2y} C_J^\Delta - 2 I_{2x} S_z S_J^\Delta$

Collect:

ρ_3	$\xrightarrow{90S,y}$	ρ_4
$2I_{1y}S_z$		$2I_{1y}S_x$
$2I_{2y}S_z$		$2I_{2y}S_x$
$-2I_{1x}S_z$		$-2I_{1x}S_x$
$-2I_{2x}S_z$		$-2I_{2x}S_x$

---

②

$\boxed{C\omega^1_I}$ $2I_{1y}S_x \xrightarrow[\Delta]{JI_{1z}S_z} X \xrightarrow[\Delta]{JI_{2z}S_z} 2I_{1y}[S_xC^{\Delta}_{J} + 2I_{2z}S_{\cancel{y}}S^{\Delta}_{J}]$

$2I_{2y}S_x \xrightarrow{JI_{1z}S_z} 2\cdot I_{2y}[S_xC^{\Delta}_{J} + 2I_{1z}S_yS^{\Delta}_{J}] \xrightarrow{JI_{1z}S_z} X$

$-2I_{1x}S_x \xrightarrow{JI_{1z}S_z} Y \xrightarrow{JI_{2z}S_z} -2I_{1x}[S_xC^{\Delta}_{J} + 2I_{2z}S_yS^{\Delta}_{J}] \xrightarrow{JI_{2z}S_z} X$

$-2I_{2x}S_x \xrightarrow{JI_{1z}S_z} -2I_{2x}[S_xC^{\Delta}_{J} + 2I_{1z}S_yS^{\Delta}_{J}]$

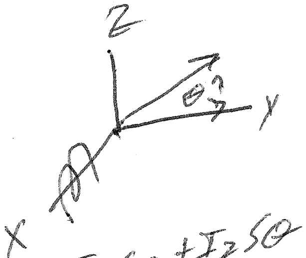
p5

$2\cancel{I_{1y}}$ $4I_{1y}I_{2z}S_{\cancel{y}}$

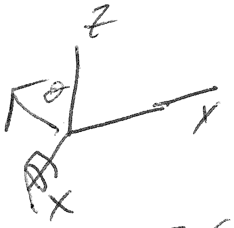
$4I_{1z}I_{2y}S_y$

$-4I_{1x}I_{2z}S_y$

$-4I_{1z}I_{2x}S_y$



$I_yC\theta + I_zS\theta$



$I_zC\theta - I_yS\theta$

---

p4 p6i

$4(I_{1y}C + I_{1z}S)(I_{2z}C - I_{2y}S)S_y$

$4[I_{1y}C(I_{2z}C - I_{2y}S) + I_{1z}S(I_{2z}C - I_{2y}S]S_y$

$4[I_{1y}I_{2z}C^2 - I_{1y}I_{2y}CS + \boxed{I_{1z}I_{2z}CS} - I_{1z}I_{2y}S^2]S_y$

all ma except

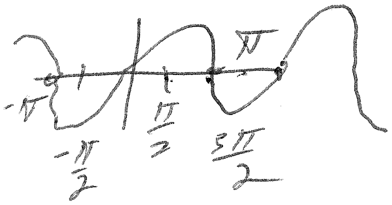
$C(\alpha)S(\beta) = \frac{S(\alpha+\beta)+S(\alpha-\beta)}{2}$

$4I_{1z}I_{2z}S_yCS = 4I_{1z}I_{2z}S_y\frac{S(2\theta)}{2}$

$= 2I_{1z}I_{2z}S_yS(2\theta)$

③ $2I_{1z}I_{2z}S_y\,S(2\theta)$

S(~~2θ~~ θ) ANGLE	S(2θ)
45	1
90	0
135	-1



$\boxed{\rho 6}$

45° $2I_{1z}I_{2z}S_y \xrightarrow{JI_{1z}S_z} \cancel{2}I_{2z}[2I_{1z}S_y C_J^0 - S_x S_J^1]$

$\boxed{C\omega_I^1}$

$-I_{2z}S_x \xrightarrow{JI_{2z}S_z} \left(-\frac{1}{2}\right)[2I_{2z}S_x C_J^0 + S_y S_J^1]$

$\rho 7 = -\frac{1}{2} S_y C\omega_I^1$

$-\frac{1}{2} C\omega_I^1 [S_y C\omega_S^2 - S_x S\omega_S^2]$

Ω

amp modulation

$4I_{1z}I_{2y}$ term $\quad 4(I_{1z}C - I_{1y}S)(I_{2y}C + I_{2z}S)S_y$

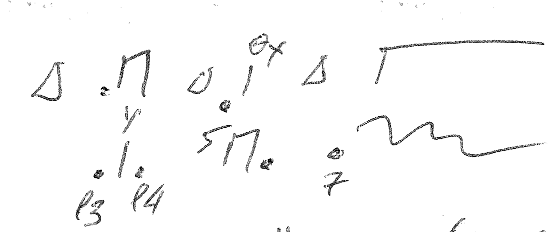
$= 4[I_{1z}C(I_{2y}C + I_{2z}S) - I_{1y}S(I_{2y}C + I_{2z}S)]S_y$

$= 4[I_{1z}I_{2y}C^2 + \boxed{I_{1z}I_{2z}CS} - I_{1y}I_{2y}CS \cancel{+} - I_{1y}I_{2z}S^2]S_y$

$2I_{1z}I_{2z}S_y\,S(2\theta)$ again...

$-4I_{1x}I_{2z}S_y \longrightarrow -4I_{1x}S_y(I_{2z}C - I_{2y}S)$ MQC — ϕ_{out}

I_3S ①



DePT - H,C cos"
Again

$I =$

$$I_{1z}+I_{2z}+I_{3z} \xrightarrow{H_r} I_{1x}+I_{2x}+I_{3x} \xrightarrow{H_{cs}} (I_{1x}+I_{2x}+I_{3x})C\omega_I'$$
$$+ (I_{1y}+I_{2y}+I_{3y})S\omega_I'$$

$C\omega_I'$ I_{1x}

$$I_{1x} \xrightarrow{JI_{1z}S_z} I_{1x}C_J^\Delta + 2I_{1y}S_zS_J^\Delta \xrightarrow{JI_{2z}S_z} \xrightarrow{JI_{3z}S_z} X$$

$$I_{2x} \xrightarrow{JI_{2z}S_z} I_{2x}C_J^\Delta + 2I_{2y}S_zS_J^\Delta \xrightarrow{JI_{1z}} \xrightarrow{JI_{3z}} X$$

$$I_{3x} \xrightarrow{JI_{3z}S_z} I_{3x}C_J^\Delta + 2I_{3y}S_zS_J^\Delta \longrightarrow \longrightarrow X$$

ρ_3: $C\omega_I'$

$$2I_{1y}S_z \xrightarrow{90x,S} 2I_{1y}S_x$$
$$2I_{2y}S_z \qquad 2I_{2y}S_x$$
$$2I_{3y}S_z \qquad 2I_{3y}S_x$$

$$2I_{1y}S_x \xrightarrow{JI_{1z}S_z} X \xrightarrow{JI_{2z}S_z} 2I_{1y}[S_xC_J^\Delta + 2I_{2z}S_yS_J^\Delta]$$

$$= 4I_{1y}I_{2z}S_y \xrightarrow{JI_{3z}S_z} 4I_{1y}I_{2z}[S_yC_J^\Delta - 2I_{3z}S_xS_J^\Delta]$$

$$= -8I_{1y}I_{2z}I_{3z}S_x$$

$$2I_{2y}S_x \xrightarrow{JI_{1z}S_z} 2I_{2y}[S_xC_J^\Delta + 2I_{1z}S_yS_J^\Delta]$$

$$= 4I_{1z}I_{2y}S_y \xrightarrow{JI_{3z}S_z} 4I_{1z}I_{2y}[S_yC_J^\Delta - 2I_{3z}S_xS_J^\Delta]$$

$$= -8I_{1z}I_{2y}I_{3z}S_x$$

② $2 I_{3y} S_x \rightarrow -8 I_{1z} I_{2z} I_{3y} S_x$

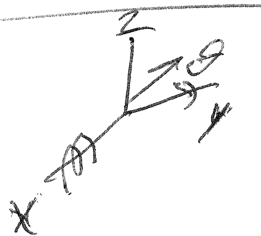
---

collect $\boxed{P5}$

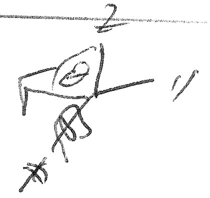
$-8 I_{1y} I_{2z} I_{3z} S_x \xrightarrow[\theta_x]{H_R}$

$-8 I_{1z} I_{2y} I_{3z} S_x$

$-8 I_{1z} I_{2z} I_{3y} S_x$



$I_y C\theta + I_z S\theta$



$I_z C\theta - I_y S\theta$

$(I_{2z}C - I_{2y}S)(I_{3z}C - I_{3y}S)]] S_x$

P6) $-8[(I_{1y}C + I_{1z}S)(I_{2z}C - I_{2y}S)][I_{3z}C - I_{3y}S) S_x$

$-8[I_{1y}C(I_{2z}C - I_{2y}S) + I_{1z}S(I_{2z}C - I_{2y}S)][I_{3z}C - I_{3y}S) S_x$

$= -8[I_{1y}I_{2z}C^2 - I_{1y}I_{2y}CS + I_{1z}I_{2z}CS - I_{1z}I_{2y}S^2]$

$= 8[I_{1y}I_{2z}I_{3z}C^3 - I_{1y}I_{2y}I_{3z}C^2S + \boxed{I_{1z}I_{2z}I_{3z}C^2S} - I_{1z}I_{2y}I_{3z}CS^2$

$- (\text{all MQ } \text{~~terms~~}) I_{3y}S) S_x$

survives

rest MQ

=

P9 $8 I_{1z} I_{2z} I_{3z} S_x C^2 S$

=

$C \cdot S = \frac{S(a+b) + S(a-b)}{2}$

$= S(2\theta)$

$C \cdot CS = C(\theta) \cdot S(2\theta)$

$\rightarrow \frac{S(3\theta) - S(-\theta)}{2}$

$S(3\theta) + S(\theta) = S(4 \cdot \theta)$

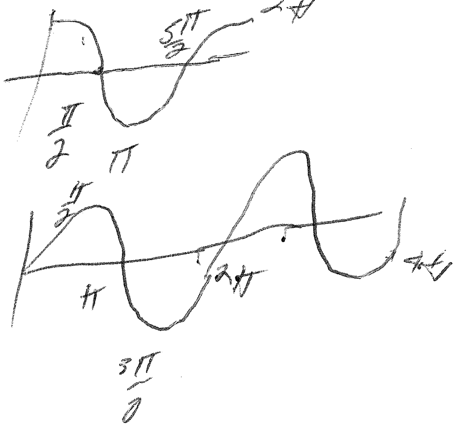
③ $c(\theta)\cdot c(\theta) s(\theta)$ $\qquad c(\theta)\cdot s(\theta) = s(2\theta)$

$$\underset{(\beta)}{c(\theta)}\underset{(\alpha)}{s(2\theta)} = \frac{s(\alpha+\beta)}{2} + \frac{s(\alpha-\beta)}{2} = \frac{s(3\theta)}{2} + \frac{s(\theta)}{2}$$

$$s(A)+s(B) = 2\sin\frac{(A+B)}{\cancel{2}}/2\,\cos\frac{(A-B)}{\cancel{2}}/2 = 2\sin\left(\frac{3\theta+\theta}{2}\right)\cos\left(\frac{2\theta-\theta}{2}\right)$$

$$= 2\sin(2\theta)\cos(\theta)$$

$2s(2\theta)c(\theta)$	θ
$+\sqrt{2}$	45
0	90
$+\sqrt{2}$	135



$\theta = 45$ $\quad 8\cdot\sqrt{2}\, I_{1z} I_{2z} I_{3z} S_x \xrightarrow{J I_{1z} S_z} \cancel{\frac{A I_{2z}}{2}}$

$2\cancel{I_{2z} I_{3z} I_{1z}}$

$$4\sqrt{2}\, I_{2z} I_{3z} \left[2 I_{1z} S_x \xrightarrow[\Delta]{J I_{1z} S_z} \left[2 I_{1z} \cancel{S_x} C_J^0 + S_y S_J^0\right] 4\sqrt{2}\, I_{2z} I_{3z}\right.$$

$$I_{3z} 2\sqrt{2} \left[2 I_{2z} S_y \xrightarrow{I_{2z} S_z} \left[2 \cancel{I_{2z} S_y} C_J^0 - S_x S_J^{\Delta}\right] I_{3z} 2\sqrt{2}\right.$$

$$-\sqrt{2}\left[2 I_z S_x\right] \xrightarrow{J I_{3z} S_z} -\sqrt{2}\left[2 I_z S_x C_J^0 + S_y S_J^{\Delta}\right]$$

$$\Rightarrow -\sqrt{2}\, S_y \xrightarrow[t_2]{H_{cs}} \cancel{-\sqrt{2}\, I}$$

⑱④

$\Rightarrow -\sqrt{2} S_y \xrightarrow[t_2]{H_{CS}} -\sqrt{2}\left[S_y C_{\omega_S}^{2} - S_y S_{\omega_S}^{2}\right]$

Final $C_{\omega_I}^{1} I_{1x}$ $\quad -\sqrt{2}\, C_{\omega_S}^{2}\, i S_y$ $\mathbb{I}$

$-\sqrt{2}\, S_{\omega_S}^{2}\, i S_x$ $\mathbb{R}$

↗

AmP modulated

Note: $-8 I_{1y} I_{2z} I_{3z} S_x \longrightarrow -\sqrt{2} S_y$

(ρ_7)

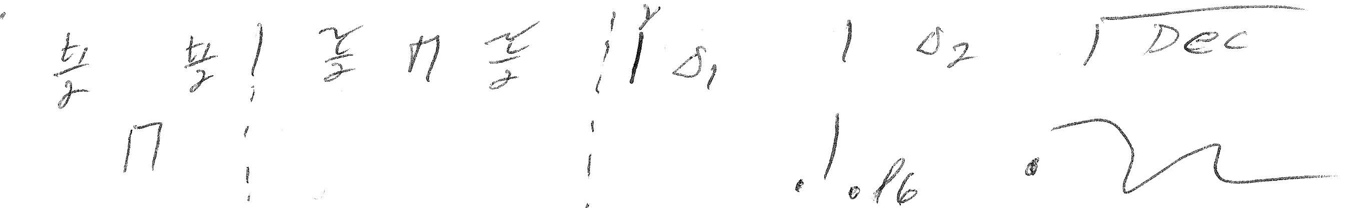
(ρ_5)

$\xrightarrow[t_2]{H_{CS}}$ all Detected

so does $-8 I_{1z} I_{2y} I_{3z} S_x \longrightarrow -\sqrt{2} S_y$

$-8 I_{1z} I_{2z} I_{3y} S_x \longrightarrow -\sqrt{2} S_y$

VI-19



Keep?

H, C-
Relay COSY

$I_{1x} C\omega_1'$
$I_{1z} S\omega_1'$

$2I_{1z}I_{2y}$

$2I_{2y}S_z$

S_x

$J_{13} = 0$

$J_{12} = I_{1z} + I_{2z}$ $J_{23} = I_{2z} + S_z$

$I_{1z} \xrightarrow{Hr} I_{1x} \xrightarrow{CS} I_{1x} C\omega_1' + I_{1y} S\omega_1' \xrightarrow{90_x I} I_{1x} C\omega_I' + I_{1z} S\omega_{I_1}'$

$\boxed{t_1 : C\omega_{I_1}' I_{1x}}$

$I_{1x} \xrightarrow[J_{12} I_{1z} I_{2z}]{J_{12}} I_{1x} C_J^\tau + 2 I_{1x} I_{2z} S_J^\tau$

$2 I_{1x} I_{2z} S_J^\tau \xrightarrow{90_y I} -2 I_{1z} I_{2y} S_J^\tau$

$-S^\tau_{J_{12}} : 2 I_{1z} I_{2y} \xrightarrow[\Delta_1]{J_{23}} 2 I_{1z} [I_{2y} C_J^\Delta - 2 I_{2x} S_z S_J^\Delta)$ ⟸ DOESN'T survive

$2 I_{1z} I_{2y} \xrightarrow[\Delta_1]{J_{12}} 2 I_{1z} I_{2y} C^\Delta_{J_{12}} - I_{2x} S^\Delta_{J_{12}}$

$S^\tau_{J_{12}} S^{\Delta_1}_{J_{12}} : + I_{2x} \xrightarrow[\Delta_1]{J_{23}} I_{2x} C^{\Delta_1}_{J_{23}} + 2 I_{2y} S_z S^\Delta_{J_{23}}$

$\xrightarrow{H_{CS}} 2 (I_{2y} C\omega_{I_2}^{\Delta_1} \mp I_{2x} S\omega_{I_2}^{\Delta_1}) S_z$

$S^\tau_{J_{12}} S^\Delta_{J_{12}} S^\Delta_{J_{23}} : 2 I_{2y} S_z$

$2 I_{2y} S_z \xrightarrow[90_x S]{90_x I} 2 I_{2z} S_y \longrightarrow$

$-2 I_{2x} S_z \longrightarrow -2 I_{2x} S_y \rightarrow$ MQ — Φ-out

② P6i

$S_{J12}^{\tau} S_{J12}^{\Delta'} S_{J23}^{\Delta 1} C_{\omega I2}^{\Delta 1}$: $2I_{2y}S_z$

$2I_{2y}S_z \xrightarrow[90_x S]{90_x I} 2I_{2z}S_y$ $-S_{J23}^{\Delta 2} S_x \xrightarrow{CS} -S_{J23}^{\Delta 2}[S_x C_{\omega S}^{\Delta 2} + S_y S_{\omega S}^{\Delta 2}]$

$2I_{2z}S_y \xrightarrow{J_{12}} X \xrightarrow{J_{13}} X$

$2I_{2z}S_y \xrightarrow{J_{23}} 2I_{2z}S_y C_{J23}^{\Delta 2} - S_x S_{J23}^{\Delta 2}$

$-S_{J12}^{\tau} S_{J12}^{\Delta 1} S_{J23}^{\Delta 1} C_{\omega I2}^{\Delta 1}$

$2I_{2z}S_y \xrightarrow[\Delta 2]{CS} 2I_{2z}[S_y C_{\omega S}^{\Delta 2} - S_x S_{\omega S}^{\Delta 2}]$

$2I_{2z}S_y C_{\omega S}^{\Delta 2} \xrightarrow{J_{23}}$ Same as Above

$-2I_{2z}S_x S_{\omega S}^{\Delta 2} \longrightarrow$

$-S_{J12}^{\tau} S_{J12}^{\Delta 1} S_{J23}^{\Delta 1} C_{\omega I2}^{\Delta 1} (-S_{J23}^{\Delta 2} C_{\omega S}^{\Delta 2})$; S_x ; $C_{\omega S}^{2} \cdot (-S_{\omega S}^{2})$

" $(-S_{J23}^{\Delta 2} S_{\omega S}^{\Delta 2}$; S_y ; $S_{\omega S}^{2} \cdot (C_{\omega S}^{2})$

"

Now still t2

$S_x \xrightarrow[t2]{CS} S_x C_{\omega S}^{2} + S_y S_{\omega S}^{2}$

$S_y \xrightarrow{CS} S_y C_{\omega S}^{2} - S_x S_{\omega S}^{2}$

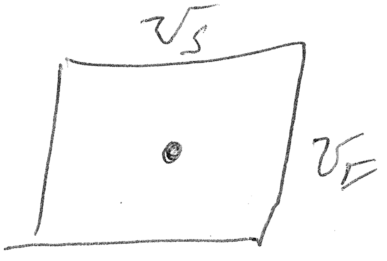
mess:

t_1 : $C_{\omega I1}$

t_2 : $C_{\omega I2}^{\Delta 1} C_{\omega S}^{2}$

⑤ start I_{1x} cw_I!

end wit $I_{2y}S_z \rightarrow S_x$ (S_x attacked to I_2

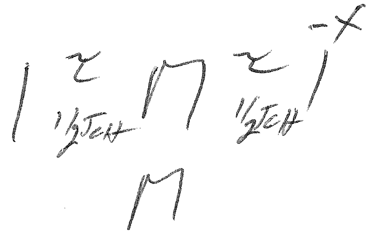


x pk = ν_I (for I_1)

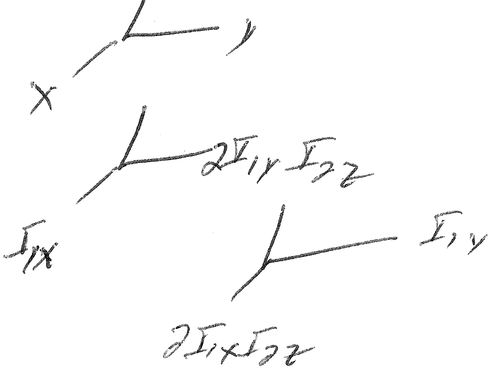
ν_S (coupled to I_2)
& not I_1

$\boxed{\text{VI-20}}$

BIRD
seQ



} Bax seQ



↑ ^{12}C − ^{13}C↑ $\xrightarrow{\text{BIRD}}$ ↑^{12}C − ^{13}C↑
↑ H   H↑   ↓H   H↑ (INVERT ^{12}C-H↑ONLY)

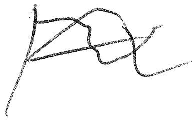
H-^{13}C

$I_{1z} \xrightarrow{90x} -I_{1y} \xrightarrow[\tau\, \cancel{2\tau}]{J I_z S_z} \overset{90\ 0}{\cancel{-I_{1y} C_\tau^\tau}} + 2 I_{1x} S_z S_\tau^\tau$

$C_\tau^\tau = c\left(\frac{J}{2} \cdot \frac{1}{2J}\right) = \frac{1}{4}$

$c(90) = 0$

$s(90) = 1$



$2I_{1x}S_z \xrightarrow[\pi_x]{\pi x} -2I_{1x}S_z$

$-2I_{1x}S_z \xrightarrow[\tau]{J I_z S_z} -[\overset{90\ 0}{\cancel{2I_{1x}S_z C_\tau}} + I_{1y}S_\tau) = -I_{1y}$

$-I_{1y} \xrightarrow[90\text{-}x]{\cancel{90x}} +I_{1z}$ ↑H-^{13}C [$I_{1z} \rightarrow I_{1z}$ no Flip)

H-^{12}C

$I_{1z} \xrightarrow{90x} -I_{1y} \xrightarrow{J I_{1z} I_{2z}} -(I_{1y} C_\tau - 2 I_{1x} I_{2z} S_\tau]$

$-I_{1y} \xrightarrow{\pi_x} +I_{1y}C_\tau \xrightarrow{\cancel{\pi x}}$ $\xrightarrow{J I_{1z} I_{2z}} C_\tau[I_{1y}C_\tau - 2I_{1x}I_{2z}S_\tau]$

$-2I_{1x}I_{2z} \xrightarrow{I_x} +2I_{1x}I_{2z}S_\tau \longrightarrow \underline{S_\tau[2I_{1x}I_{2z}C_\tau + I_{1y}S_\tau]}$

$= I_{1y}C_\tau^2 - 2I_{1x}I_{2z}C_\tau S_\tau$

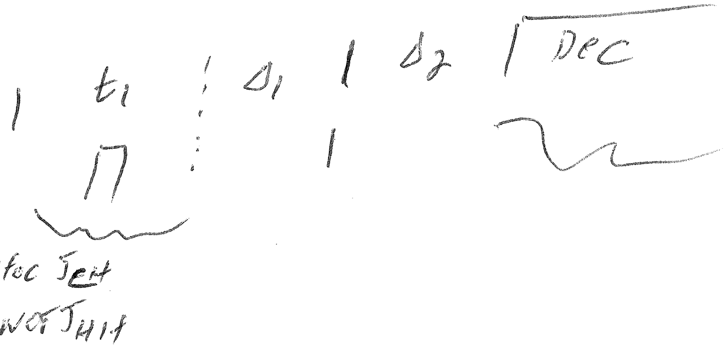
$I_{1y}S_\tau^2 + 2I_{1x}I_{2z}C_\tau S_\tau$

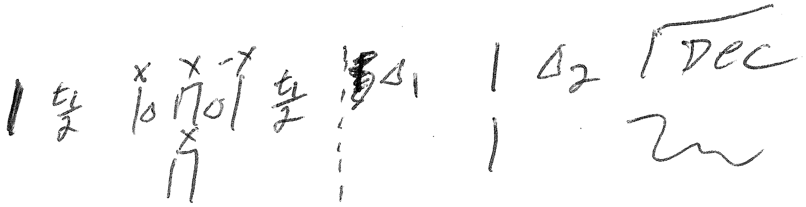
$= I_{1y} \xrightarrow{90x} -I_{1z}$

II-20) use BIRD in INEPT HX-COSY

ii)

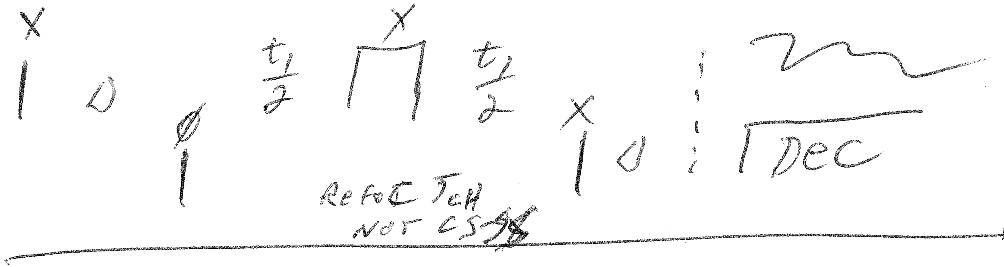
INEPT
COSY
prog 19

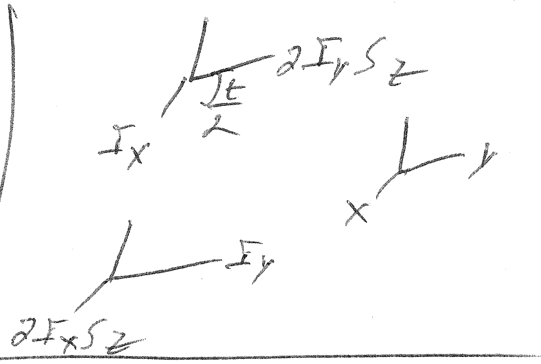




sep'd t1

II-21) i) calc Ix Funcs HMQC





$$I_z \xrightarrow{90x} -I_y \xrightarrow[\Delta=\frac{1}{2J_{CH}}]{JI_zS_z} -\cancel{I_y C_J}^{0} + 2I_xS_zS_J$$

$$C\left(\frac{J}{2}\cdot\frac{1}{2J}\right) = C\left(\frac{\pi}{2}\right) = 0$$

$$\Delta = \frac{1}{2J_{CH}}$$

$$2I_xS_z \xrightarrow{90x^S} -2I_xS_y \xrightarrow{CS-S} -2I_x(S_yC_\omega^1 - S_xS_\omega^1)$$

$$-2I_xS_yC_{\omega S}^1 + 2I_xS_xS_{\omega S}^1 \xrightarrow{90x^S} -2I_xS_zC_{\omega S}^1 + \cancel{2I_xS_xS_\omega}^{0}\ (\text{MQC})$$

Lose 1/2 Sig

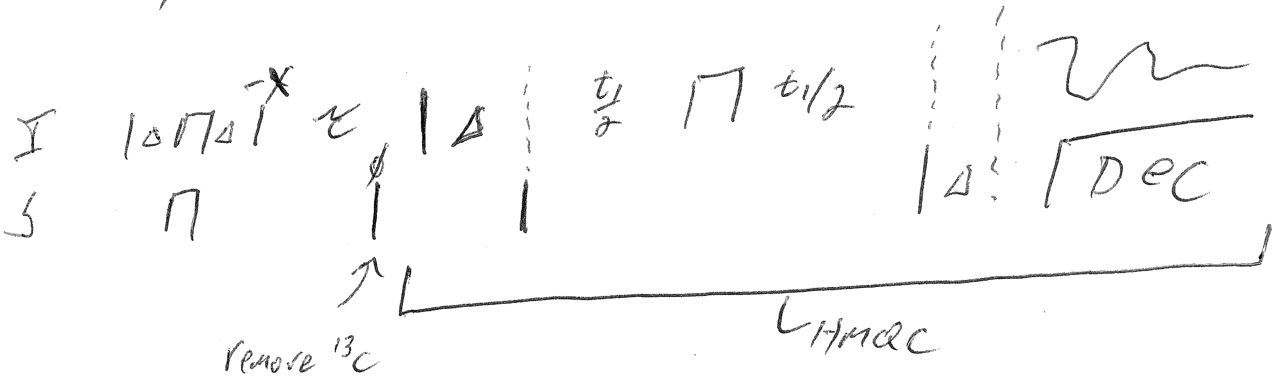
$$-2I_xS_zC_{\omega S}^1 \xrightarrow[\Delta]{JI_zS_z} -\left[\cancel{2I_xS_zC_J}^{0} + I_yS_J\right]C_{\omega S}^1$$

$$\xrightarrow{\text{Detect}} -I_yC_{\omega S}^1 \xrightarrow{CS-I} -C_{\omega S}^1\left[I_yC_{\omega I}^2 - I_xS_{\omega I}^2\right]$$

AMP-mod eg) States

~~VI~~-2~~4~~ ii) use BIRD in ~~INEPT~~-seq HMQC for H,H t_1 decoupling

*Bax, JMR, 67, p565, 1986



$\tau = 1.3\,T_1$ ∴ $H-^{12}C$ signal near its null (saturation) at beginning of expt, like a presat

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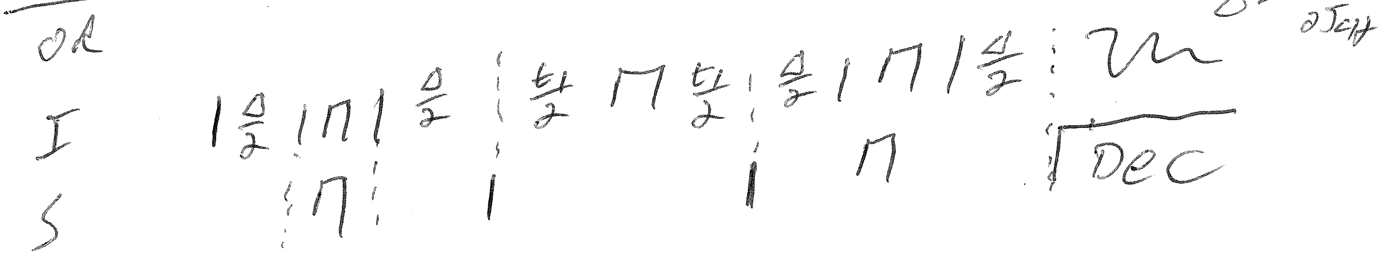
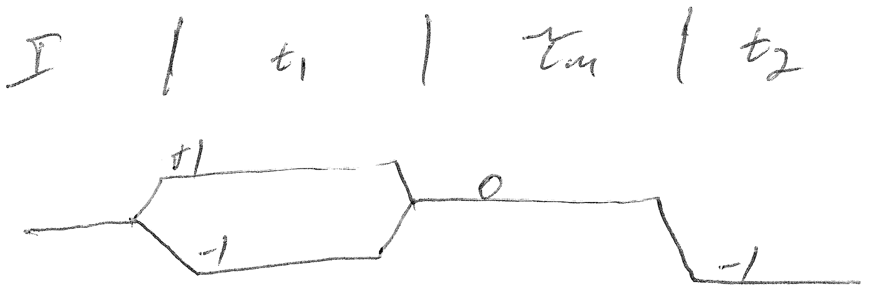
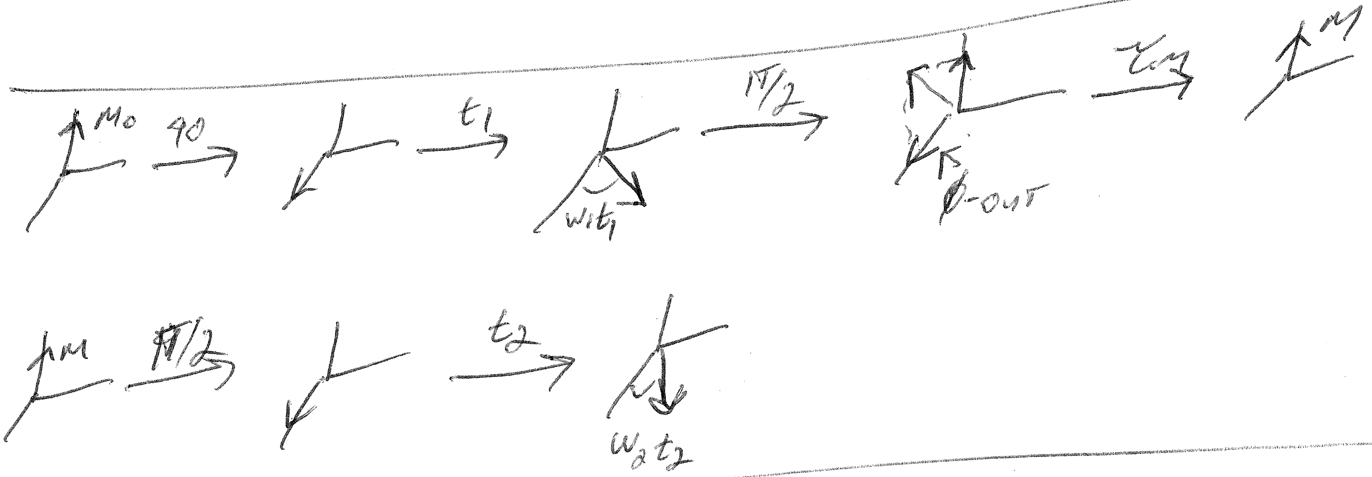
OR



VI 22 2D-exchange

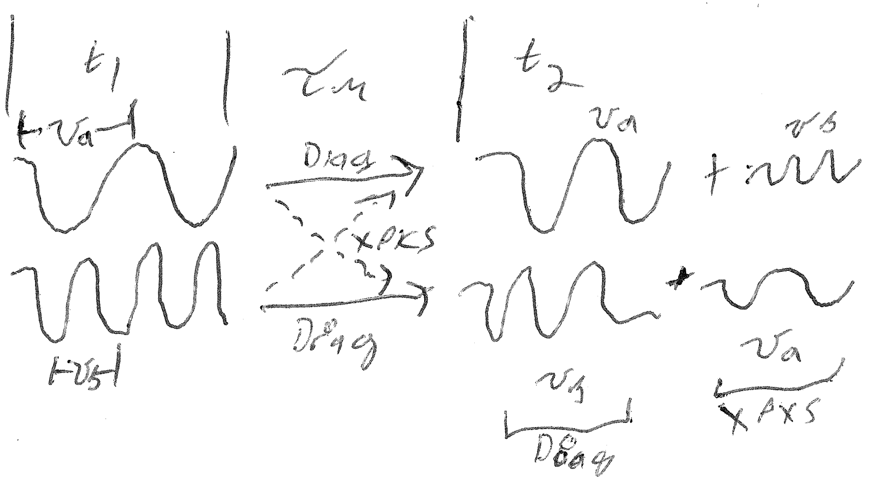
*uncoupled spins





$$A \underset{}{\overset{K}{\rightleftharpoons}} B \qquad K << |\nu_A - \nu_B|$$

slow exchange



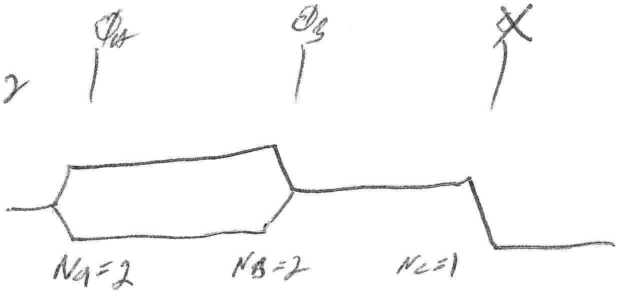
For $P_A = P_B$

linear appx for xchange

$$\boxed{\frac{I_{Diag}}{I_{xpk}} = \frac{1 - K\cdot\tau_m}{K\cdot\tau_m}}$$

— 1st order kinetics

② / VI-22



$\phi_{Path} = \phi_A \Delta P_A + \phi_B \Delta P_B + \phi_C \Delta P_C + \phi_{Dig} = 0$

Simul ~~AE~~ $= \phi_A(-1) + \phi_B(+1) + 0 + \phi_{Dig} = 0$

$\phi_{Dig} = \phi_A - \phi_B$

✓

ϕ_A	ϕ_B	ϕ_C	ϕ_{Dig}
0	0	0	0
2	0	0	2
0	2	0	2
2	2	0	0

AE $N_A=2$ $N_B=4$ $N_C=1$

$\phi_{Path} = \phi_A(-1) + \phi_B(+1) + 0 + \phi_{Dig} = 0$

$\phi_{Dig} = \phi_A - \phi_B$

ϕ_A	ϕ_B	ϕ_C	ϕ_{Di}
0	0	0	0
2	0	0	2
2	1	0	3
2	1	0	1
0	2	0	2
2	2	0	0
0	3	0	1
2	3	0	3

Echo $N_A=2$ $N_B=4$ $N_C=1$

$\phi_S = \phi_A(+1) + \phi_B(-1) + \phi_C(-1) + \phi_{Dig}$

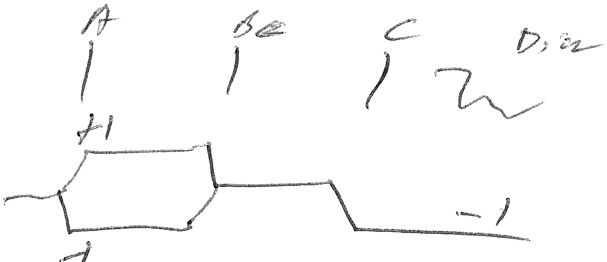
$= \phi_A - \phi_B + \phi_D = 0$

$\phi_D = \phi_B - \phi_A$

ϕ_A	ϕ_B	ϕ_C	ϕ_D
0	0	0	0
2	0	0	2
0	1	0	1
2	1	0	3
0	2	0	2
2	2	0	0
0	3	0	3
2	3	0	1

$\phi_{Ar5} = \Delta P_A$

$\phi_{Ar5 4}$



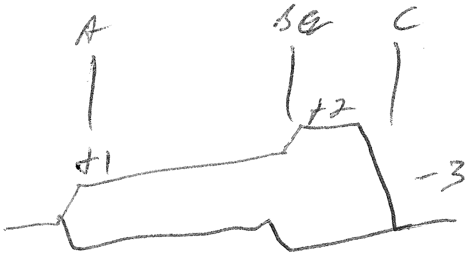
$\Delta P = 1$ $\Delta P = -1$

$N_A = 2$ $N_B = 1$ $N_C = 2$

$$\phi_{Pat} = \phi_A \Delta P_A + \phi_B \Delta P_B + \phi_C \Delta P_C$$

$$= \phi_A \cdot 1 + 0 + \phi_C(-1)$$

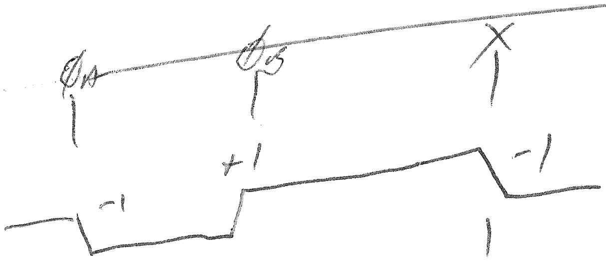
$$= \phi_A - \phi_C$$



$$\phi_{PA} = \phi_A \Delta P_A + \phi_B \Delta P_B + \phi_C \Delta P_C$$

$$= \phi_A$$

$N_a = 2$ $N_B = 1$ $N_C = 4$



ϕ_A	ϕ_B	ϕ_C	ϕ_D
0	0	0	0
2	0	0	2
0	2	0	2
2	2	0	0

$N_a = 2$ 2

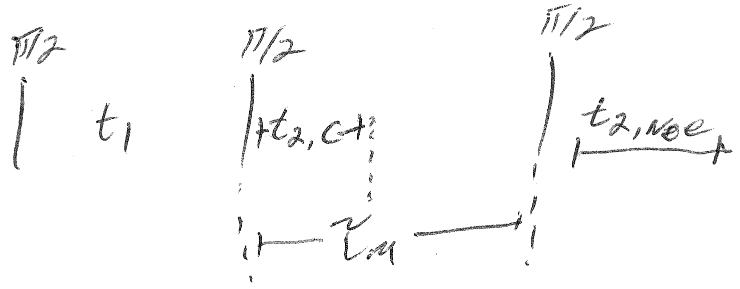
$$\phi_P = \phi_A(-1) + \phi_B(+1) + \phi_C(-1) + \phi_{dig}$$

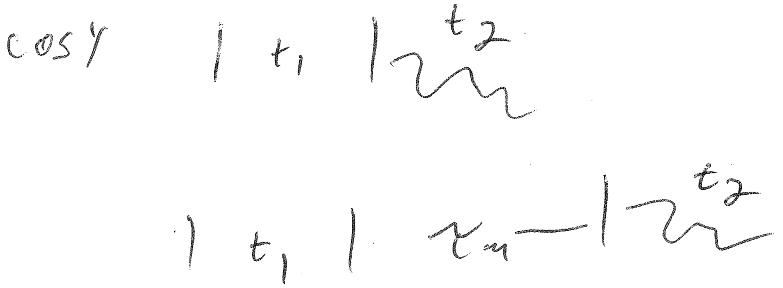
$$\phi_P = -\phi_A + \phi_B + 0 + \phi_{Dig} = 0$$

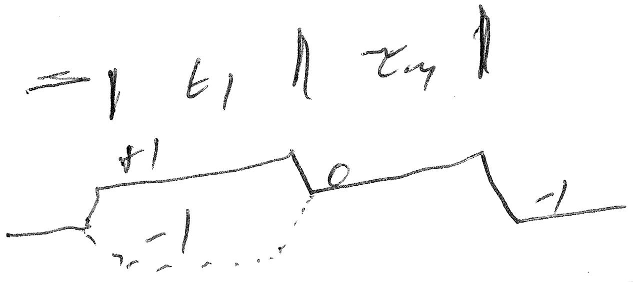
~~ϕ_{Dig}~~ =

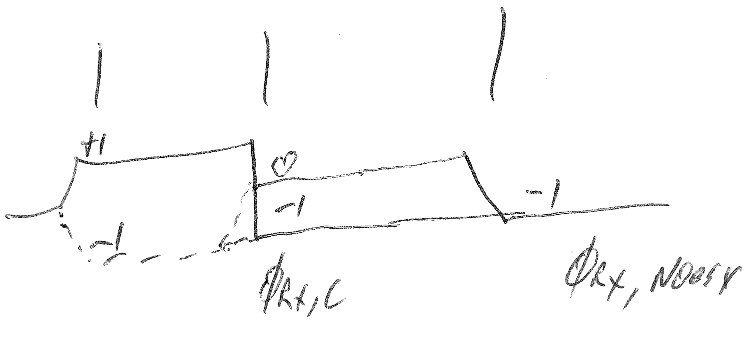
$$\phi_{Dig} = \phi_A - \phi_B$$

VI-23) COCONOESY - combined COSY/NOESY





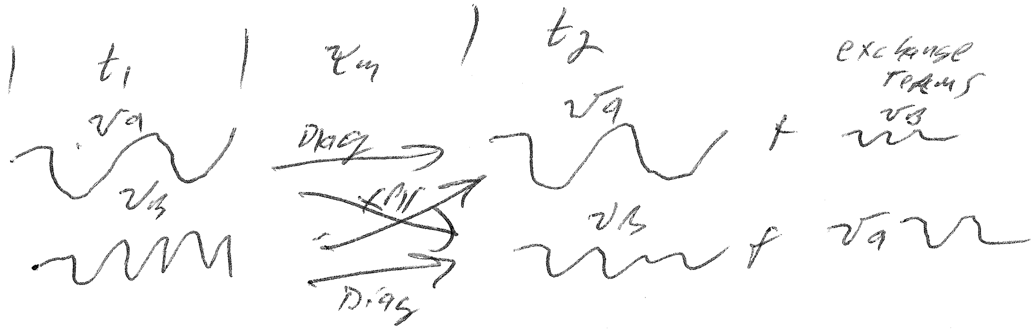




VI-24 explain the origin & dependence of xpks on τ_m

For $SnCl_4 : SnBr_4$ 1:1 soln

Notes:



* as τ_m increases the time for observable chemical exchange increases too. ∴ we see more & more xpks grow in, However it is T1 limited

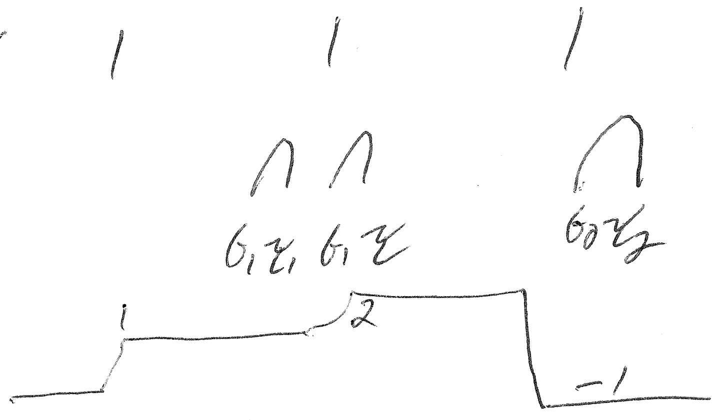
The 1st order behavior is:

$$\boxed{\frac{I_{\cancel{Diag}\ xpk}}{I_{Diag\ \cancel{xpks}}} = \frac{1 - k \cdot \tau_m}{k \cdot \tau_m}}$$

* So for this Sn mixture the exchange of Br & Cl is seen which changes the chem shifts in turn...

VI-25) explain how following seqs achieve coh pathway needed.
& what should Gz or τ be?

1) DQF-COSY
echo



$\phi = \gamma G_z \cdot \tau \cdot p$

* note +2 coh wraps twice as fast as +1
+1

$\phi = (+1)G_1\tau + (+2)G_1\tau_1 + (-1)G_2\tau_2$

Let $\tau_1 = \tau_2$

$= G_1\tau_1 + 2G_1\tau_1 - G_2\tau_2 = 0$

$= G_1\tau + 2G_1\tau - G_2\tau = 0$

$= 3G_1\tau - G_2\tau = 0 \Rightarrow G_2 = 3G_1$

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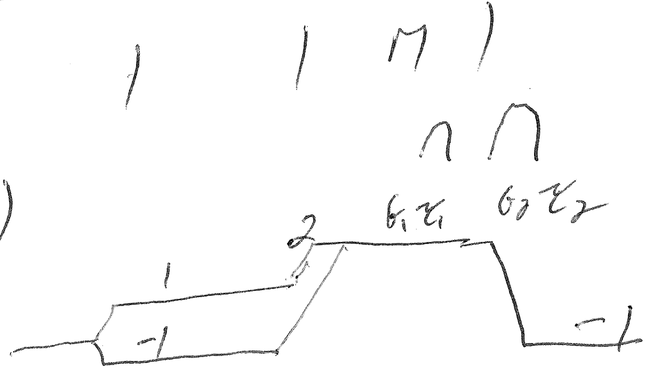
2) DQF-COSY
E/AE (
(Amp-modulated)



Let $\tau_1 = \tau_2$

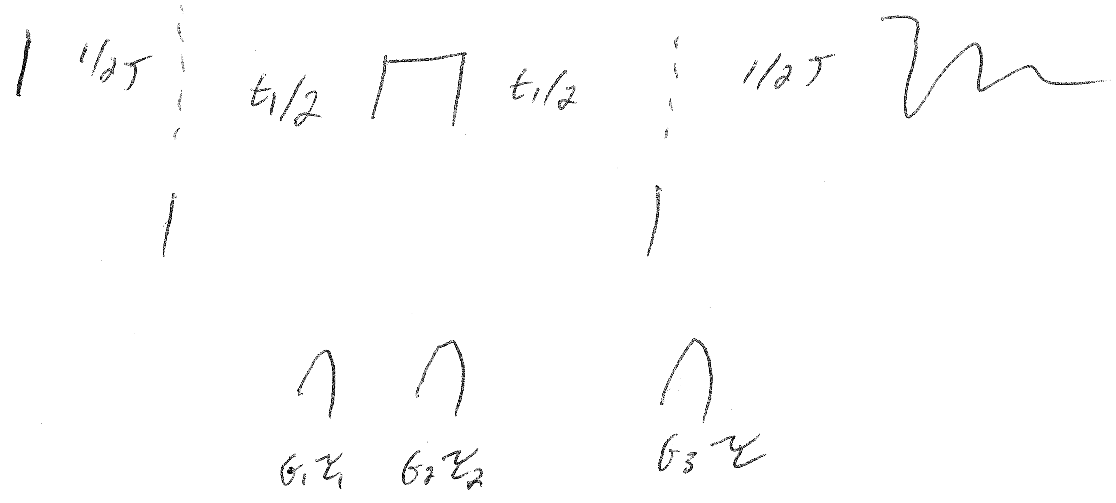
$\phi = (+2)G_1\tau_1 + (-1)G_2\tau_2$

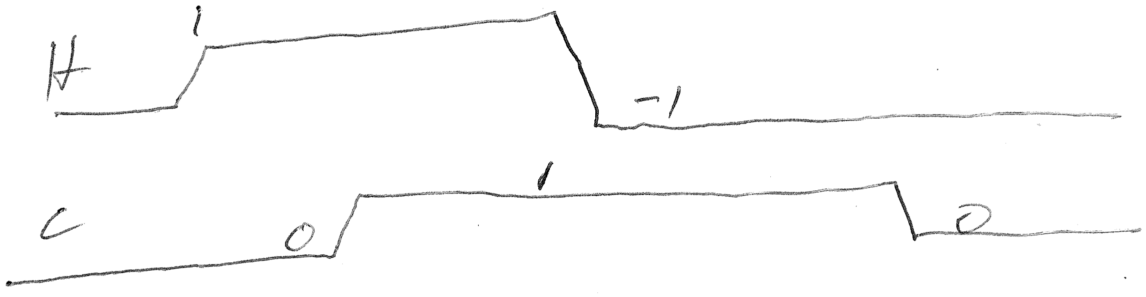
$= 2G_1\tau - G_2\tau = 0$

$\therefore 2G_1 = G_2$

* note p=0 at ~~after~~ 2nd pulse can only go → ±1
∴ Axial is Filtered

IV-25)
iii)





$\phi = (+1)\gamma_H G_1 \tau_1 + (+1)\gamma_c G_1 \tau_1 + (-1)\gamma_H G_2 \tau_2 + (+1)\gamma_c G_2 \tau_2 + (-1)\gamma_H G_3 \tau_3 = 0$

let $\tau = \tau_1 = \tau_2 = \tau_3$

$\phi = \gamma_H G_1 + \gamma_c G_1 - \gamma_H G_2 + \gamma_c G_2 - \gamma_H G_3 = 0$

$\boxed{\phi = \gamma_H (G_1 - G_2 - G_3) + \gamma_c (G_1 + G_2) = 0}$ } could be general case eg) $\gamma_c \rightarrow \gamma_N$

$\phi = 4(G_1 - G_2 - G_3) + G_1 + G_2 = 0$

let $G_1 = G_2$

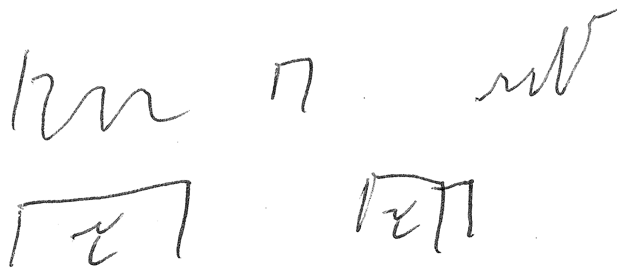
$\phi = 5G_1 - 3G_2 - 4G_3 = 0$

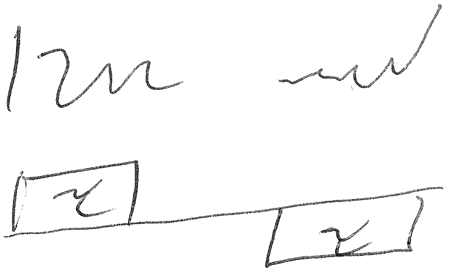
$\therefore \phi = 5G_1 - 3G_1 - 4G_3 = 0$

$\Rightarrow 2G_1 - 4G_3 = 0$

$G_1 = 2G_3$

Gradient Selection   refocus!





$\Phi_1 = \gamma_1 G_z^1 P_1 \tau_1$ P_1 = coh order γ = gamma

τ = length G_z - Grad Amp

$\Phi_1 + \Phi_2 = 0$ = refocus

$\gamma_1 G_z^1 P_1 \tau_1 + \gamma_2 G_z^2 P_2 \tau_2 = 0$ $\therefore \boxed{\frac{P_2}{P_1} = \frac{-\gamma_1 G_{z1} \tau_1}{\gamma_2 G_z^2 \tau_2}}$

$\gamma_1 G_z^1 P_1 \tau_1 = -\gamma_2 G_z^2 P_2 \tau_2$

└ coh. ratio selected

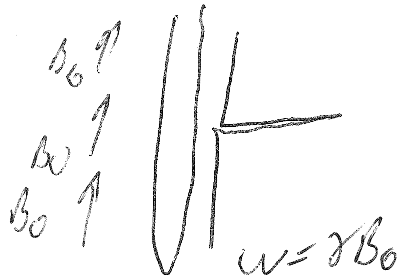
~~35~~

OR JUST follow coh effects ~~thus~~ thru BY adding as needed

$\Phi = (\gamma G) P \tau$

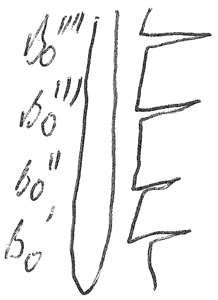
ADDITIONAL Phase
cycling NOTES From
Levitts Book & some
Gradient NOTES

① **Gradients**



$\omega = \gamma B_0$

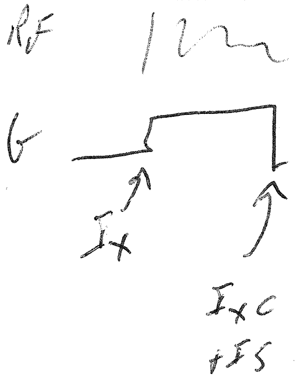
$\uparrow z$



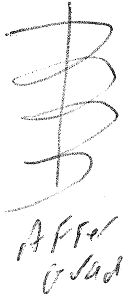
$B = B_0 z + G_z \cdot z$

$G_z = \frac{\partial B_z}{\partial z}$

$\omega = \gamma G_z \cdot z$



$$\left.\begin{array}{l} I_x\, c(\gamma G_z \cdot z\, t) \\ + I_y\, s(\gamma G_z \cdot z t) \end{array}\right\}$$



Sig is coiled

$\langle M \rangle \sim 0$

$= I_x c(G_z z \gamma t) + I_y s()$

$$\langle M_x(t) = \frac{1}{l}\int_{-l/2}^{l/2} c(\gamma G_z \cdot z t)\, dz = \frac{\sin(\gamma G_z \cdot z t)}{\gamma G_z \cdot z t} = \text{sinc}$$

$l = 1\text{cm}$ $\quad \gamma G_z = \frac{50\text{kHz}}{\text{cm}}$, $t = 3\text{ms} \Rightarrow M_x = 10^{-3} - 10^{-4}$

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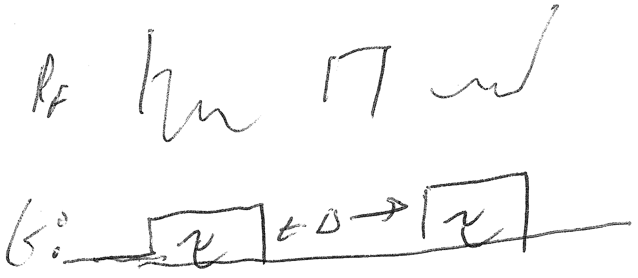
spherical ops under G_z

$$\boxed{G_p \xrightarrow{\gamma G_r r t} G_p e^{-i p \gamma G_r t}}$$

ZQ → No effect!

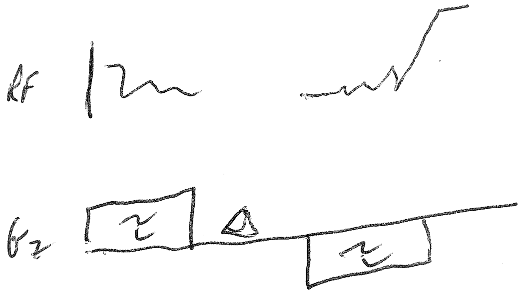
DQ → dephase twice as fast

Ⓠ



RF + Grad

RF+Grad → echo



Gradient echo!

For coh order change, echo occurs when $\phi_1+\phi_2=0$

$p_1 \rightarrow p_2$

~~$\phi_2 = \gamma_2$~~

$$\phi_1 = \gamma_1 G_z^1 z\, p_1 \tau_1$$

$$\phi_2 = \gamma_2 G_z^2 z\, p_2 \tau_2$$

~~Take time~~

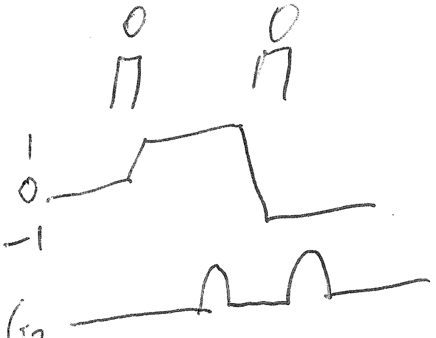
$$\therefore \phi_1+\phi_2 \Rightarrow \gamma_1 G_z^1 p_1 \tau_1 + \gamma_2 G_z^2 p_2 \tau_2 = 0$$

$$\gamma_1 G_z^1 p_1 \tau_1 = -\gamma_2 G_z^2 p_2 \tau_2$$

Coherence selection for single scan

$$\boxed{\frac{p_2}{p_1} = \frac{-\gamma_1 G_z^1 \tau_1}{\gamma_2 G_z^2 \tau_2}}$$

Depends on G_z, τ & γ!



~~$\gamma_1 = G_2$~~

~~$G_z^1 = G_z^2$~~

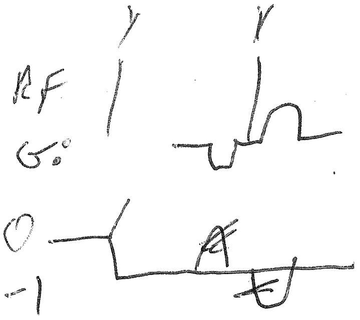
~~$\tau_1 = \tau_2$~~

$$\frac{p_2}{p_1} = \frac{1}{-1}$$

$$-1 = \frac{-\cancel{\gamma_1}^1 G_z^1 \tau_1}{\cancel{\gamma_2} G_z^2 \tau_2}$$

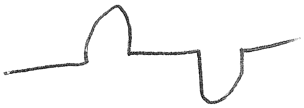
Keep $G_z^1 = G_z^2$ & $\tau_1 = \tau_2$?

∴ Single scan coh selec



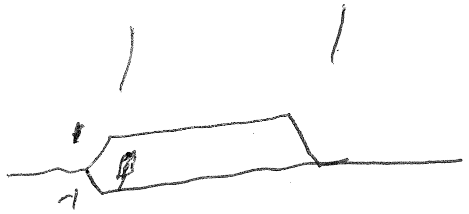
$$\cancel{\frac{\rho_1}{\rho_2}} \quad \frac{\rho_2}{\rho_1} = \frac{-1}{-1} = \frac{-\gamma_1 G_{z_1} \tau_1}{\gamma_2 G_{z_2} \tau_2}$$

$$1 = \frac{(-G_{z_1} \tau_1)}{(+G_{z_2} \tau_2)}$$



ML - Phase cycling

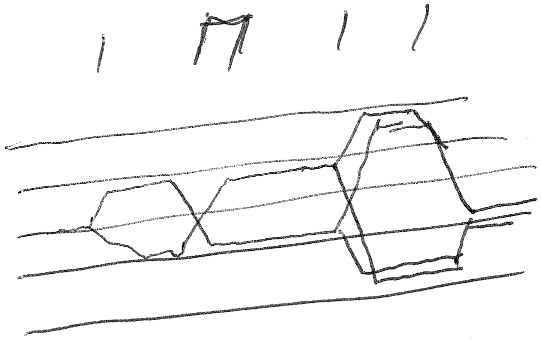
1) Draw coh path 1st (CTP)



0 → 1 → -1 } This is 6
0 → -1 → -1 }

2) +1 & -1 both necessary in t1 (states!)

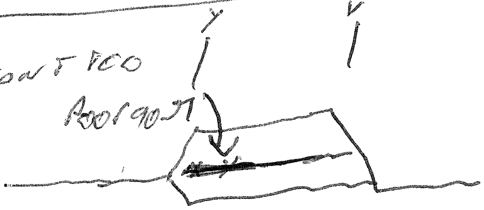
INAD



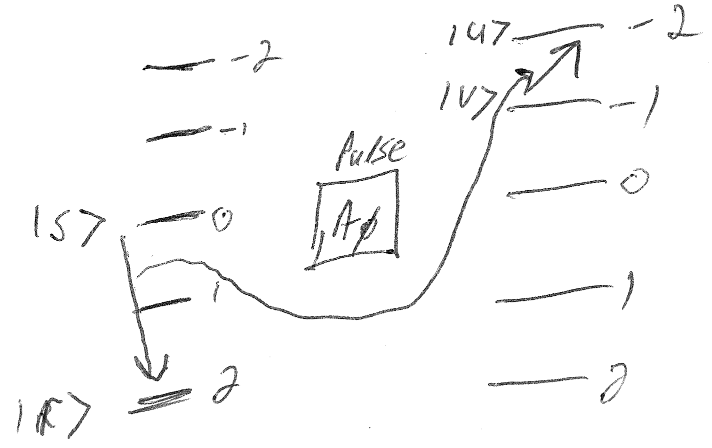
0 → 1 → -1 → 2 → -1
0 → 1 → -1 → -2 → -1
0 → -1 → 1 → 2 → -1
0 → -1 → 1 → -2 → -1

} desired

#undesired important PCO



Poor 90 1st pulse
→ pops I_0
$\Omega_1 = 0$ in 2D



$P_{rs} = +2$

$\hat{A}_\phi$ = Hamil / Prolog of pulse A w/ ϕ

Z_ϕ = complex #, coh transfer amp!

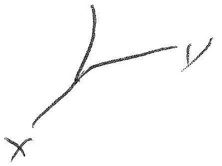
$$\boxed{\hat{A}_\phi |r\rangle\langle s| \hat{A}_\phi^{+} = Z\phi\, |u\rangle\langle v|}$$

mult by $\langle u|\ \ |v\rangle$ →

$$\boxed{\langle u|\hat{A}_\phi|r\rangle\langle s|\hat{A}_\phi^{+}|v\rangle = Z\phi}$$

② relates $Z\phi$ (coh Tx Amp) to the product of 2-operator matrix elements $\cancel{\begin{pmatrix}* & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}0 & *\\ 0 & 0\end{pmatrix}}$

17.3 how does Z_ϕ depend on ϕ



$\hat{A}_\phi = \hat{R}_z(\phi)\hat{A}_0 R_z(-\phi)$ R_z = rotation of about z

recall $\boxed{Z\phi = \langle u|\hat{A}_\phi|r\rangle\langle s|\hat{A}_\phi^{+}|v\rangle}$

$\therefore Z\phi = \langle u|\hat{R}_z^{\phi}\hat{A}_0\hat{R}_z^{-\phi}|r\rangle\langle s|R_z^{\phi}\hat{A}_0^{+}R_z^{-\phi}|v\rangle$

$|r\rangle|s\rangle|u\rangle|v\rangle$ are ES of z-ang mom

$I_z|r\rangle = M_r|r\rangle$

$I_z|s\rangle = M_s|s\rangle$

$I_z|u\rangle = M_u|u\rangle$

$I_z|v\rangle = M_v|v\rangle$

$R_z(-\phi) = e^{iI_z\phi}$ $R_z(+\phi) = e^{-i\phi I_z}$

$\therefore R_z^{-\phi}|r\rangle = e^{iM_r\phi}$ $\langle u|R_z^{\phi} = \langle u|e^{-iM_u\phi}$

$R_z^{-\phi}|v\rangle = e^{iM_v\phi}$ $\langle s|R_z^{\phi} = \langle s|e^{-iM_s\phi}$

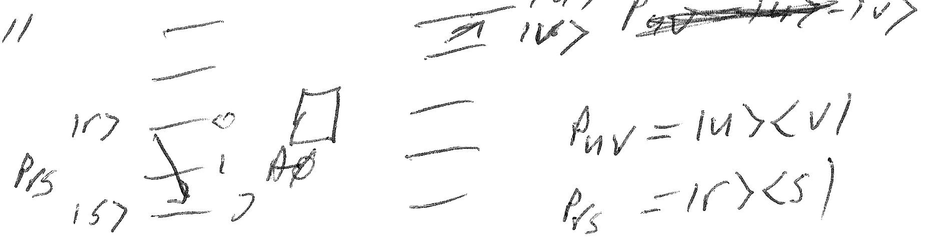
$\langle u|e^{-iM_u\phi}\hat{A}_0 e^{iM_r\phi}|r\rangle\langle s|e^{-M_s\phi}\hat{A}_0^{+}e^{iM_v\phi}|v\rangle = Z\phi$

$= \langle u|\hat{A}_0|r\rangle\langle s|\hat{A}_0^{+}|v\rangle e^{i(M_R-M_u)\phi}\, e^{i(M_v-M_s)\phi} = Z\phi$

③ $P_{uv} = M_u - M_v$

$P_{rs} = M_r - M_s$

recall



$P_{uv} = |u\rangle\langle v|$

$P_{rs} = |r\rangle\langle s|$

$$Z\phi = Z(0)\, e^{i(Mr - Mu + Mv - MS)}$$

$$= Z(0)\, e^{-i(Mu - Mv + Ms - MR)\phi} = Z\phi\, e^{-i(P_{uv} - P_{RS})}$$

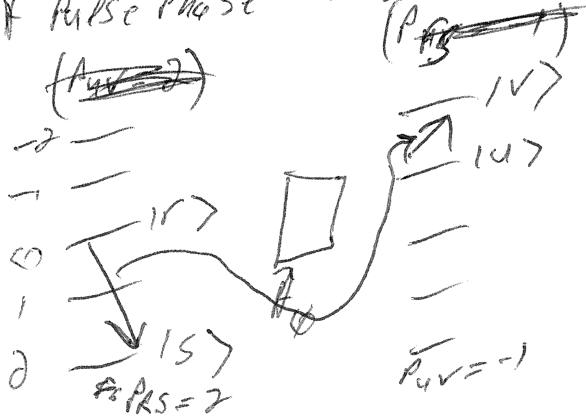
$$\boxed{Z\phi = Z0\, e^{-i(\Delta P)\phi}}$$

$\Delta P = P_{uv} - P_{rs}$

$$\boxed{Z\phi = Z_0\, e^{-i\Delta P\phi}}$$

— comlex # for CT AMPlitude

∗ Pulse Phase changes coh Tx AMP by $e^{-i\Delta P\phi}$ complex #



$P_{uv} = -1$ $|u\rangle\langle v|$

$P_{rs} = 2$ $|r\rangle\langle s|$

~~$\Delta P = P_{uv} - P_{rs}$~~ → $\Delta P = P_{uv} - P_{rs}$

$= -1 - 2$

$\Delta P = -3$

∴ $\boxed{Z\phi = z_0\, e^{+i3\phi}}$

$\Delta P = P_{uv} - P_{rs}$

$$Z\phi = e^{-i\Delta P\phi}$$

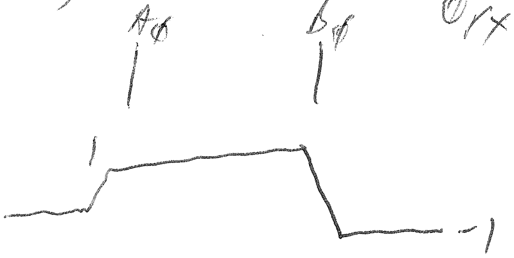
$$= e^{-i(-1-2)\phi}$$

$$\boxed{Z\phi = e^{-i3\phi} z_0}$$

$Z\phi = z_0 e^{-i3\phi}$

④ (17-10-4) Pathway Selection

ϕ_{rx}, ϕ_{dig}



$$s(t : \phi_A, \phi_B, \phi_{Rx}) = \sum_{path} S_{path}(t ; \phi_a, \phi_b, \phi_{rx})$$ } many paths here including above

* Now take ref sig w/ $\phi = 0$...

$$s(t : 0\,0\,0) = \sum_{path} S_p(t : 0\,0\,0)$$

$$\boxed{\text{use: } \quad z_\phi = z_0 e^{-i \Delta P \phi}}$$

$$\boxed{\begin{aligned} &S_{path}(t : \phi_A \phi_B \phi_{Rx}) = S_{path}(t : 0\,0\,0)\, e^{-i\phi_{path}} \\ &\phi_{path} - \Delta P_A \phi_A + \Delta P_B \phi_R + \phi_{Rx} \end{aligned}}$$

in above: $\Delta P_A = 1$ $\quad \therefore \phi_{path} = +\phi_A - 2\phi_B + \phi_{Rx}$

$\Delta P_B = -2$

(17.10.5) Sum Theorem

(1) $S = 1 + X + X^2 + X^3 + X^{n-2} + X^{n-1}$

$$\boxed{X = e^{i\left(\frac{2\pi p}{n}\right)}}$$

$S = 0$ if $p \neq n * \text{integer}$

$S = 1$ if $p = n * \text{integer}$

Proof: Mult (1) by X

$SX = X + X^2 + .. X^{n-1} + X^n$

$X \cdot X = X \cdot e^{i\left(\frac{2\pi p}{n}\right)}$

$X = e^{(i 2\pi p)\cancel{n}/\cancel{n}}$

$$\boxed{X^n = e^{i 2\pi p}}$$

⑤ $S = 1 + x + x^2, x^{n-1} \overset{x}{\Rightarrow} X S =$

$Sx = x + x^2 X^{n-4} = x + x^2 x^{n-1} + 1)$

$\therefore S = SX$

$0 = S(X-1)$

$$S = \begin{cases} 0 & \text{if } x \neq 1 \\ n & \text{if } X = 1 \end{cases}$$

S must vanish IF $X \neq 1$

$X = e^{i2\pi P/n}$ $\therefore \frac{P}{n} = 1 \neq$ integer For $S = n$ else no sig

---

10-6) Pathway selection

* can use Σ Theorem For φ-cycle selection

eq) m	ϕ_A	ϕ_B	ϕ_{Rx}
0	0	0	0
1	$\pi/2$	0	0
2	π	0	0
3	$3\pi/2$	0	0

Formulae: $\frac{2\pi \cdot m}{4}$ here

$\frac{2\pi 0}{4}$ $\frac{2\pi \cdot 1}{4}$ $\frac{2\pi \cdot 2}{4}$ $\frac{2\pi \cdot 3}{4}$

0 $\frac{\pi}{2}$ π $\frac{3\pi}{3}$

scans = N = 4

m = modulus(m, 4)   counter: m = 0, 1, .(N-1)

---

all Phases taken modulo 2π

* computers like 0 → 2π

⑥ $S_{path}(t,m) = S_{path}(t,0)\, e^{-i\phi_{path}(m)}$

$\phi_{path} = \Delta P_a \phi_A + \Delta P_b \phi_b + \phi_{Rx}$

From Formulae:

here all $\phi = 0$ except ϕ_A =

$\therefore \phi_{path} = \Delta P_a \phi_A = \Delta P_a \cdot \left(\frac{2\pi \cdot m}{4}\right)$

$$S_{tot,path}(t) = \sum_{m=0}^{N-1=3} S_{path}(t,m)$$

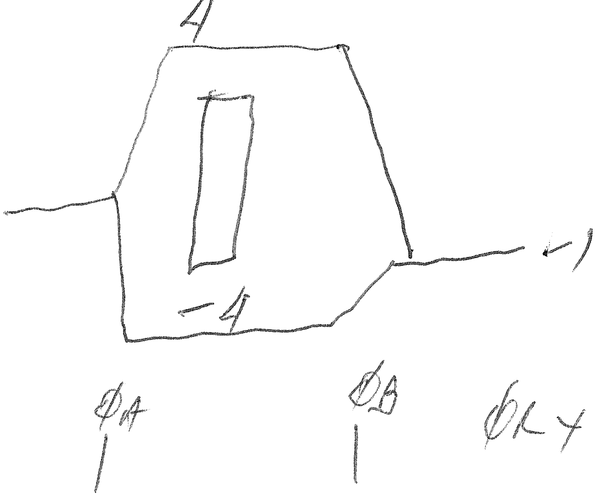
$$= S_{path}(t,0) \sum_{m=0} e^{(-i\phi_{path})}\,^{\cancel{-i\Delta\phi}m} = \sum_{m=0} e^{-i\Delta P_a\left(\frac{2\pi \cdot m}{4}\right)} \cdot S_{path}(t,0)$$

$X = e^{i\frac{2\pi P}{N}} \Rightarrow S = \begin{cases} 0 & \text{if } P \neq N * \text{integ} \\ 1 & \text{if } P = N * \text{integ} \end{cases}$ $\frac{2\pi P}{N}$ vs $\frac{2\pi P m}{4}$ $(N=4)$

$S_{tot,path} = \sum_{m=0} e^{-i\frac{2\pi \Delta P_a m}{4}}$ $S_{tot\,path} = \begin{cases} 0 & \text{if } \Delta P_A \neq 4 * \text{integ} \\ 1 & \text{if } \Delta P_A = 4 * \text{integ} \end{cases}$

$\therefore$ only $P = 4 * \text{integ}$ gets thru For:

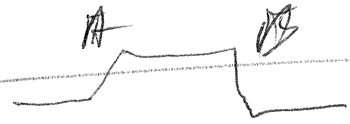
M =	ϕ_A	ϕ_B	ϕ_{Rx}
0	0	0	0
1	$\pi/2$	0	0
2	π	0	0
3	$3\pi/2$	4	4



⑦ $X = e^{i\frac{2\pi p}{N}} \Rightarrow S =$ 0 IF $p \neq N \times$ integ
1 IF $p = N \times$ integ

$S = 1 + X + X^2 + \ldots X^{N-2} + X^{N-1}$

$S(X-1) = 0$



0 → +1 → -1

17-10-2) Path Selection 2

m	ϕ_A	ϕ_s	ϕ_{Rx}	ϕ_{path} (0→1→-1)
0	0	0	0	0
1	π/2	0	0	π/2
2	π	0	0	π
3	3π/2	0	0	3π/2

remember
$Z\phi = Z0\, e^{-ip\phi}$

$\phi_{path} = \Delta p_a \phi_A + \Delta p_s \phi_s + \phi_{rx}$
$= 1\phi_A - 2\phi_s + \phi_r$

~~Next Now the~~ Above 0→1→-1 cancel out exactly

~~I~~ want to keep ϕ_{path} = const for our pathway 0→1→-1

∴

m	ϕ_A	ϕ_s	ϕ_{Rx}	ϕ_{Dig}	ϕ_{path}
0	0	0	0	0	0
1	π/2	0	0	-π/2	0
2	π	0	0	-π	0
3	3π/2	0	0	-3π/2	0

been leaving out ↓

$\phi_{path} = \phi_A - 2\phi_s + (\phi_{Dig} + \phi_{Rx})$

Keep in interval 0→2π tho,
$-\pi/2 = 3\pi/2$
$-\pi = \pi$ etc

Note 0→1→-1 gets thru but so does
$\Delta p_A = 1 + 4 * INT \Rightarrow \Delta p_A =$ -3, 1, 5, 9

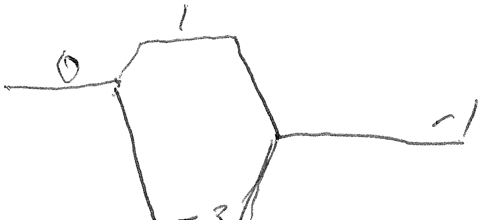
$e^{-i\Delta p_A\left(\frac{2\pi m}{4}\right)}$

p = 4*int

$\frac{2\pi p}{N}$ vs $\frac{2\pi p}{4}$

+4 & -4 get thru w/out ϕ_{rx}

using 4 step cycles



8)

*note 4 step selects cohs in steps of 4

*-however ϕ_{Dig} changed centre pos of selection

From $0 \to +1$

$\phi_A = \frac{2\pi \cdot m}{4}$ $\phi_B = \phi_{Rx} = 0$

ϕ_{Dig}: adjusted for const tot phase ~~of~~ for $0 \to 1 \to -1$

$\Delta p_A = 1$ $\Delta p_B = -2$

$$\therefore \phi_{path} = \phi_A \Delta p_A + \phi_B \Delta p_B + \phi_{Rx} + \phi_{Dig}$$

$$= \phi_A - 2\phi_B + \phi_{Dig}$$

$$= \phi_A + \phi_{Dig} \Rightarrow 0 \text{ in this selection}$$

$$\therefore \boxed{\phi_{dig} = -\phi_A = \frac{-2\pi m}{4} = \frac{-\pi m}{2}}$$

A general principle now:

1) write out desired CTP
2) Design # steps according to # neighboring paths suppressed
3) adjust ϕ_{Dig} to ϕ_{path} ~~so as~~, on each step of cycle so as to select desired CTP.

17-10-8) CTP select III

$\phi_A = \phi_{Rx} = 0$

$\phi_B = \frac{2\pi m}{4}$

$\phi_P = -2\phi_B + \phi_{Dig}$

$\phi_P = -2\phi_B$

$0 \to 1 \to +1$

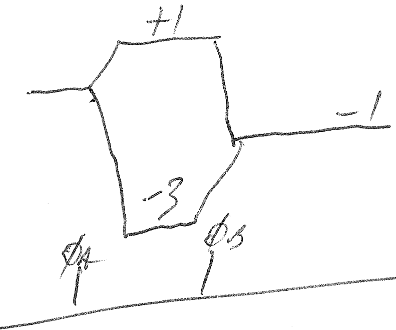
$\Delta p_A = 1$ $\Delta p_B = -2$

$\phi_{path} = \Delta p_A \phi_A + \Delta p_B \phi_B + \phi_{Rx} + \phi_{Dig}$

$= 0$ ~~+~~ $-2\phi_B$

M	ϕ_A	ϕ_B	ϕ_{Rx}	ϕ_{Dig}	ϕ_{Path}
0	0	0	0	0	0
1	0	$\pi/2$	0	π ~~$\pi/2$~~	~~$3\pi/2$~~ π
2	0	π	0	~~0~~ 0	$2\pi = 0$
3	6	$3\pi/2$	0	π	~~$\pi/2$~~ $3\pi = \pi$

⑨



For above cycle

17-10-9) Selection of a single pathway

$n \geq 8$ For success $P \leq 4$

just 4 Quantum

eg) $0 \to (-3) \to (-1)$

$$S_{path} = S_{path}(t,0)\, e^{-i\phi_{path}(m)}$$

Formulae:

$m = \mathrm{mod}(m, 8)$ $\quad \frac{2\pi \cdot m}{8}$

$m = 0, .. (N-1)$

$$\Rightarrow e^{\frac{i2\pi p}{N}} \text{ vs } e^{i2\pi pm/8}$$

$$\therefore \phi_{path} = \Delta p_a \phi_A + \Delta p_b \phi_B + \phi_{rx} + \phi_{dig}$$

~~$= \phi_B + \phi_{dig}$~~

$$\phi_{pa} = \Delta p_a \phi_A + \Delta p_b \phi_B + \phi_{rx} + \phi_{dig}$$

$$= 0 + 2\phi_B + \phi_{dig}$$

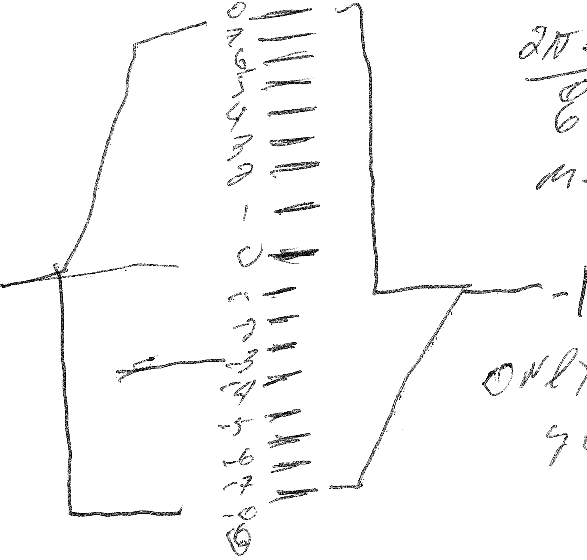
$$S_t = \begin{cases} 0 \text{ if } p \neq N * \text{integ} \\ 1 \text{ if } p = N * \text{integer} \end{cases}$$

For $\mathrm{mod}(m, 8) \Rightarrow$

$$S_t = \begin{cases} 0 \text{ if } p \neq 8 * \text{Integer} \\ 1 \text{ if } p = 8 * \text{Integer} \end{cases}$$

---

m	ϕ_A	ϕ_B	ϕ_{RX}	ϕ_{Dig}
0	0	0	0	0
1	0	$\pi/4$	0	0
2	0	$2\pi/4$	0	0
3	0	$3\pi/4$	0	0
4	0	$4\pi/4$	0	0
5	0	$5\pi/4$	0	0
6	0	$6\pi/4$	0	0
7	0	$7\pi/4$	0	0



$\frac{2\pi \cdot m}{8} = \frac{\pi \cdot m}{4}$

$m = 0 .. 7$

Only +8 & -8 get thru

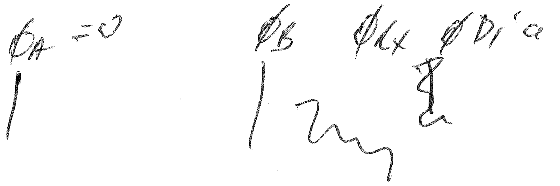
10) however, remember can change center of ± 8 via ϕ_{Dig}

$$\phi_{path} = \phi_A \Delta P_a + \phi_B \Delta P_b + \phi_{rx} + \phi_{Dig}$$

$$= -3\phi_A + 2\phi_B + \phi_r + \phi_D$$

$0 \longrightarrow -3 \longrightarrow -1$

$\Delta P = -3 \quad \Delta P = +2$



$$\phi_{path} = 2\phi_B + \phi_D = 0$$

$$\therefore \boxed{\phi_D = -2\phi_B}$$

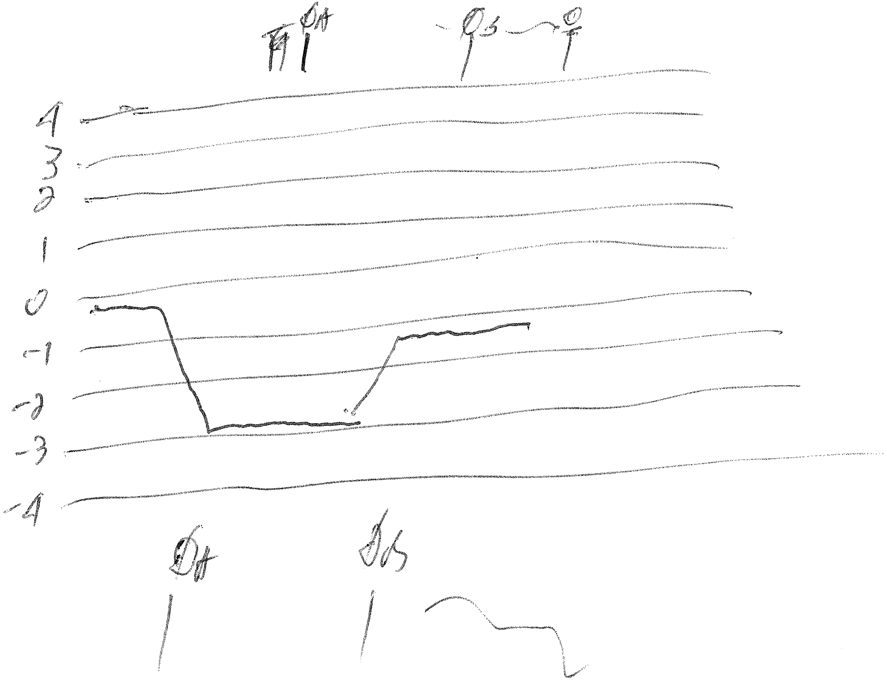
~~ΔP = m~~

$m = mod(m, 8)$

$$\frac{2\pi \cdot m}{8} = \frac{\pi m}{4}$$

∴

m	ϕ_B	ϕ_{A}	ϕ_R	ϕ_D		ϕ_{path}
0	0	0	0	0	0	0 0
1	$\pi/4$	0	0	$-\pi/2$	$3\pi/2$	0
2	$2\pi/4$	0	0	$-\pi$	π	0
3	$3\pi/4$	0	0	$-\frac{6\pi}{4}$	$\pi/2$	0
4	$4\pi/4$	0	0	$-\frac{8\pi}{4}$	0	0
5	$5\pi/4$	0	0	$-10\pi/4$	$3\pi/2$	0
6	$6\pi/4$	0	0	$-12\pi/4$	π	6
7	$7\pi/4$	0	6	$-14\pi/4$	$\pi/2$	



-3 + 8 Get thru step

-3 - 8

or 5, -13 = P

Hardware Restrictions

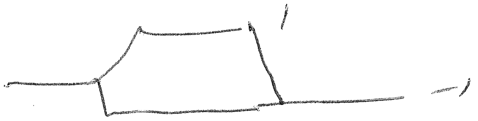
$$\phi_{dig} = int * \frac{\pi}{2}$$

* ∴ if $\phi_A \neq 0$ we would need $\phi_{DIG} = \pi/4$

NOT recommended

① 17-10-11 Dual Path Selection

$0 \rightarrow 1 \rightarrow -1$



$0 \rightarrow -1 \rightarrow -1$

* Done by ~~selection~~ setten m = # steps = to the diff in order ∴ ~~Other~~ $\Delta P = 2$

∴ $m =$ $\frac{2\pi}{m}$

m	ϕ_A	ϕ_B	ϕ_C	ϕ_D
0	0	0	0	0
1	π	0	0	π

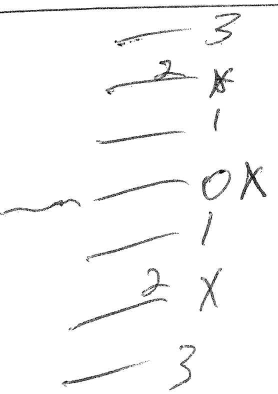
Formal selection is done by choosing one of paths – doesn't matter which ∴ $P = -1$

$\phi = \frac{2\pi m}{2} = \pi \cdot m$ $\quad 0 \rightarrow -1 \rightarrow -1$

$$\phi_P = -\phi_A - 0\phi_B + \phi_C + \phi_D$$

$$= -\phi_A + \phi_D = 0 \quad \therefore \quad \phi_A = \phi_D$$

Note 2 step 0-π



0,1,3 etc Get Thru

$e^{i\pi m P/2}$

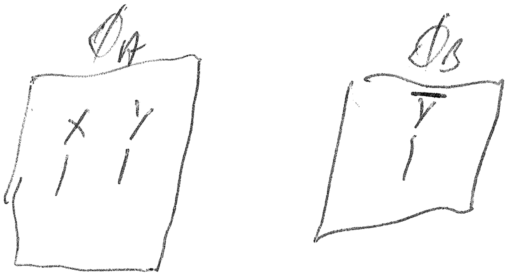
∴ P

$S = \phi$ IF $P = 2 * \text{Int}$

2 Step → $P \pm 2 \cdot$ Integ

4 Step → $P \mp 4 *$ Integ

② 17-10-12 internal phases



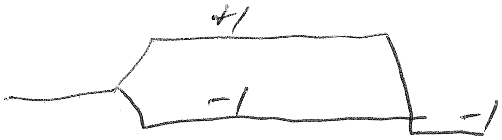
X3 pulses in 2Φ blocks

m	ϕ_1	ϕ_2	ϕ_3	ϕ_{rx}	ϕ_D
0	0	$\pi/2$	$3\pi/2$	0	0
1	π	$3\pi/2$	$3\pi/2$	0	π

$\phi_1 = \phi_A$

$\phi_2 = \phi_A + \pi/2$

$\phi_3 = \phi_B + 3\pi/2$



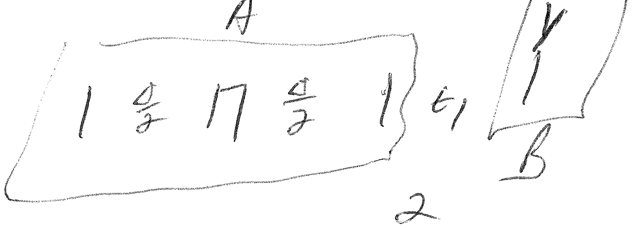
m	ϕ_A	ϕ_B	ϕ_r	ϕ_D
0	0	0	0	0
1	π	0	0	π

$\phi_p = 0 \rightarrow 1 \rightarrow -1$

$\phi_p = -\phi_A + \phi_D$

$\therefore\ \phi_D = \phi_A$

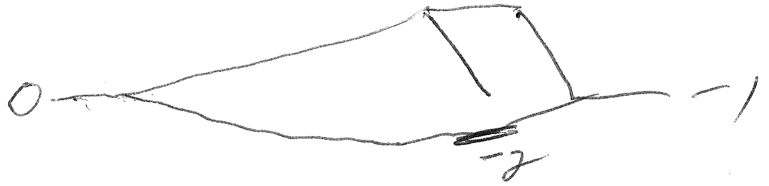
17-10-12 inadequate int phases



4-step

$e^{2\pi \frac{mp}{4}}$ $p \pm 4 \times$ int

get th/4



$\phi_p = \phi_A \Delta p_A + \phi_B \Delta p_B + \phi_D$

$= 2\phi_B + \phi_r$

$\phi_D = 2\phi_B$

$\phi_1 = \phi_A + 0$

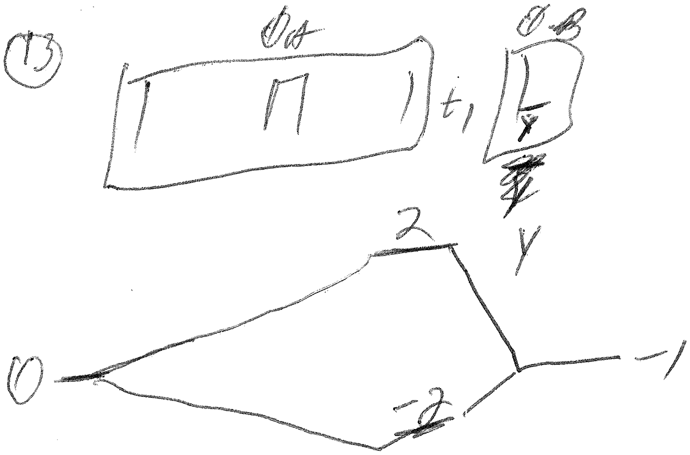
$\phi_2 = \phi_A + 0$

$\phi_3 = \phi_A + 0$

$\phi_4 = \phi_B + \pi/2$

m	ϕ_A	ϕ_B	ϕ_r	ϕ_D	ϕ_{int}
0	0	0	0	0	0
1	0	$\pi/2$	6	π	0
2	0	π	ϕ	0	0
3	6	$3\pi/2$	6	π	6

⑬



INADEQUATE

$\phi_A = \phi_A \Delta P_A + \phi_B \Delta P_B + \phi_D + \phi_R$

$\phi_A = 0 + ~~3~~ 1\phi_B + \phi_r$

$\therefore \phi_r = -\phi_B$

4 step $\therefore$ P ± 4·INT gets thru

$\therefore$ 2 − 4 = −2 as well

M	ϕ_A	ϕ_B	ϕ_r	ϕ_D
0	0	0	0	0
1	0	1	0	3
2	0	2	0	2
3	0	3	0	1

$\phi_1 = \phi_A + 0$

$\phi_2 = \phi_A + 0$

$\phi_3 = \phi_A + 0$

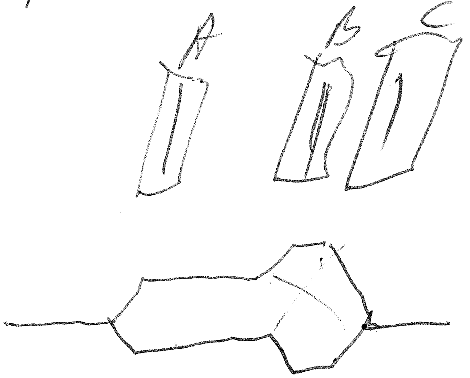
$\phi_4 = \phi_B + 1$

M	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_r	ϕ_D
0	0	0	0	~~3~~ 1	0	~~1~~ 0
1	0	0	0	~~0~~ 2	0	~~0~~ 3
2	0	0	0	3	0	~~2 3~~ 2
3	0	0	0	~~2~~ 0	0	~~2~~ 1

⑭ Nested Phase cycling

* More than one stage of CTP needed

DQ-COSY



nested every block in C requires A tobe fixed.

$\Delta P_A = \pm 1$

∴ 4 step

$\Delta P_C = 3$

$\Delta P_C = 1$

∴ 4 step

floor(X) = largest int that is not > X. Rounds down

eg) $fl(0.9)=0$ $fl(1.9)=1$ $fl(1)=1$ $fl(-1.9)=-2$

∴ 2 step ϕ_A nested in 4-step ϕ_C can be specified

$$\phi_A = \frac{2\pi m}{2} = \pi m \quad m = 0, 1$$

$$\phi_B = 0$$

$$\phi_C = \frac{2\pi\, fl(m/2)}{4} = \frac{\pi}{2} fl\left(\frac{m}{2}\right)$$

$\phi_X = 0$

$$0 \xrightarrow[\Delta P=1]{} 1 \xrightarrow[\Delta P=1]{} 2 \xrightarrow[\Delta P=3]{} -1$$

$$\phi_R = \Delta P_A \phi_A + \Delta P_B \phi_B + \Delta P_C \phi_C + \phi_D$$

$$\phi_R = \phi_A + 3\phi_C + \phi_{Dig}$$

$$\therefore \phi_D = -\phi_A + 3\phi_C$$

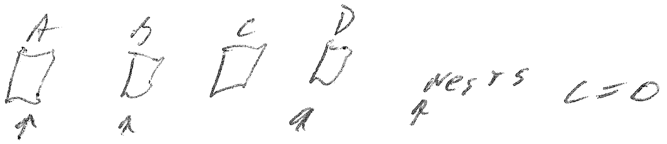
$$= -\phi_A + 3\left(\frac{\pi}{2} fl\left(\frac{m}{2}\right)\right)$$

$$\phi_D = -\phi_A + 3\, fl(m/2)$$

$=$

m	$fl(\frac{m}{2})$	ϕ_A	ϕ_B	ϕ_C	ϕ_r	ϕ_D
0	0	0	0	0	0	~~2~~ 0
1	0	2	0	0	0	2
2	1	0	0	1	0	3
3	1	2	0	1	0	1
4	2	0	0	2	0	0 2
5	2	2	0	2	0	0 0
6	3	0	0	3	0	3 1
7	3	2	0	3	0	3 3

⑮ 17.10.15 Nested 11



$c=0$

$$\phi_A = \frac{2\pi \cdot m}{n_a}$$

$n = n_a \cdot n_b \cdot n_d$

* note fl ÷ all prev steps $\frac{m}{n_a n_b}$ eg)

$$\phi_B = \frac{2\pi}{n_b} fl\left(\frac{m}{n_a}\right)$$

$$fl\left(\frac{m}{n_a}\right) = fl\left(\frac{m}{2}\right)$$

$$\phi_C = 0$$

$$\phi_D = \frac{2\pi}{n_D} fl\left(\frac{m}{n_a n_b}\right)$$

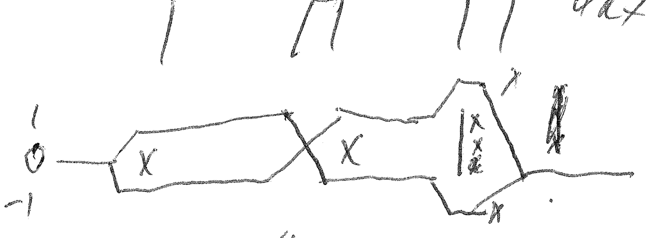
ϕ_A nested in ϕ_B

ϕ_B nested in ϕ_D

eg) $n_a = 2$ $n_b = 2$ $n_d = 4$ ∴ $n = 16$

m	$fl(m/2)$	$fl(\frac{m}{4})$	ϕ_A	ϕ_B	ϕ_C	ϕ_D	ϕ_D	ϕ_{RF}	ϕ_{DIG}
0	0	0	0	0	0	0			
1	0	0	2	0	0	0			
2	1	0	0	2	0	0			
3	1	0	2	2	0	6			
4	2	1	0	0	0	1			
5	2	1	2	0	0	1			
6	3	1	0	2	0	1			
7	3	1	2	2	0	1			
8	0	2	0	0	0	2			
9	0	2	2	0	0	2			
10	1	2	0	2	0	2			
11	1	2	2	2	0	2			
12	2	3	0	0	0	3			
13	2	3	2	6	0	3			
14	3	3	0	2	0	3			
15	3	3	2	2	6	3			

16) (a) 1N9D $\overset{X}{\phi_A}$ $\overset{X}{\phi_B}$ $\overset{X}{\phi_C}$ $\overset{Y}{\phi_D}$ $\phi_d + \phi_{Dig}$



2 4

$\Delta P = \pm 1$ $\Delta P = \pm 2'$ ~~$\phi \rightarrow$~~ $\Delta P = -3$

1

2 4 4

$\phi_1 = \phi_A$

$\phi_2 = \phi_B$

$\phi_3 = \phi_C + 0$

$\phi_4 = \phi_D + 1$

$$\phi_A = \frac{2\pi \cdot m}{n_a} = \frac{2\pi}{2} \cdot m = \pi \cdot m$$

$$\phi_B = \frac{2\pi}{n_B} fl\left(\frac{m}{n_a}\right) = \frac{2\pi}{4} fl\left(\frac{m}{n_a}\right) = \frac{\pi}{2} fl\left(\frac{m}{\cancel{2} n_a}\right)$$

6

$$\phi_C = 0$$

$$\phi_D = \frac{2\pi}{n_d} fl\left(\frac{m}{n_a \cdot n_B}\right) = \frac{2\pi}{4} fl\left(\frac{m}{8}\right) = \frac{\pi}{2} fl\left(\frac{m}{8}\right)$$

$$n_T = n_a \cdot n_B \cdot n_d = 32$$

$$\phi_B = 1 \cdot fl\left(\frac{m}{2}\right)$$

$$\phi_D = 1 \cdot fl\left(\frac{m}{8}\right) + 1$$

$0 \rightarrow 1 \rightarrow -1 \rightarrow -2 \rightarrow -1$

$\Delta P = 1$ -2 -1 $+1$

$\phi_P = \phi_1 \Delta P_1 + \phi_2 \Delta P_2 + \phi_3 \Delta P_3 + \phi_4 \Delta P_4 + \phi_r + \phi_{Dig}$

= Remember select P_1 & P_4 ∴ Take dif($1 - -1 = 2$

= ~~$\phi_2 \cdot 2$~~ + $\phi_P =$

⑰

m	$\frac{m}{2}$ fl($\frac{m}{2}$)	$\frac{m}{8}$ fl($\frac{m}{8}$)	ϕ_A	ϕ_B	ϕ_C	ϕ_D	ϕ_{Dig}
0	0	0	0	0	0	1	0
1	0	0	2	0	0	1	2
2	1	0	0	1	0	1	2
3	1	0	2	1	0	1	0
4 0	2	0	0	2	0	1	0
5 1	2	0	2	2	0	1	2
6	3	0	0	3	0	1	2
7 3	3	0	2	3	0	1	0
8 (0)	0	1	0	0	0	2	3
9 (1)	0	1	2	0	0	2	1
10 (2)	1	1	0	1	0	2	1
11 (3)	1	1	2	1	0	2	3
12 (0)	2	1	0	2	0	2	3
13 (1)	2	1	2	2	0	2	1
14 (2)	3	1	0	3	0	2	1
15 (3)	3	1	2	3	0	2	3
16	0	2	0	0	0	3	2
17	0	2	2	0	0	3	0
18	1	2	0	1	0	3	0
19	1	2	2	1	0	3	2
20	2	2	0	2	0	3	2
21	2	2	2	2	0	3	0
22	3	2	0	3	0	3	0
23	3	2	2	3	0	3	2
24	0	3	0	0	0	0	1
25	0	3	2	0	0	0	3
26	1	3	0	1	0	0	3
27	1	3	2	1	0	0	1
28	2	3	0	2	0	0	1
29	2	3	2	2	0	0	3
30	3	3	0	3	0	0	3
31	3	3	2	3	0	0	1

$\phi_{Dig} = -\phi_A + 2\phi_B - \phi_D$

$0 \rightarrow 1 \rightarrow -1 \rightarrow -2 \rightarrow -1$

$\Delta\rho_1 = 1 \quad \Delta\rho_2 = -2 \quad \Delta\rho_3 = -1 \quad \Delta\rho_4 = +1$

$\phi_0 = \phi_A \Delta\rho_1 + \phi_B \Delta\rho_2 + \phi_C \Delta\rho_3 + \phi_D \Delta\rho_4$

$= \phi_A - 2\phi_B - \phi_C + \phi_D$

$= \pi \cdot m - \pi \, fl(\frac{m}{2}) - 0 + \frac{\pi}{2} fl(\frac{m}{8})$

$\phi_1 = \pi \cdot m$
$- \pi \, fl(\frac{m}{2})$
$+ \frac{\pi}{2} fl(\frac{m}{8})$

$= 2 \cdot m$
$- 2 \cdot fl(m/2)$
$+1 \, fl(\frac{m}{8})$ ~~0~~

$+ \phi_{Dig} = 0$

or $\phi_r = -\phi_A + 2\phi_B - \phi_D$

$$\boxed{\phi_{Dig} = -2m + 2 \, fl(\frac{m}{2}) - 1 fl(\frac{m}{8})}$$

⑱

$\phi_D = -2(9) + 0 - 1$

$= -18 - 1 = -\frac{19}{4} = -4\,1/4 =$ ~~$1/4$~~

ϕ 4 − x
8 − x
12
16
20
24

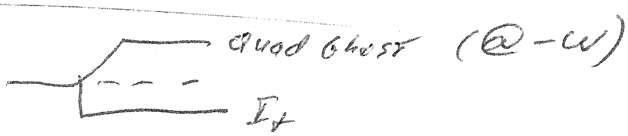
$-2 \cdot 7 + 2 \cdot 3 = -14 + 6 = -8 = 0$

$-2 \cdot 10 \quad 2 \cdot 1 \quad -1$

$-20 + 2 - 1 = -19 \rightarrow 1$

$-2 \cdot 11 \quad 2 \cdot 1 \quad -1 = -22 + 2 - 1 = -21 \rightarrow 3$

* use program to calc...

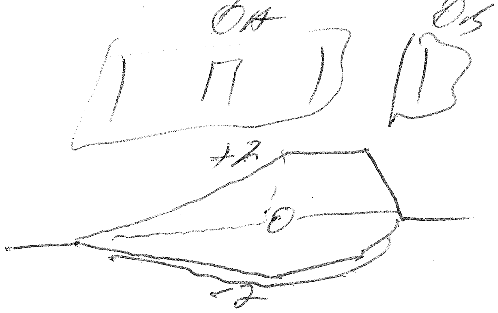


R_x Artefacts

* remove R_x-offset by ϕ-cycling it $0 \rightarrow 3$

recall 4-step quad $0 \rightarrow 2 \rightarrow -1$ & $0 \rightarrow -2 \rightarrow -1$

m	ϕ_A	ϕ_B	ϕ_{Rx}	ϕ_{DIG}
0	0	0	0	0
1	0	1	0	3
2	0	2	0	2
3	0	3	0	1



$\phi_{path} = \Delta p_1 \phi_A + \Delta p_2 \phi_B$
$= 0 + 1 \cdot \phi_B + \phi_{Rx}$

$\phi \quad \therefore \phi_{DIG} = -\phi_B$

or $\phi_{DIG} = 3\phi_B$

⑲

M
0
1
2
3

$\Phi_1 = \Phi_A$

$\Phi_2 = \Phi_A$

$\Phi_3 = \Phi_A$

$\Phi_4 = \Phi_B + \pi/2$

$\Phi_A \rightarrow \overset{\Phi_A}{\boxed{1 \quad \Pi \quad 1}}$

M =	Φ_A	Φ_B	Φ_{RX}	Φ_{DIG}
0	0	~~0~~ ~~1~~ 0	0	~~3~~ 0
1	0	~~1~~ ~~2~~ 1	0	~~2~~ 3
2	0	~~2~~ ~~3~~ 2	0	~~1~~ 2
3	0	~~3~~ ~~0~~ 3		~~0~~ 1
4	0	~~1~~ 0	1	3
5	0	~~2~~ 1	1	2
6	0	~~3~~ 2	1	1
7	0	~~0~~ 3	1	0
8	0	1 0	2	2
9	0	2 1	2	1
10	0	3 2	2	0
11	0	~~0~~ 3	2	3
12	0	~~1~~ 0	3	1
13	0	~~2~~ 1	3	~~0~~ [illegible]
14	0	~~3~~ 2	3	~~3~~ 3
15	0	~~0~~ 3	3	~~1~~ 2

$\Phi_{DIG} = -\Phi_B \mp \Phi_{RX}$ NOW

①

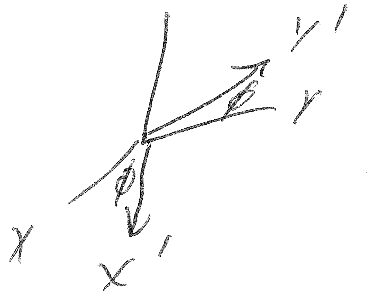
Phase cycling Notes

ZQC (e^0)	SQC e	DQC
I_0 (e^0)	I_+	I_+S_+
S_0	I_-	I_-S_-
I_-S_+	S_+	
I_+S_-	S_-	
I_0S_0	I_+S_0	
$\mathbb{1}$	I_0S_+	
Doesn't change	I_-S_0	
	I_0S_-	
σ_0	σ_1	σ_2 ← New basis w/ ϕ shift

$$\cancel{\rho(t)(\phi)}\ \rho_t(\phi=0)=\sum_{p=-2}^{2}\sigma_p \rightarrow$$

Phase shift	σ_{-2}	σ_{-1}	σ_0	σ_1	σ_2
	I_-S_-	I_- S_- I_0S_- I_-S_0	$\mathbb{1}$ I_0 S_0 I_0S_0 I_+S_- I_-S_+	I_+ S_+ I_0S_+ I_+S_0	I_+S_+
Phase shift	$e^{i2\phi}$	$e^{i\phi}$	e^0	$e^{-i\phi}$	$e^{-i2\phi}$

*remember RF phase redefines rot. frame



②

1) Start w/ σ_0 $I_z + S_z$

2) 1^{st} Pulse $\rightarrow$ σ_1

$\sigma_0 \rightarrow$ signal left on (z or $-z$)

σ_{-1}

3) σ_p is conserved during H_J & H_{cs} etc evolution

4) If we have N-spins, 2^{nd} pulse creates, $\sigma_N \rightarrow \sigma_{-N}$
& all start from $\sigma_1, \sigma_0, \sigma_{-1}$

Density matrix phase-shifted

5) phase shifts $\rightarrow$ $\sigma_p \overset{\phi}{\Rightarrow} \sigma_p e^{-iP\phi}$

$$\text{or } \rho_t(0) = \sum_{P=-N}^{N} \sigma_P \quad \text{to} \quad \boxed{\rho_t(\phi) = \sum_{P=-N}^{N} \sigma_p e^{-i\phi P}}$$

Looks like FT!

* can now follow evolutions of a particular coh.

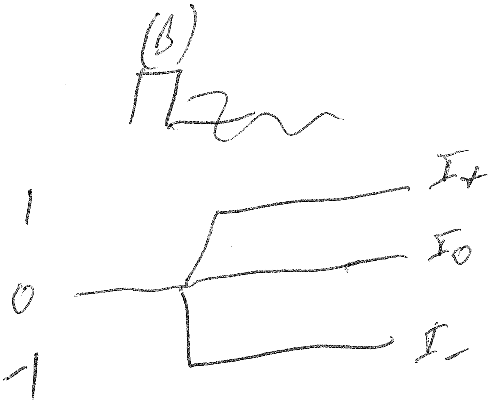
Detect S: $M = 2N+1$ phase shifted expts
& combine signals by

$$\boxed{\sigma_p = \sum_{K=1}^{M} S(\phi_K) e^{iP\phi_K} \; ; \; \phi_K = \frac{2\pi(K-1)}{M} \quad (K=1,2,3..)}$$

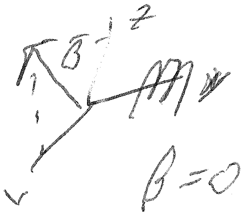
P = coherence order, eg) $-1, 0, 1$ ...

σ_p = all sph. ops according to P, see table

(a) $\rho(\phi=0) = c(\beta)\cdot I_0 + s(\beta)e^{-i\omega t} I_+ + s(\beta)e^{i\omega t} I_-$



I_- : detect $Tr(\rho\cdot I_+)$?
$Tr(\rho\cdot I_-)$



$\beta = 0$

$c(\beta) I_0 = I_0$

$s(\beta) I_+ = 0$

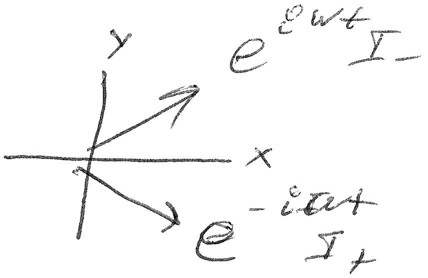
$s(\beta) I_- = 0$

---

remember

$I_x \xrightarrow{H_{cs}} I_x c(\omega t) + I_y s(\omega t)$

$= \frac{1}{2}\left[I_+ e^{-i\omega t} + I_- e^{i\omega t} \right]$.



Now shift RF ($\phi=\pi$)

$\rho(\phi=\pi) = c(\beta)\cdot I_0 \cdot e^0 + s(\beta)e^{-i\omega t}\cdot I_+ \cdot \underbrace{e^{-i\pi}}_{-1} + s(\beta)e^{i\omega t}\cdot I_- \cdot \underbrace{e^{i\pi}}_{-1}$

$e^{i\pi} = c(\pi) + i s(\pi)$
$= -1 + 0$

$\Rightarrow \rho(\phi=0) = c(\beta) I_0 + s(\beta)e^{-i\omega t} I_+ + s(\beta)e^{i\omega t} I^-$

$-\rho(\phi=\pi) = -c(\beta) I_0 + s(\beta)e^{-i\omega t} I_+ + s(\beta)e^{i\omega t} I^-$

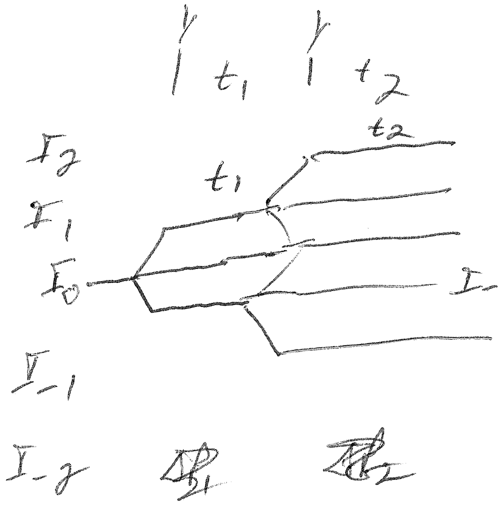
$\rho_0 - \rho_\pi \quad = 0 + 2s(\beta)e^{-i\omega t} I_+ + 2s(\beta)e^{i\omega t} I_-$

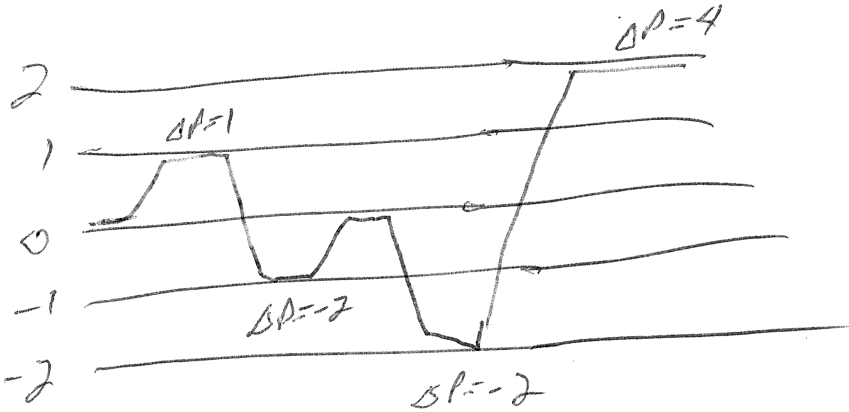
* usually done in software

2D NMR Phasing

* Free evol is just orders of coh.

$S(t) = Tr(\rho \cdot I_+)$





$\Delta\phi_i$ = change in RF ϕ

ΔP_i = change in coh orde

$\Rightarrow$ Density matrix changes

$$\boxed{e^{-i\Delta\phi_i \Delta P_i} = \rho(\Delta P)}$$

~~Cong~~ group ϕ-shifts of expt into a vector $\vec{\phi}$

$$\vec{\Delta\phi} = (\Delta\phi_1, \Delta\phi_2, \Delta\phi_3 .. \Delta\phi_N)$$

Now express Final Dens mat interms of absence of phase shifts (ie $\Delta\phi = 0$)

$$\boxed{\rho(\Delta\phi) = \sum_{\Delta P} \rho(\vec{\Delta P}, \vec{\Delta\phi} = 0) e^{-i\vec{\Delta P}\vec{\Delta\phi}}}$$

Suppose we want to detect sig $\rho(\Delta P)$

* Sig also depends on ϕ_{rx} $\quad S(t) = Tr(\rho \cdot F_+) e^{i(\phi_{Tx} - \phi_{Rx})}$

we only want to Finish @ & $p=-1$

Detect $Tr(\rho I_+) \equiv (p=-1)$

$$\sum_{i=1}^{N} \Delta p_i = -1$$

$$\boxed{s(t) = \rho(\vec{\Delta p}, \vec{\Delta\phi}=0)\, e^{i\underbrace{(-\vec{\Delta p}\cdot\vec{\Delta\phi})}_{\phi_{Rx}}}\, e^{-i\phi_{Rx}}}$$

This $\rightarrow\rightarrow$ leads to $-\vec{\Delta p}\cdot\vec{\Delta\phi} - \phi_{Rx} = 0$

$$s(t) = \rho(\vec{\Delta p}, \vec{\Delta\phi}=0)\, e^{0}$$

$$s(t) = \rho($$

$$\boxed{\phi_{Rx} = -\sum_{i=1}^{N} \Delta p_i \Delta\phi_i}$$

Fullfill this & $I_0 \rightarrow I_-$ start Finish

N = # of expts

---

remember $\Delta\phi_i = \frac{2\pi}{k_g}$ $\quad G_p = \sum_{k=1}^{M} s(\phi_k)\, e^{ip\phi_k}$

$$\phi_K = \frac{2\pi(K-1)}{M}$$

$M = 2N+1 = \#$ expts

N = # of spins coupled

---

when we phase shift we let a manifold of coh (p) thru.

$$\phi_i = \frac{2\pi(K-1)}{M} \qquad p_i,\ p_i \pm k_i,\ p_i \pm 2k_i \text{ etc}$$

ⓔ $\rho_0 \Rightarrow \quad I_0 \quad I_+ \quad I_-$

$\rho_1 \Rightarrow I_0 e^{-i\pi/3} \quad I_+ e^{-i2\pi/3} \quad I_-$

$\rho_2 \Rightarrow I_0 e^{-i2\pi/3} \quad I_+ e^{-i4\pi/3} \quad I_-$

$$S(t) = 3I_- + I_0\left(e^0 + e^{-i\pi/3} + e^{-i2\pi/3}\right) + I_+\left(e^0 + e^{-i\pi/3} + e^{-i2\pi/3}\right)$$

$$= 3I' + I_0 \begin{pmatrix} 1 \\ -0.5 - i0.8 \\ -0.5 + i0.8 \end{pmatrix} + I_+ \begin{pmatrix} 1 \\ -0.5 - 0.8i \\ -0.5 + 0.8i \end{pmatrix}$$

$S(t) = 3I_-$ Much like A FT

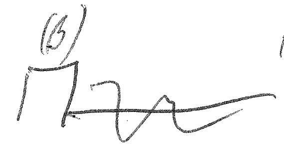
$$S(t) = \underset{\nearrow}{\rho(\vec{\Delta\rho})}\, e^{i\phi_{TX}} \cdot e^{-i\phi_{RX}}$$

eg) $\left.\begin{matrix} I_+ \\ I_- \end{matrix}\right\} = \rho(\Delta\rho)$ = what you select

---

$\phi = \frac{2\pi(k-1)}{M}$ eg) if $M=2$ $\phi = \pi$

$\phi_k = \cancel{21} \sum_{k=1}^{M} \frac{2\pi(k-1)}{M}$



~~$\rho(\pi)(t) = c(\beta) I_0$~~ $= \rho_0 - \rho(\pi)$ again

$\phi_{k} \Rightarrow \sum_{k=1}^{M} \frac{2\pi(k-1)}{M} - 0, \pi$

$\rho(0) = c(\beta) I_0 + s(\beta) I_+ e^{-(i\omega t)} I_+ e^0 + s(\beta) I_- e^0 e^{i\omega t}$

$= \cancel{c\beta} I_0 c\beta + s\beta I_+ e^0 + s\beta e^0 I_-$

$e^{\pm i\pi} = -1$

$\rho(\pi) = I_0 c\beta + s\beta I_+ e^{-i\pi} + s\beta I_- e^{i\pi}$

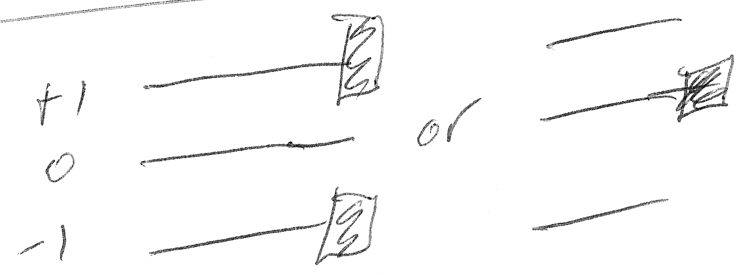
$\rho_0 = I_0 + I_+ + I_-$

add → I_0

sub → I_+ & I_-

$\rho_\pi = I_0 - I_+ - I_-$

$\rho_0 =$



$\rho_0 = I_+ + I_0 + I_-$

M=3 can elim Quad ghost

$\rho_{\pi/3} =$

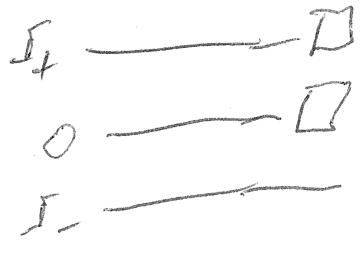
$c(\cancel{\tfrac{2\pi}{3}})$

$c(\frac{\pi}{3}) = -0.5$

$s(\frac{\pi}{3}) = 0.86$

$c(\frac{2\pi}{3}) = -0.5$

$s(\frac{2\pi}{3}) = -0.86$



① **Phase notes** ϕ_A ϕ_s

$\phi_{path} = \phi_A \Delta_a + \phi_s \Delta_s + \phi_{Dig}$

$e^{\frac{i 2\pi i p}{1}}$

$0 \to 1 \to -1$

$\Delta_a = 1$ $\Delta_s = -2$

=

$n_a = 1$

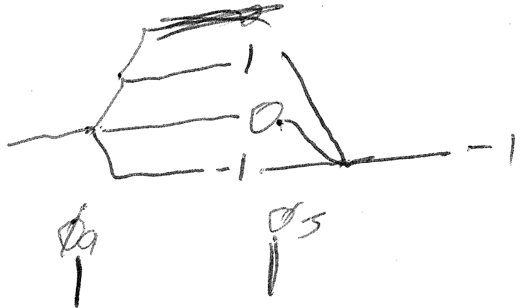
m	ϕ_A	ϕ_s	ϕ_R	ϕ_D
0	0	0	0	0

$\phi_A = \frac{2\pi}{1} \cdot (m)$

$m = 0, 1 \ (n_a - 1)$

$= 0$

$\nrightarrow S \begin{cases} 0 \text{ if } p \neq \text{int} \times 1 \\ 1 \text{ if } p = \text{int} \times 1 \end{cases}$

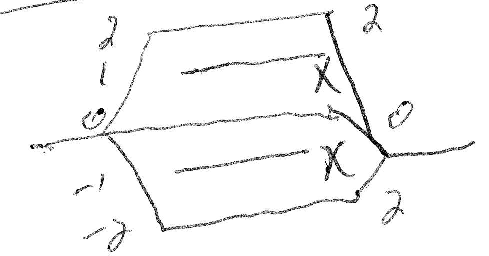


So $n_a = 1$

1
0 get thru
-1

$\phi = 0$

$n_a = 2$



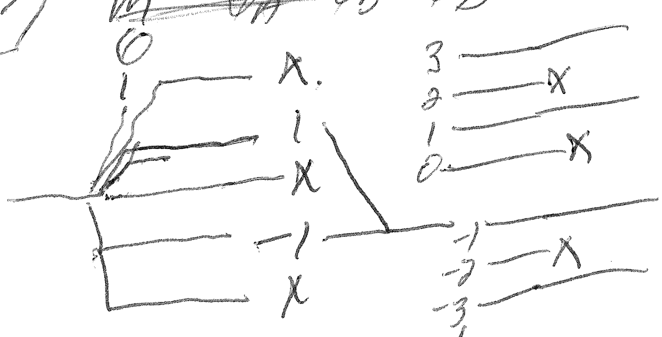
2
0 get thru
-2

$\phi = 0, \pi$

m	ϕ_A	ϕ_s	ϕ_D
0	0	0	0
1	π	0	0

$\phi_{Dig} \to$ changes p center $= 1 \ q-1$

~~m ϕ_A ϕ_s ϕ_D~~



$n_a = 2$

$\phi_p = \Delta_a \phi_1 + \Delta_s \phi_s + \phi_D$

$0 \to 1 \to -1$

$\phi_D = \phi_A - \phi_s + \phi_{Dig}$

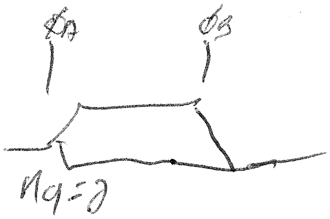
$\therefore \phi_{Dig} = -\phi_A + \phi_s$

m	ϕ_A	ϕ_s	ϕ_{Dig}
0	0	0	0
1	π	0	π

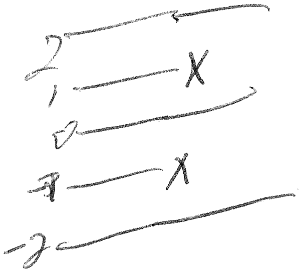
② ϕ_A ϕ_B

m	ϕ_A	ϕ_B	ϕ_D
0	0	0	0

$\phi_A = \frac{2\pi}{n_a}$



m	ϕ_A	ϕ_B	ϕ_D
0	0	0	0
1	π	0	0



$e^{i2\pi p/2} \Rightarrow S \{ \cancel{...}$

$\Rightarrow S = \begin{cases} 0 \text{ IF } p \neq \text{INT} * 2 \\ 1 \text{ IF } p = \text{INT} * 2 \end{cases}$

$\phi_{path} = 0 \to 0 \to -1$

$\Delta p = 0 \quad = -1$

$\phi_R = \phi_A \cdot 0 + \phi_B \cdot (-1) + \phi_D$

$\phi_{Dig} = -\phi_B$

← can select ±1 off 1st pulse too

$\Delta p_a = 1 \quad \Delta p_b = -2$

$\Delta p_a = -1 \quad \Delta p_b = 0$

$0 \to 1 \to -1$

$n_a = 2$ = $0 \to -1 \to -1$

$n_a = 2 \quad n_b = 1$

$\phi_A = \frac{2\pi \cdot m}{n_a} \quad \frac{2\pi \cdot m}{n_b}$

$= 0, \pi \quad 0$

$\phi_{path} = \phi_A \cdot 1 + \phi_B \cdot (-2) + \phi_{Dig}$

$\phi_{path} =$ ~~B~~

$\phi_{path} = \phi_A - 2\phi_B + \phi_{Dig}$

(for $0 \to 1 \to -1$)

m	ϕ_A	ϕ_B	ϕ_{Dig}
0	0	0	0
1	π	0	π

$\phi_{Dig} = -\phi_A$

③

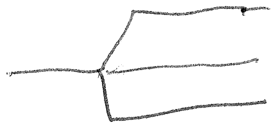
$$\phi_{Path} = \frac{2\pi}{na} \Delta P_a \cdot m \qquad m = 0, \ldots (Na-1)$$

$$S_{Sorh} = S_{Path}(t,0)\, e^{\left(-i\frac{2\pi \cdot m\, \Delta P_a}{na}\right)}$$

$$= S \begin{cases} 0 \text{ IF } \Delta P_a \neq \text{INT} * na \\ 1 \text{ IF } \Delta P_a = \text{INT} * na \end{cases}$$

$$X = e^{i\frac{2\pi P}{n}}$$

$$~~\S~~\ S = \begin{cases} 0 \text{ IF } P \neq \text{INT} * n \\ 1, \text{IF } P = \text{INT} * n \end{cases}$$



$$e^{i 2\pi \Delta P_a / na} = e^{i\frac{2\pi}{2}\cdot 1} = e^{i 2\pi \Delta P_a m / na}$$

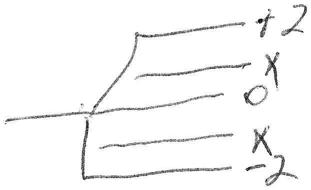
$$S = \begin{cases} 0 \text{ IF } \Delta P_a \neq 2 * \text{INT} \\ 1 \text{ IF } \Delta P = 2 * \text{INT} \\ \quad\quad \text{INC } 0 \end{cases}$$

$\Delta P_a = 1$

$na = 2$

	ϕ_A	ϕ_B	ϕ_{Rx}	ϕ_D
i. ~~#~~Pulse N:	1	1		

m	ϕ_A	ϕ_B	ϕ_C	ϕ_D
0	0	0	0	0
1	π	0	0	0

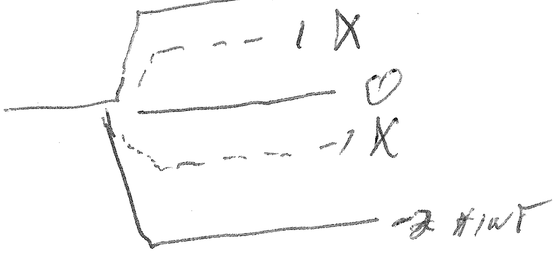


$$\phi_P = \phi_A \Delta P_a + \cancel{\phi_B \Delta P_B}^{0} + \cancel{\phi \Delta P_g}^{0}$$

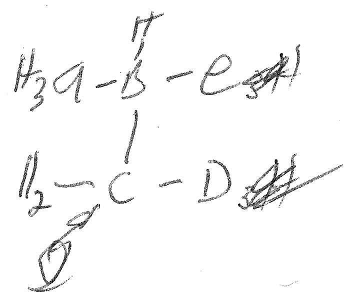
$$\phi_P = \phi_A \Delta P_a$$

$$S = \begin{cases} 0 \text{ IF } \Delta P_a \neq 2 * \text{INT} \\ 1 \text{ IF } \Delta P = 2 * \text{INT} \end{cases}$$

$$e^{i 2\pi \frac{\Delta P_a}{2} m}$$



II-16)

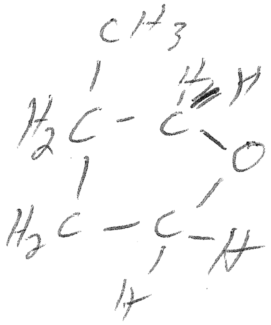


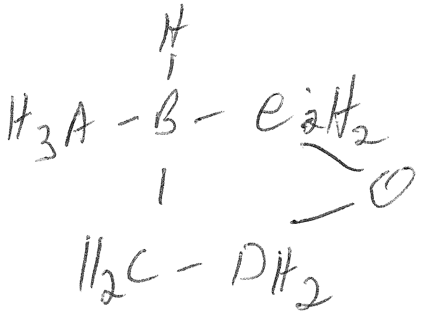
$C_5H_{10}O$

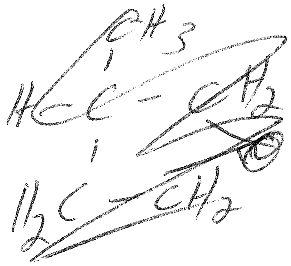
$a = 4$

$b = 2$

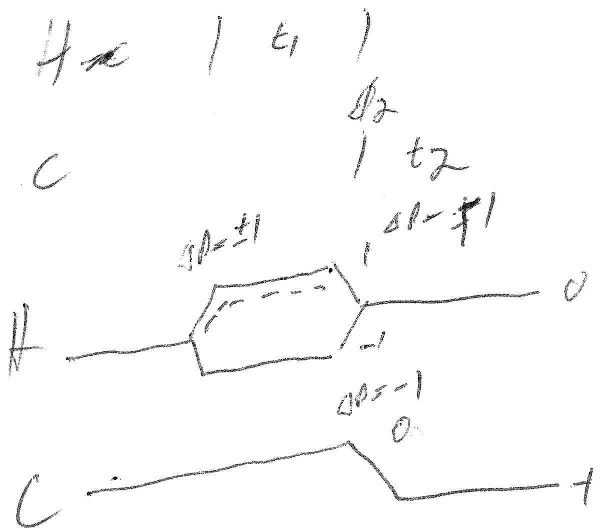
$d = c = e = 3$



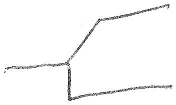




II-17)



$\frac{2\pi}{2} - \pi \cdot m$



$\Delta P = +1$ $\quad \Delta P = 0$

$= -1$ $\quad \Delta P = 2$

$N_a = 4$ $\quad n_c = 2$

$$S_{path}(t,m) = S_{path}(t,0)\, e^{-i\phi_{path}(m)}$$

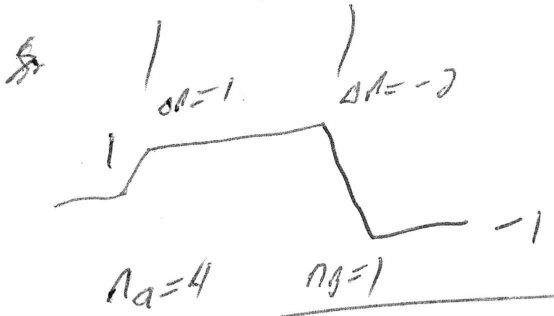
$$\phi_{path} = \Delta P_a\, \phi_A = \frac{2\pi}{n_a} \cdot m\, \phi_A \Delta P$$

~~$= +\phi_A$~~

$$\boxed{\phi_{path} = \frac{2\pi}{n_a} \cdot m \cdot \Delta P \quad m = 0, .. (n_a - 1)}$$

$n_a = 2 =$ ²

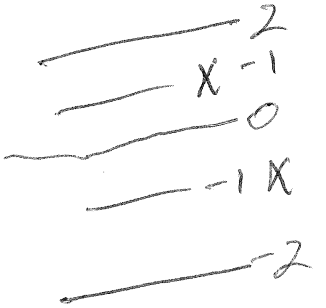
④ $S_p = S_{p0}\, e^{-i\phi_p}$ $\phi_p = \phi_A \Delta P_a + \phi_B \Delta P_b + \phi_{Rx} + \phi_{Dig}$

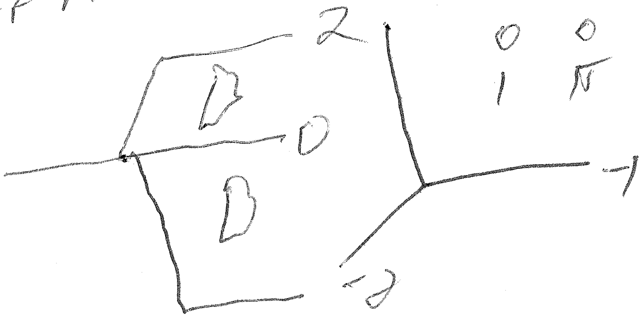


$\phi_p = \phi_A - 2\phi_B + \phi_{Rx} + \phi_{Dig}$

$$e^{i\left(\frac{2\pi P}{n}\right)} \Rightarrow S \begin{cases} =0 & \text{IF } P \neq \text{INT} * n \\ 1 & \text{IF } P = \text{INT} * n \end{cases}$$

$$n=2 \quad e^{i\frac{2\pi P}{2}} \begin{cases} S=0 & \text{IF } P \neq \text{INT} * 2 \\ S=1 & \text{IF } P = \text{INT} * 2 \end{cases}$$





m	ϕ_A	ϕ_B	ϕ_D
0	0	0	0
1	π	0	0

$S_p = S_{p0}\, e^{-i\phi_{path}}$ $\phi_{path} = \Delta P_a \phi_A + \Delta P_b \phi_A + \phi_{Rx} + \phi_{Dig}$

$\phi_{path} = \frac{2\pi}{n} \cdot m \Delta P$, . .

$\phi_p = 2\phi_A + \phi_{Dig}$ $\phi_{Dig} = -\phi_A$

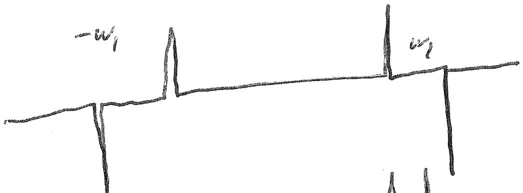
$n_a = 2 \quad \phi_A = \frac{2\pi}{2} \times m$

$= \pi m$

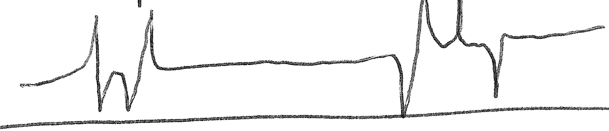
m	ϕ_A	ϕ_B	ϕ_D
0	0	0	0
1	π	0	0

Keep

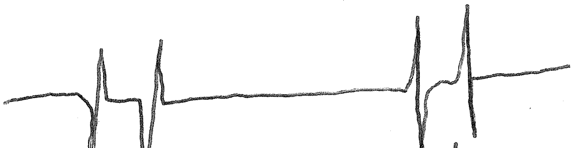
IR $s(\omega_1 t_1)\, s(\frac{J_{12} t_1}{2}) \xrightarrow{\cos FFT}$



$= s(\omega_1 - J) + s(\omega_1 + J) \xrightarrow{\sin FFT}$

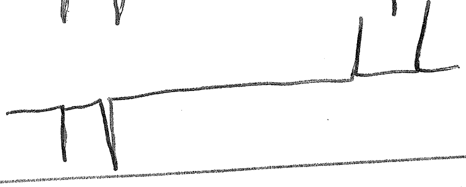


IR $s(\omega_1 t_1)\, c(\frac{J_{12} t}{2}) \xrightarrow{\cos FFT}$

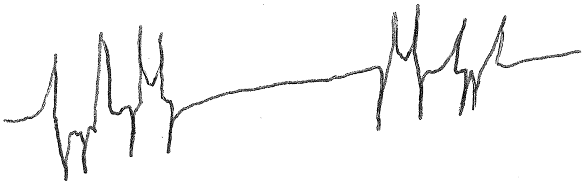


$= c(\omega_1 - J)t_1 - c(\omega_1 + J)t_1$

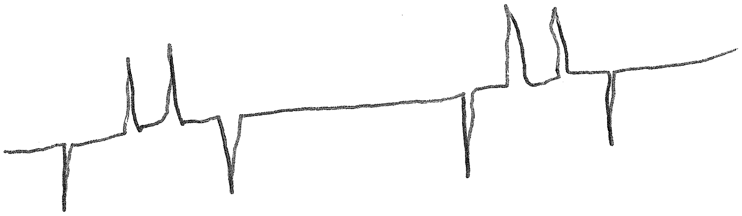
$\xrightarrow{\sin FFT}$



IR $s(\omega_1 t_1)\, s(J_{12} t_1)\, s(J_{13} t_1) \xrightarrow{\cos FFT}$

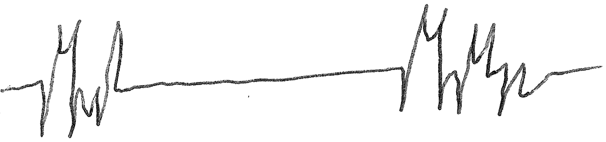


IR $c(\omega_1 t_1)\, s(J_{12} t_1)\, s(J_{13} t_1) \xrightarrow{\cos FF}$

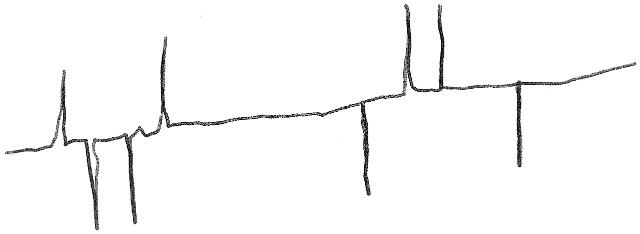


A

~~$s(\omega_1$~~ IR $c(\omega_1 t_1)\, c(J_{12} t_1)\, s(J_{13} t.) \xrightarrow{\cos FFT}$

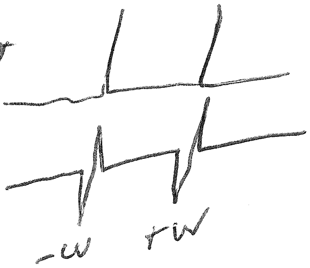


IR $s(\omega_1 t_1\, s(J_{12} t_1)\, s(J_{13} t_1) \xrightarrow{\sin FFT}$



A) ~~C~~ ℝ cos $\xrightarrow{\cos FFT}$

𝕀 φ $\xrightarrow{\sin FFT}$

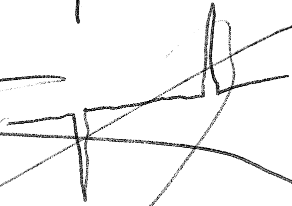


B) ℝ sin $\xrightarrow{\cos FFT}$

𝕀 0 $\xrightarrow{\sin FFT}$

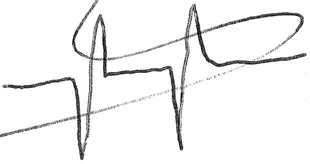
C) ~~R 0~~

~~𝕀 sin~~



D) ~~ℝ 0~~

~~𝕀 cos~~



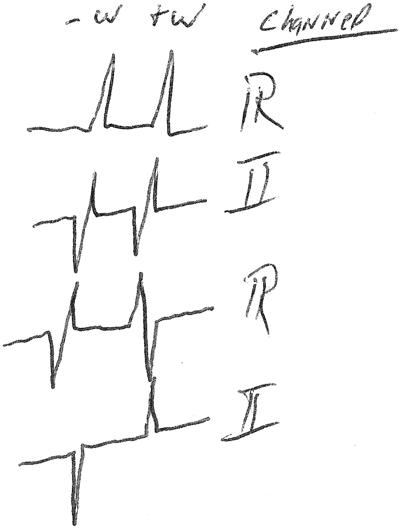
This is correct

c(wt) $\xrightarrow{cFFT}$

c(wt) $\xrightarrow{\sin FFT}$

s(wt) $\xrightarrow{\cos FFT}$

s(wt) $\xrightarrow{\sin FFT}$



FFT

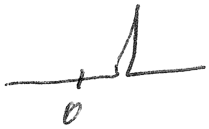
R = cos FT

𝕀 = sin FT

→ S(t) = ℝ + 𝕀

(shown on left)

A+C ⟹



ie) cos + sin $\xrightarrow{FFT}$