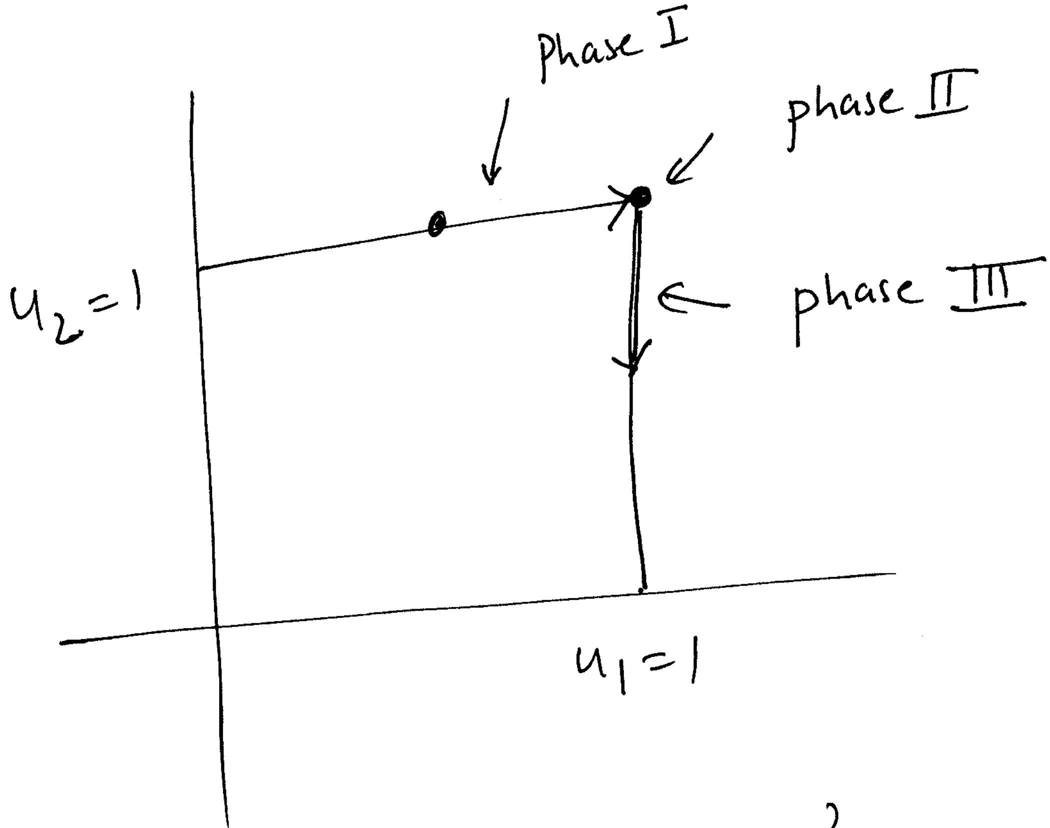
Applications & Examples of Maximum principle and Dynamic programming (HJB)



$$\begin{pmatrix} \dot{\gamma}_1 \\ \dot{\gamma}_2 \end{pmatrix} = \begin{pmatrix} -\xi u_1^2 & -u_1 u_2 \\ u_1 u_2 & -\xi u_2^2 \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}$$

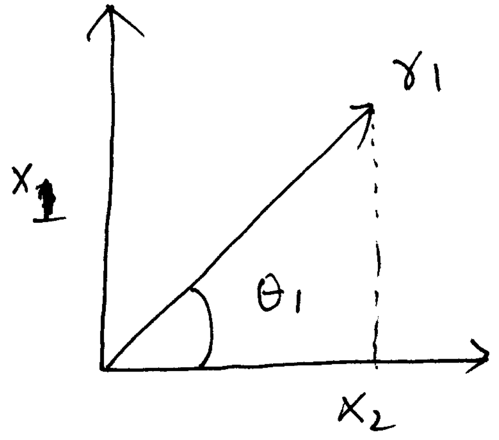
$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & -u & & \\ u & -k & -J & \\ & J & -k & -v \\ & & v & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

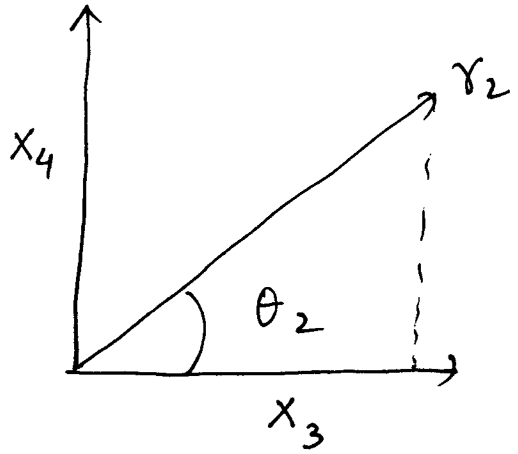
$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 0 \\ 0 \\ \eta \end{bmatrix} \qquad \max \eta$$

$u, v \gg k, J$ (Sepration of time scale)

States reached by just Using u, v are therefore Controls !

$u_1 = \cos\theta_1$
$U_2 = \cos\theta_2$





$$\frac{d}{dt}\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} -ku_1^2 & -Ju_1u_2 \\ Ju_1u_2 & -ku_2^2 \end{bmatrix}\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$$

rescale time

$$\frac{d}{dt}\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} -\xi u_1^2 & -u_1u_2 \\ u_1u_2 & -\xi u_2^2 \end{bmatrix}\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} \qquad \xi = \frac{k}{J}$$

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 0 \\ \eta \end{bmatrix} \qquad \max \eta$$

Terminal cost $\phi(\gamma_1, \gamma_2) = \gamma_2$

Hamiltonian

$$H = \begin{bmatrix} \lambda_1 & \lambda_2 \end{bmatrix}\begin{bmatrix} \dot{\gamma}_1 \\ \dot{\gamma}_2 \end{bmatrix}$$

$$H = \begin{bmatrix} \lambda_1 & \lambda_2 \end{bmatrix} \begin{bmatrix} -\xi u_1^2 & -u_1 u_2 \\ u_1 u_2 & -\xi u_2^2 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$$

$$= \begin{bmatrix} u_1 & u_2 \end{bmatrix} \overbrace{\begin{bmatrix} -\xi \lambda_1 r_1 & -\lambda_1 r_2 \\ \lambda_2 r_1 & -\xi \lambda_2 r_2 \end{bmatrix}}^{A} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$\max_{u_1, u_2} H(u_1, u_2) = 0$$

$$= \begin{bmatrix} u_1 & u_2 \end{bmatrix} \underbrace{\begin{bmatrix} -\xi \lambda_1 r_1 & \frac{\lambda_2 r_1 - \lambda_1 r_2}{2} \\ \frac{\lambda_2 r_1 - \lambda_1 r_2}{2} & -\xi \lambda_2 r_2 \end{bmatrix}}_{B} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$B \begin{bmatrix} u_1^* \\ u_2^* \end{bmatrix} = 0 \qquad \text{and} \qquad \det B = 0$$

$$\left(\frac{\lambda_2\gamma_1 - \lambda_1\gamma_2}{2}\right)^2 = \xi^2 \lambda_1 \lambda_2 \gamma_1 \gamma_2 \qquad (*)$$

$$\frac{\lambda_2}{\lambda_1} = a \quad \text{and} \quad \frac{\gamma_2}{\gamma_1} = b.$$

$$(*) \Rightarrow \left(\underbrace{\sqrt{\frac{a}{b}}}_{x} - \sqrt{\frac{b}{a}}\right)^2 = 4\xi^2$$

$$x - \frac{1}{x} = 2\xi \quad \Rightarrow \quad x^2 - 2\xi x - 1 = 0$$

$$x = \xi + \sqrt{1+\xi^2}$$

$$B \begin{bmatrix} u_1^* \\ u_2^* \end{bmatrix} = 0 \quad \Rightarrow$$

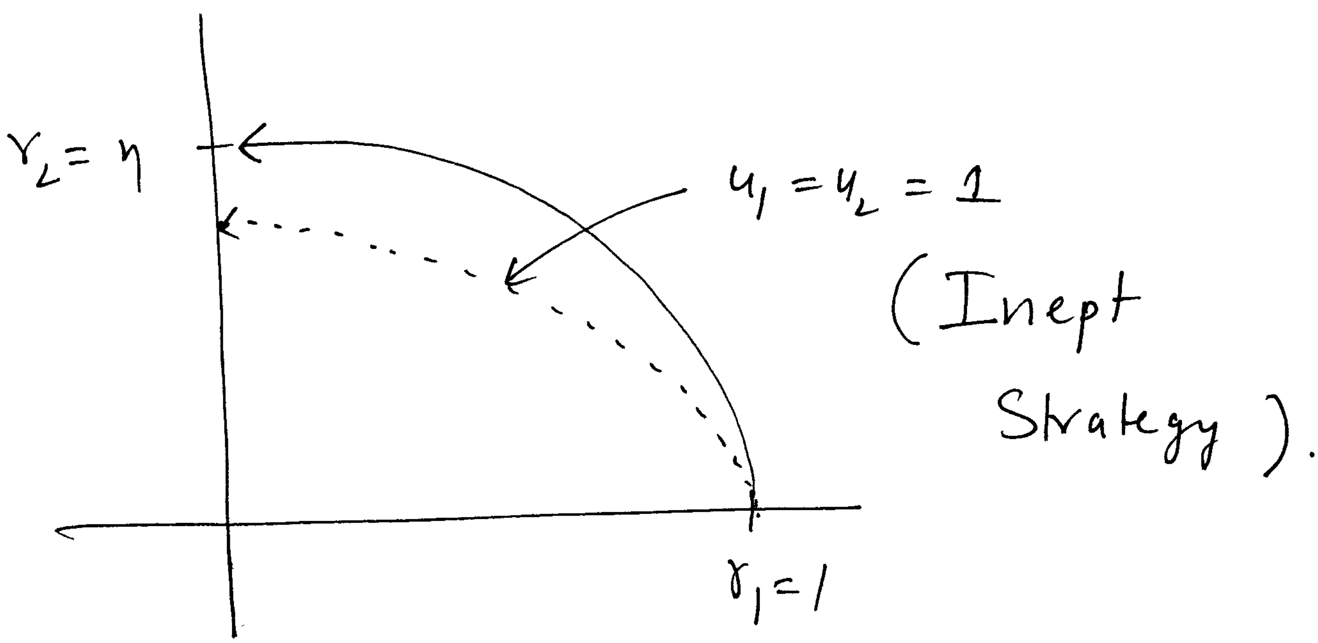
$$\left(\frac{\lambda_2\gamma_1 - \lambda_1\gamma_2}{2}\right) u_2 = \xi u_1 \lambda_1 \gamma_1$$

$$\frac{u_1 r_1}{u_2 r_2} = \left(\frac{a}{b} - 1\right)\frac{1}{2\xi} = (x^2 - 1)\frac{1}{2\xi}$$

$$= \frac{2\xi x}{2\xi} = x$$

$$\boxed{\frac{u_2 r_2}{u_1 r_1} = x^{-1} = \sqrt{1+\xi^2} - \xi}$$

Feedback Control law.



$$p_1 = r_1^2/2 \qquad p_2 = r_2^2/2$$

$$\dot{p}_1 = -\xi u_1^2 r_1^2 \;\cancel{+}\; u_1 u_2 r_1 r_2$$

**

$$\dot{p}_2 = +u_1 u_2 r_1 r_2 - \xi u_2^2 r_2^2$$

rescaling by $u_1^2 r_1^2$ (time)

$$\dot{p}_1 = -\xi - \eta$$

$$\dot{p}_2 = \eta - \eta^2 \xi$$

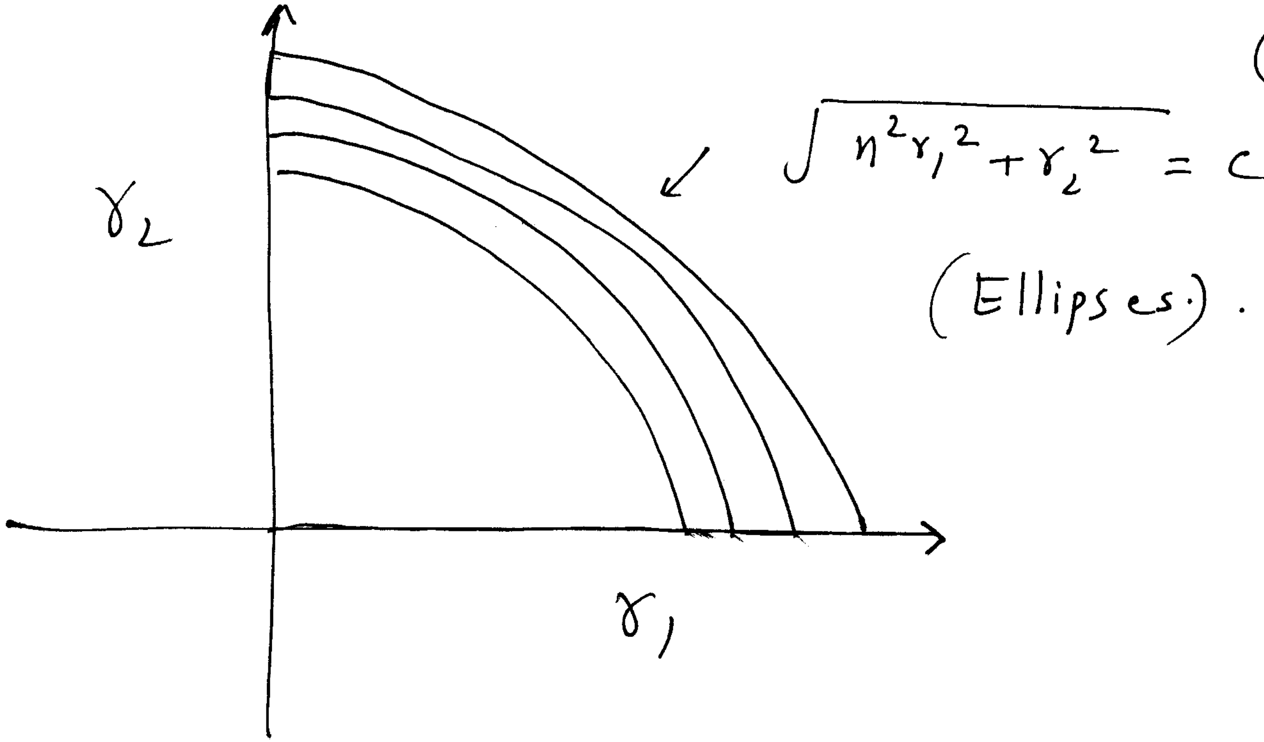
$$\frac{d}{dt}\left(\eta^2 p_1 + p_2 \right) = \eta - \eta^2 \xi - \eta^2 \xi - \eta^3$$

$$= 0$$

$\eta^2 r_1^2 + r_2^2$ is constant

$$V(r_1, r_2) = \sqrt{\eta^2 r_1^2 + r_2^2}$$

(Any unused r_1 can be put in r_2).



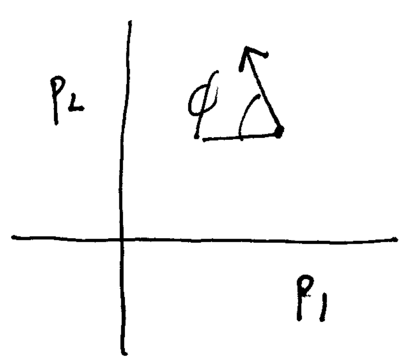
Infact this solution is obvious in (P_1, P_2) co-ordinates as

Let $\dfrac{u_2 r_2}{u_1 r_1} = w(t)$

Then from (**) we have after rescaling by $(u_1 r_1)^2$.

$$\dot{p}_1 = -\xi - w$$

$$\dot{p}_2 = w - w^2 \xi .$$



goal is to maximize P_2

$$\frac{w - w^2 \xi}{\xi + w}$$ should be maximized.

Simple differentiation gives.

$$w = \sqrt{1+\xi^2} - \xi = \eta.$$

In the (P_1, P_2) plane optimal control is simply follow the line with largest ϕ.

Eq. of the line is $\eta^2 P_1 + P_2 = C$

$\uparrow$

Constant

Finite time case

$$\begin{pmatrix} \dot{\gamma}_1 \\ \dot{\gamma}_2 \end{pmatrix} = \begin{pmatrix} -\xi u_1^2 & -u_1 u_2 \\ u_1 u_2 & -\xi u_2^2 \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} \quad (a)$$

$$H = \lambda_1 \dot{\gamma}_1 + \lambda_2 \dot{\gamma}_2$$

$$\dot{\lambda}_1 = -\frac{\partial H}{\partial \gamma_1}, \quad \dot{\lambda}_2 = -\frac{\partial H}{\partial \gamma_2}$$

$$\lambda_1(T) = \frac{\partial \Phi}{\partial \gamma_1} = 0 \qquad \lambda_2(T) = \frac{\partial \Phi}{\partial \gamma_2} = 1$$

$$\begin{pmatrix} \dot{\lambda}_1 \\ \dot{\lambda}_2 \end{pmatrix} = \begin{pmatrix} \xi u_1^2 & -u_1 u_2 \\ u_1 u_2 & \xi u_2^2 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} \quad (b)$$

~~running~~ first observe that $\lambda_1 \gamma_1 + \lambda_2 \gamma_2$ is constant (just differentiate).

Running λ backwards in time, we have

$$\begin{pmatrix} \dot{\tilde{\lambda}}_1 \\ \dot{\tilde{\lambda}}_2 \end{pmatrix} = \begin{pmatrix} -\xi \tilde{u}_1^2 & \tilde{u}_1 \tilde{u}_2 \\ -\tilde{u}_1 \tilde{u}_2 & -\xi \tilde{u}_2^2 \end{pmatrix} \begin{pmatrix} \tilde{\lambda}_1 \\ \tilde{\lambda}_2 \end{pmatrix}$$

$$\tilde{\lambda}(\sigma) = \lambda(T-\sigma).$$

Rewriting we get.

$$\frac{d}{dt}\begin{pmatrix} \tilde{\lambda}_2 \\ \tilde{\lambda}_1 \end{pmatrix} = \begin{pmatrix} -\xi \tilde{u}_2^2 & -\tilde{u}_1 \tilde{u}_2 \\ \tilde{u}_1 \tilde{u}_2 & -\xi \tilde{u}_1^2 \end{pmatrix} \begin{pmatrix} \tilde{\lambda}_2 \\ \tilde{\lambda}_1 \end{pmatrix} \quad \text{C}$$

Note $\tilde{\lambda}_2(0) = 1$ and $\tilde{\lambda}_1(0) = 0$.

$V = \lambda_1 \gamma_1 + \lambda_2 \gamma_2$ Starts with $\gamma_2 = 0$, $\gamma_1 = 1$

at $t = 0$ $V(0) = \lambda_1$

At final time $V(T) = \gamma_2$.

$$\boxed{\lambda_1^{(0)} = \gamma_2(T)} \quad \text{or} \quad \boxed{\tilde{\lambda}_1(T) = \gamma_2(T)}$$

Problems (a) and (c) (11)

are identical

maximizing $\gamma_2(T)$ is same as

maximizing $\tilde{\lambda}_1(T)$.

$$\Rightarrow \quad \boxed{u_1(t) = u_2(T-t)} \quad ! \; !$$

Let us as before define

$$a(t) = \frac{\lambda_2(t)}{\lambda_1(t)}, \qquad b(t) = \frac{\gamma_2(t)}{\gamma_1(t)}.$$

$$b(0) = 0 \qquad a^{-1}(T) = 0$$

$$a(T-t) \cdot b(t) = 1$$

In particular $ab\left(\frac{T}{2}\right) = 1$

$$\gamma_1(t) = \lambda_2(T-t)$$
$$\gamma_2(t) = \lambda_2(T-t).$$

Writing the Hamiltonian.

$$H = \lambda_1 \dot{r}_1 + \lambda_2 \dot{r}_2 = -\xi u_1^2 \lambda_1 r_1 - \xi u_2^2 \lambda_2 r_2 - u_1 u_2 \left[\lambda_1 r_2 - \lambda_2 r_1\right]$$

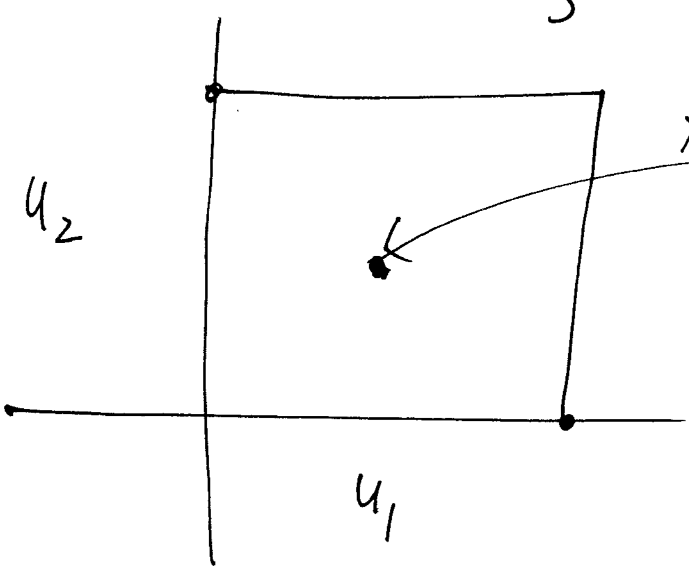
$$= -\xi \lambda_1 r_1 \left[\underbrace{u_1^2 + ab\, u_2^2 + 2 u_1 u_2 \left[\frac{b-a}{2\xi}\right]}_{*} \right]$$

$*$ should be minimized and the minimum < 0

$$\begin{bmatrix} u_1 & u_2 \end{bmatrix} \begin{bmatrix} 1 & \frac{b-a}{2\xi} \\ \frac{b-a}{2\xi} & ab \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

(else trivial solution).

$$\Rightarrow \quad ab - \frac{(a-b)^2}{4\xi^2} < 0 \qquad \text{A1}$$



A1 implies that minimum cannot be in the interior

So it must be on edges.

Three cases arise. then

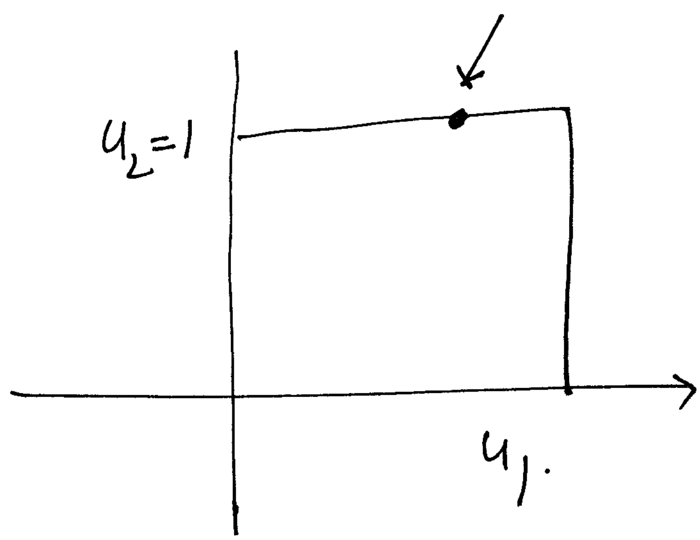
(1) $$\frac{a-b}{2\xi} \leq 1$$

In this case (*) can be written as.

$$\left(u_1 - \frac{(a-b)}{2\xi} u_2\right)^2 + \left\{ab - \frac{(a-b)^2}{4\xi^2}\right\} u_2^2$$

Clearly minimum is $u_2 = 1$

and $u_1 = \left(\frac{a-b}{2\xi}\right) u_2$



(2) $\dfrac{a-b}{2\xi ab} \lll 1.$

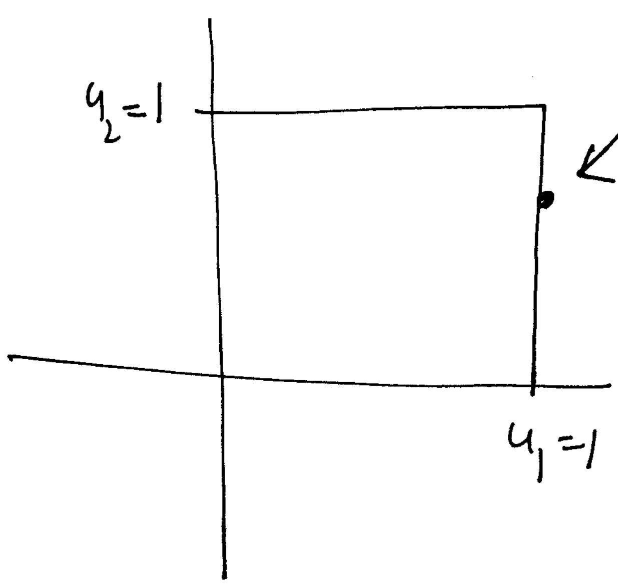
In this case (*) can be written as.

$$u_1^2 + ab\left[u_2 - \left(\frac{a-b}{2\xi ab}\right)u_1\right]^2 - \frac{(a-b)^2}{4\xi^2 ab}u_1^2$$

$$= u_1^2\left[1 - \frac{(a-b)^2}{4\xi^2 ab}\right] + ab\left[u_2 - \left(\frac{a-b}{2\xi ab}\right)u_1\right]^2$$

Clearly minimum =

$$u_2 = \left(\frac{b^{-1} - a^{-1}}{2\xi}\right)u_1 \qquad u_1 = 1$$

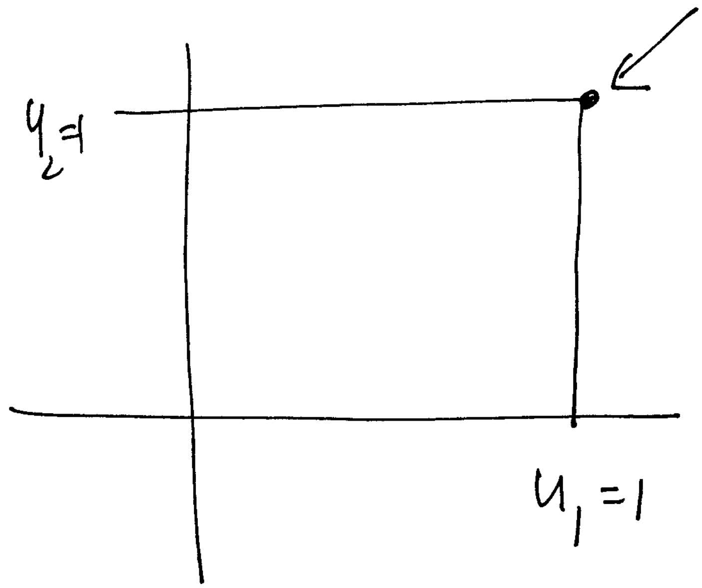


if

$$\frac{a-b}{2\xi} \geq 1$$

$$\frac{b^{-1}-a^{-1}}{2\xi} \geq 1$$

Then $u_1^* = u_2^* = 1$



We know that $\dfrac{(a-b)^2}{4\xi^2} > ab.$

at $t = \frac{T}{2}$ $ab = 1.$

$\Rightarrow$ $\dfrac{a-b}{2\xi} \geq 1$ $\dfrac{b^{-1}-a^{-1}}{2\xi} \geq 1$

at time $T/2$ we are in case $\underline{\overline{\text{III}}}$

At time $t=0$ $b(0)$.

if $\frac{a(0)}{2\xi} < 1$ then we are in case 1

At $t\uparrow$ $a\downarrow$ and $b\uparrow$

$\Rightarrow$ $\frac{a-b}{2\xi}\uparrow$

After time τ $\frac{a-b}{2\xi} = 1$

Swich from case I $\longrightarrow$ Case III.

While in case I. Let $k(t) = b/a\,(t)$

then using $u_1 = \left(\frac{a-b}{2\xi}\right) u_2$, we get

$$\dot{k}(t) = \frac{k^2-2k+1}{2\xi} - 2\xi k \qquad k(0)=0$$

Riccatti Equation

$$k(t) = 1 + 2\xi^2 - 2\xi\sqrt{1+\xi^2}\,\coth\left(\sqrt{1+\xi^2}\,t + 2\beta\right)$$

$$\sinh\beta = \xi$$

When $\dfrac{(a-b)}{2\xi} = 1$; we get

$$\frac{k^{-1}(\tau)-1}{2\xi} = \frac{1}{b} \Rightarrow b = \frac{2\xi}{k^{-1}(\tau)-1}$$

$$\Rightarrow \frac{2\xi\, k(\tau)}{1-k(\tau)} = b(\tau)$$

$$\frac{\gamma_2}{\gamma_1}(\tau) = \frac{2\xi\, k(\tau)}{1-k(\tau)}.$$

Now $u_1 = u_2 = 1$ and ab is increasing till $ab = 1$ at $t = T/2$.

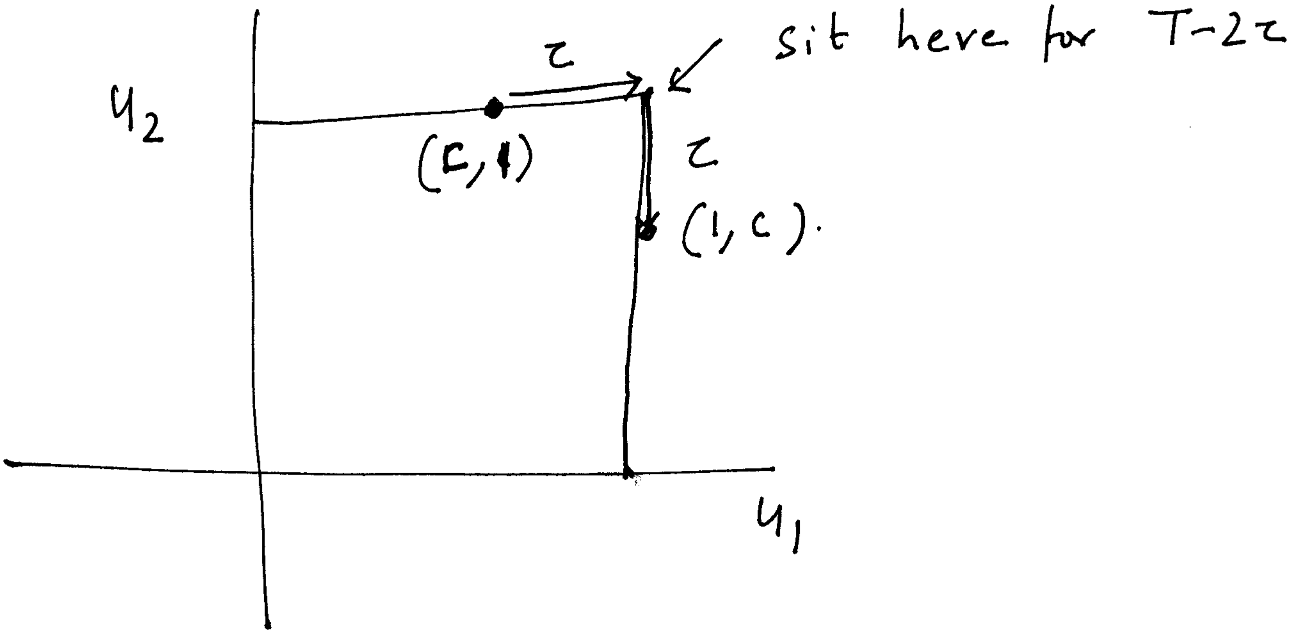
After that using symmetry.

$$u_2\left(\tfrac{T}{2} + \tau'\right) = u_1\left(\tfrac{T}{2} - \tau'\right).$$

$$u_1\left(\tfrac{T}{2} + \tau'\right) = u_2\left(\tfrac{T}{2} - \tau'\right).$$

To compute τ, we have to just (18)

see the control trajectory



Switching from case $\underline{\overline{III}} \longrightarrow \underline{\overline{II}}$ occurs.

at time $T-\tau$ when

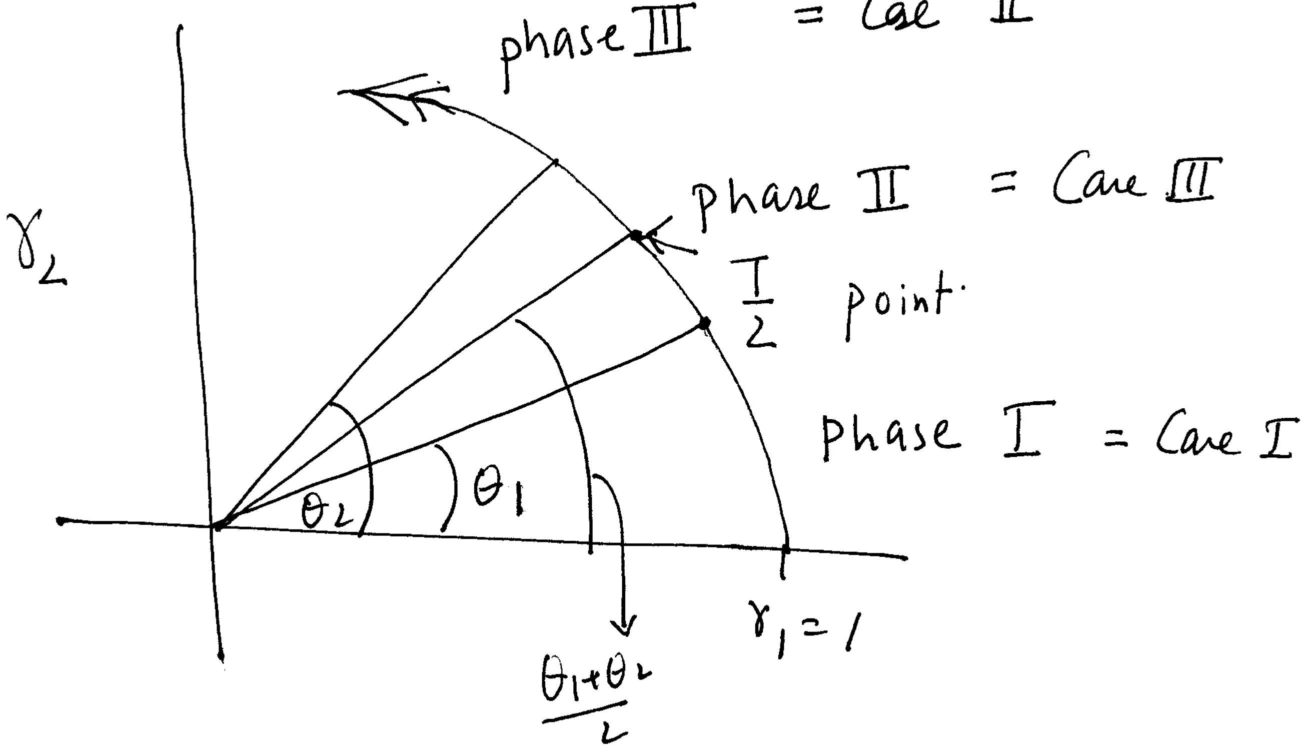
$$\frac{b^{-1} - a^{-1}}{2\xi}(T-\tau) = 1.$$

$$b(T-\tau) = \frac{1 - k(T-\tau)}{2\xi} \Rightarrow \frac{\gamma_2}{\gamma_1}(T-\tau) = \frac{1-k(\tau)}{2\xi}$$

but $k(T-\tau) = k(\tau)$

(19)

If we look at trajectory for (γ_1, γ_2)



$$\operatorname{Tan}\theta_1 = \frac{2\xi\, k(\tau)}{1-k(\tau)}$$

$$\operatorname{Tan}\theta_2 = \frac{1-k(\tau)}{2\xi}$$

In phase II (γ_1, γ_2) just rotates and dissipa[te]

Then $\cancel{\operatorname{Tan}\theta_2 - \operatorname{Tan}\theta_1}$ $= T - 2\tau$

$\theta_2 - \theta_1$

(20)

$$T - 2\tau = \operatorname{Tan}^{-1}\left(\frac{1-k(\tau)}{2\xi}\right) - \operatorname{Tan}^{-1}\frac{2\xi k(\tau)}{1-k(\tau)} \qquad \text{(E1)}$$

Clearly RHS is maximum at $\tau = 0$.

if $\operatorname{Tan} T \le \frac{1}{2\xi}$ no solution

for τ (Always in Case III).

Else solve (E1) for τ.

Since $\underline{\lambda_1 \gamma_1 + \lambda_2 \gamma_2}$ is constant

at time $\frac{T}{2}$ $\searrow$ $2\gamma_1\left(\frac{T}{2}\right)\gamma_2\left(\frac{T}{2}\right)$.

$$\frac{\gamma_2}{\gamma_1} = \tan\left(\frac{\theta_1 + \theta_2}{2}\right) \Rightarrow \boxed{V = R_2^2 \sin(\theta_1 + \theta_2)}$$

$$R_2^2 = \sqrt{\gamma_1^2\left(\tfrac{T}{2}\right) + \gamma_2^2\left(\tfrac{T}{2}\right)}$$

A compulation shows that

$t \geqslant T-\tau$ we have

$$V(t) = \sqrt{\gamma_2^2(t) + k(T-t)\gamma_1^2(t)} \quad \text{is Constant}$$

at $t = T$ $\quad V(T) = \gamma_2(T)$

$$V(T-\tau) = R_1 \sqrt{1 - \xi \sin 2\theta}$$

$$R_1 = R_2 \exp\left(-\left(\tfrac{T}{2} - \tau\right)\right).$$

Hence the ~~proof~~ Solution for R_2

But note this gives all controls.

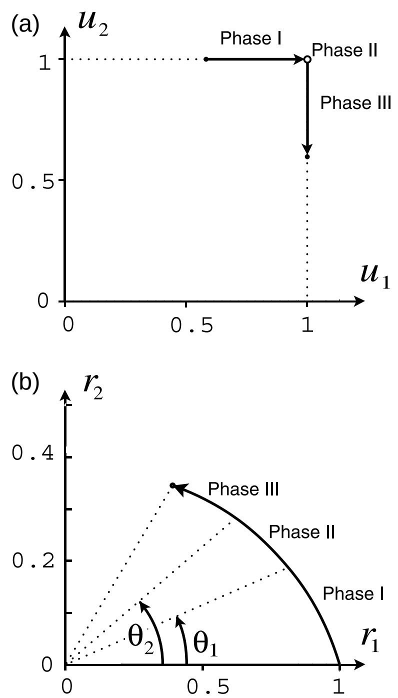


Fig. 5. Phase trajectory of the controls u_1 and u_2 (panel a) and $\vec{r}(t)$ (panel b) for a finite-time ROPE sequence ($\xi = 1$).

$$\kappa(\tau) = 1 + 2\xi^2 - 2\xi\sqrt{1+\xi^2}\coth\left(\pi J\sqrt{1+\xi^2}\tau + 2\sinh^{-1}\xi\right).$$

At time τ, the optimal trajectory (r_1, r_2) passes from phase I to II and makes an angle θ_1 with the r_1 axis and at time $T - \tau$ the optimal trajectory passes from phase II to phase III and makes an angle θ_2 with the r_1 axis (see Fig. 5b). The optimal efficiency η_T for the finite time T is expressed in terms of these angles as

$$\eta_T = \frac{\exp(\xi(\theta_1 - \theta_2))(1 - \xi\sin 2\theta_2)}{\sin(\theta_1 + \theta_2)}. \tag{11}$$

In the limit, T goes to infinity $\tau = T/2$ and $\theta_1 = \theta_2 = \tan^{-1}\sqrt{1+\xi^2} - \xi$ and η_T approaches η in (6). This corresponds to the unconstrained time case we discussed initially. For the general finite time problem, we can analytically characterize the optimal controls (see Fig. 6a) and the optimal rf pulse elements (see Fig. 6b) as following.

For $0 \leqslant t \leqslant \tau$, the optimal control is given by

$$u_1(t) = \sqrt{\frac{R_1^2\{1 + \cosh(\phi(t))\}}{(BR_1^2 + 2A^2R_2^2) - R_1^2\cosh(\phi(t))}},$$

where $A = \sinh\phi(\tau/2)$, $B = \cosh\phi(\tau)$, and $\phi(t) = 2\sinh^{-1}\xi + 2\pi Jt\sqrt{1+\xi^2}$. The optimal trajectory crosses from region II to region III at the point

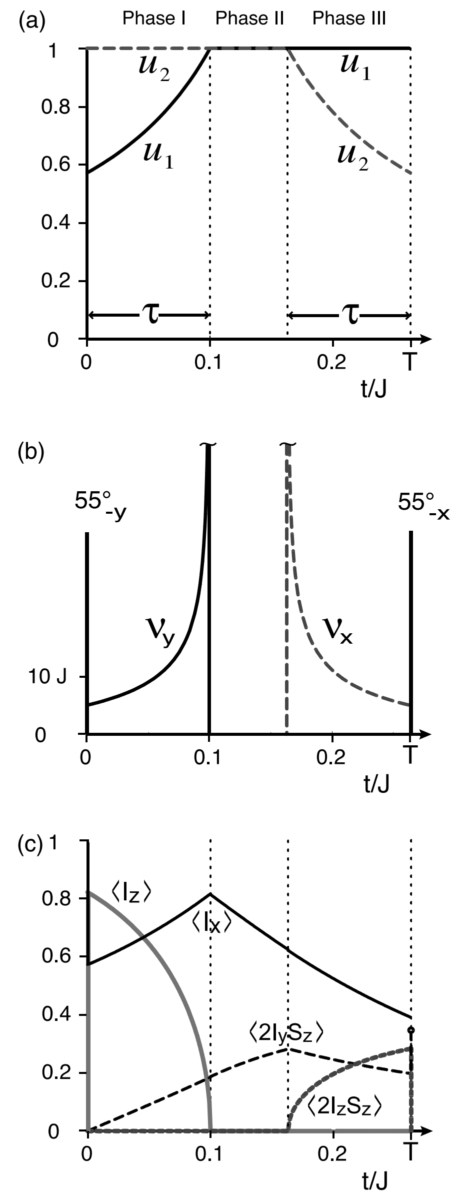


Fig. 6. Controls u_1 and u_2 (panel a), the corresponding rf pulse sequence (panel b) and the expectation values $\langle I_z\rangle$, $\langle I_x\rangle$, $\langle 2I_yS_z\rangle$, and $\langle 2I_zS_z\rangle$ (panel c) are shown for a finite-time ROPE sequence ($\xi = 1$, $\tau = 0.1J^{-1}$, $T = 0.263J^{-1}$) that optimizes the transfer $I_x \to 2I_yS_z$. In panel b, the initial hard $55_{-y}°$ pulse establishes $u_1(0) = 0.572$ (see panel a) and the final hard $55_{-x}°$ pulse completes the transfer. During phase I and III, the optimal rf amplitudes $B_{x,y}^{\mathrm{rf}}(t)$ are given in frequency units ($\nu_{x,y}(t) = \gamma_I B_{x,y}^{\mathrm{rf}}(t)/2\pi$, where γ_I is the gyromagnetic ratio of spin I). During phase II no rf pulses are applied. Approaching phase II (Panel b) the rf amplitude becomes large for a very short time period. This can experimentally be very well approximated by a hard pulse of small flip angle.

$$(R_1, R_2) = \left(\frac{\eta_T}{\sqrt{\tan^2\theta_2 + \kappa(\tau)}}, \frac{\eta_T}{\sqrt{1 + (\kappa(\tau)/\tan^2\theta_2)}}\right)$$

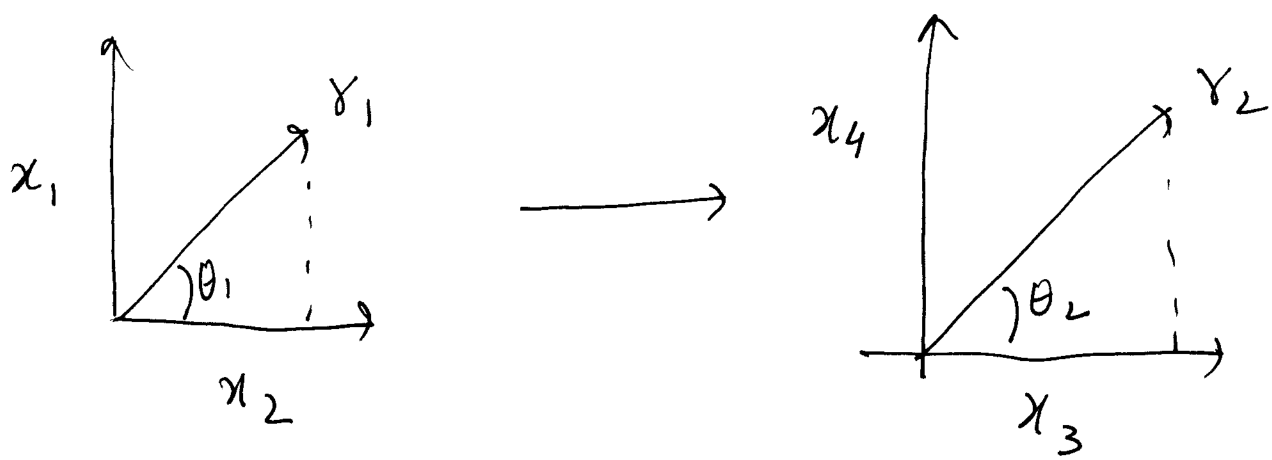
(as depicted in Fig. 5). For $t > \tau$, we have $u_1(t) = 1$ and $u_2(t) = u_1(T - t)$. The explicit expression for the rf-amplitude ν_y for phase I in panel b of Fig. 6 in terms of u_1 is

Optimal Control of coupled spins in presence of longitudinal & transverse relaxation

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -k_1 & -u & & \\ u & -k & -J & \\ & -J & -k & -v \\ & & v & -k_2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

maximize x_4 starting from $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

Again using sepration of time scale.



$$u_1 = \cos\theta_1 \; ; \quad u_2 = \cos\theta_2$$

$$\begin{bmatrix} \dot{r}_1 \\ \dot{r}_2 \end{bmatrix} = \begin{bmatrix} -\xi_1 u_1^2 - \bar{\xi}_1 & -u_1 u_2 \\ u_1 u_2 & -\xi_2 u_2^2 - \bar{\xi}_2 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}.$$

$$\xi_1 = \frac{k - k_1}{J}, \quad \bar{\xi}_1 = \frac{k_1}{J}$$

$$\xi_2 = \frac{k - k_2}{J} \qquad \bar{\xi}_2 = \frac{k_2}{J}$$

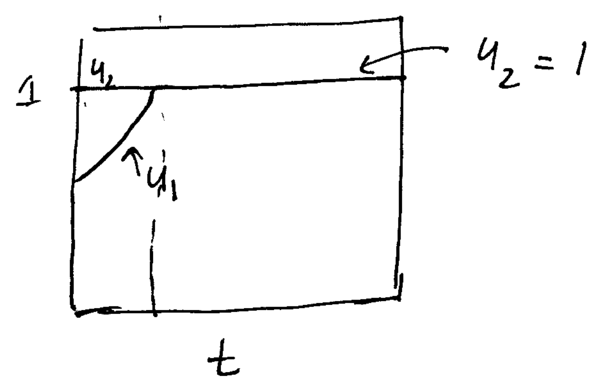
maximize $r_2(T)$.

Assume $k_1 < k_2$.

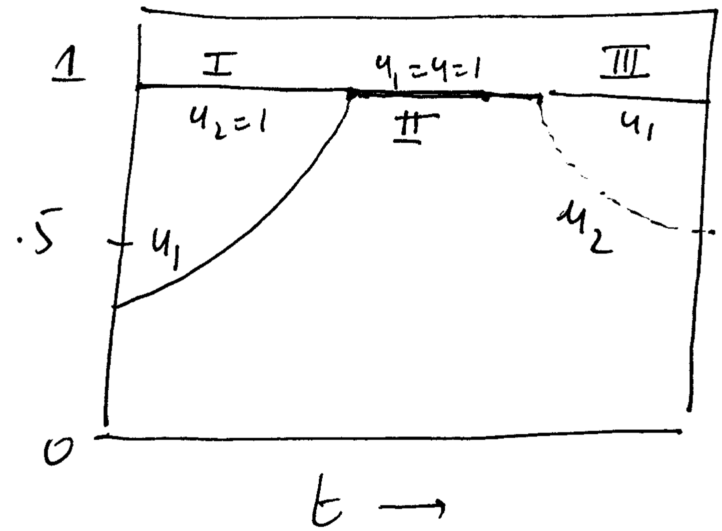
Then 3 cases.

1). $T \leq T_A$ $\quad u_1 = u_2 = 1.$

2) $T_A < T \leq T_B$.



3) $T > T_B$



As before, we form the Hamiltonian.

$$H(u_1, u_2) = -\lambda_1 \gamma_1 \left[+\xi_1 u_1^2 - (a-b) u_1 u_2 + ab\,\xi_2 u_2^2 + \bar{\xi}_1 + ab\,\bar{\xi}_2 \right]$$

As before $\lambda_1, \lambda_2 \geq 0$, $0 \leq u_1, u_2 \leq 1$.

All we have to do is to minimize the quadratic form.

$$\boxed{Q(u_1, u_2) = \xi_1 u_1^2 - (a-b) u_1 u_2 + ab\,\xi_2 u_2^2}$$

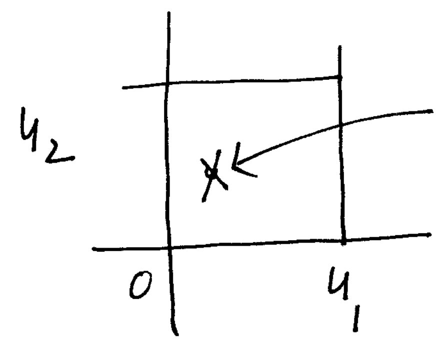
24

Again we need $(a-b)^2 > 4\xi_1 \xi_2 ab.$ (*)

$a-b > 0$

for there to be non-trivial $u_1 = u_2 = 0$ solution.

From (*) we find that no optimal in the interior.



not optimal.

We consider three Case

a) $(a-b) < 2\xi_1$

$$Q(u_1, u_2) = \xi_1 \left[\left(u_1 - \frac{(a-b)u_2}{2\xi_1}\right)^2 + \left(\frac{ab\xi_2}{\xi_1} - \frac{(a-b)^2}{4\xi_1^2}\right)u_2^2 \right]$$

Clearly minimum at $u_2 = 1$

$$u_1 = \frac{(a-b)}{2\xi_1}$$

2). Case II

$$(a-b) \geq 2\xi_1 \quad \text{and} \quad \frac{a-b}{ab} \geq 2\xi_2$$

minimum at $\quad u_1 = u_2 = 1$

3). Case III $\quad (a-b) \geq 2\xi_1$ and

$\frac{a-b}{ab} < 2\xi_2$ then minimum of

$$Q \Rightarrow \begin{array}{l} u_1 = 1 \\ u_2 = \dfrac{a-b}{2ab\,\xi_2} \end{array}$$

Equation for λ

$$\frac{d}{dt}\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} \xi_1 u_1^2 + \bar{\xi}_1 & -u_1 u_2 \\ u_1 u_2 & \xi_2 u_2^2 + \bar{\xi}_2 \end{bmatrix}\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}$$

26

Again $\lambda_1 r_1 + \lambda_2 r_2 = \text{Constant}$

$\lambda_1(T) = 0$, $\lambda_2(T) = 1$

The dual problem is.

$$\frac{d}{dt}\begin{bmatrix}\tilde{\lambda}_2 \\ \tilde{\lambda}_1\end{bmatrix} = \begin{bmatrix} -\xi_2 \tilde{u}_2^2 - \bar{\xi}_2 & -\tilde{u}_1\tilde{u}_2 \\ \tilde{u}_1\tilde{u}_2 & -\xi_1\tilde{u}_1^2 - \bar{\xi}_1 \end{bmatrix}\begin{bmatrix}\tilde{\lambda}_2 \\ \tilde{\lambda}_1\end{bmatrix}$$

maximize $\tilde{\lambda}_1(T)$.

$\tilde{u}_1(\sigma) = u_1(T-\sigma)$; $\tilde{u}_2(\sigma) = u_2(T-\sigma)$.

Now we loose symmetry.

$u_1(T-\sigma) \neq u_2(\sigma)$ in general.

Suppose

1). $a(0) \geqslant 2\xi_1$ then we start in

$u_1 = u_2 = 1$ and we can show

that $b^{-1}(t) - a^{-1}(t) = \dfrac{a(t) - b(t)}{ab}$

$\geqslant 2\xi_2$

So we stay there as $a - b \uparrow$

2) If $a(0) < 2\xi_1$ then.

we we are in case $\overline{\underline{I}}$

$u_1 = \left(\dfrac{a-b}{2\xi_1}\right) u_2$ $u_2 = 1$.

At time T_1 we switch to case $\overline{\underline{II}}$

At time $T - \cancel{t_2}$ we switch to case $\overline{\underline{III}}$

Optimal control of coupled spins in the presence of longitudinal and transverse relaxation

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In this paper, we develop methods for optimal manipulation of coupled spin dynamics in the presence of relaxation. These methods are used to compute analytical bounds for the optimal efficiency of coherence transfer between coupled nuclear spins in presence of longitudinal and transverse relaxation. We derive relaxation optimized pulse sequences which achieve these bounds and maximize the sensitivity of the experiments in spectroscopic applications. This paper is a continuation of our previous work. Here, we take into account both the longitudinal and the transverse relaxation mechanisms, thus generalizing our previous results, where the former had been neglected.

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I. INTRODUCTION

In applications involving control and manipulation of quantum phenomena, the system of interest is not isolated but interacts with its environment. This leads to the phenomenon of relaxation, which in practice results in signal loss and ultimately limits the range of applications. Manipulating quantum systems in a manner that minimizes relaxation losses poses an important practical problem. A premier example is the transfer of coherence between coupled spins in NMR spectroscopy [1]. Presence of relaxation limits the efficiency of coherence transfer between coupled spins and results in poor sensitivity of the experiments. The problem becomes pronounced in NMR spectroscopy of large biomolecules. With increasing size of molecules or molecular complexes, the rotational tumbling of the molecules becomes slower and leads to increased relaxation losses. When these relaxation rates become comparable to the spin-spin couplings, the efficiency of coherence transfer is considerably reduced, leading to poor sensitivity and significantly increased measurement times.

This negative effect of relaxation on the efficiency of coherence transfer automatically gives rise to some important practical (and theoretical) problems.

(1) What is the theoretical upper limit for the coherence transfer efficiency in the presence of relaxation?

(2) How can this theoretical upper limit be reached experimentally?

In our previous work, we answered the above questions for a coupled two-spin system under the presence of transverse relaxation [2,3] (neglecting and including cross-correlation effects, respectively). In this manuscript, we extend these results to the case where both longitudinal and transverse relaxation mechanisms are important, and we cannot neglect the former.

The methods developed here are also useful for answering important questions in quantum information theory. It is a fundamental problem to understand the extent to which an open quantum system can be controlled, i.e., where all the state of a quantum-mechanical system can be steered in the presence of relaxation? How much entanglement can be produced in presence of decoherence and dissipation and what is the optimal way to synthesize unitary gates in open quantum systems so as to maximize their fidelity? All these problems are related to optimal control of quantum-mechanical systems in presence of relaxation.

II. RELAXATION IN NMR IN LIQUIDS

As a model system, we consider optimal control of ensembles of nuclear spins in NMR spectroscopy. We use ρ to denote the density matrix for the spin ensemble. The density matrix of a closed quantum system ($\hbar=1$) evolves as

$$\frac{d\rho}{dt}=-i[H(t),\rho], \tag{1}$$

where $H(t)$ is the Hamiltonian of the system.

For an open quantum system, the evolution is no longer unitary. In many applications of interest, the environment can be approximated as an infinite thermostat, whose own state never changes. Under this assumption, also called the Markovian approximation, it is possible to write the evolution of the density matrix of the system (master equation) alone in the (Lindblad) form [4]

$$\frac{d\rho}{dt}=-i[H(t),\rho]+L(\rho), \tag{2}$$

where the term $L(\rho)$ is linear in ρ and models relaxation. The general form of L is

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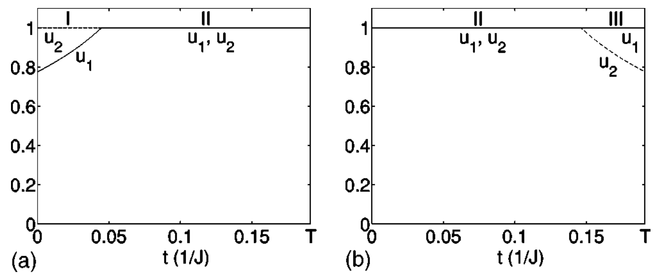


FIG. 2. Optimal pulse sequence when $T_A < T \leqslant T_B$ for (a) $k_1 < k_2$ and (b) $k_1 > k_2$. For case (b) we just interchanged the values of k_1, k_2 from case (a), keeping the same k. Observe the symmetry in the optimal controls.

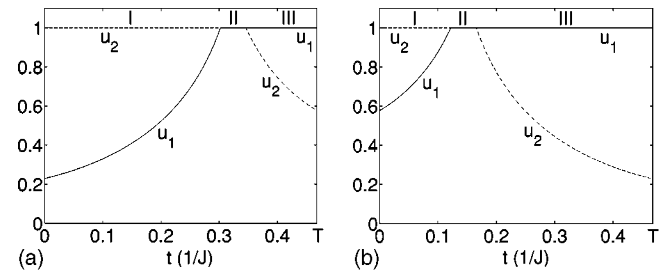


FIG. 3. Optimal pulse sequence when $T > T_B$ for (a) $k_1 < k_2$ and (b) $k_1 > k_2$. Again, for case (b) we just interchanged the values of k_1, k_2. The symmetry in the controls appears again. Note that the duration T has been set equal to the optimal duration T_{opt}, which maximizes the optimal transfer efficiency η_T. For the values $k = J, k_1 = 0.05J, k_2 = 0.25J$ that we used in (a), it is $T_{opt} \simeq 0.468 J^{-1}$. For case (b), T_{opt} is the same.

corresponding magnetic-field components $B_x(t), B_y(t)$, which achieve the maximum efficiency.

IV. THEORETICAL RESULTS

The optimal control problem is solved in Appendix A. Here, we describe the characteristics of the optimal pulse sequence for the case $\xi_1 > \xi_2$, i.e., for $k_1 < k_2$. The results for $k_1 > k_2$ are analogous. Presence of finite longitudinal relaxation rates results in an optimal transfer duration T_{opt} in which the maximum transfer efficiency is achieved. We compute this T_{opt} by finding the optimal pulse sequence for every choice of transfer duration T and then locating the T that gives the best transfer efficiency. Depending on the values of the problem parameters, we find three important cases in the optimal solution.

(1) $T \leqslant T_A$ (case A) [$T_A = \cot^{-1}(2\xi_1)/\pi J$, for $\xi_1 > \xi_2$]: In this case $u_1(t) = u_2(t) = 1$ throughout, i.e., β_1 and β_2 in Fig. 1 are always kept zero and this solution corresponds to the INEPT pulse sequence.

(2) $T_A < T \leqslant T_B$ (case B1) (we describe how we calculate T_B below): In this case the optimal pulse sequence has two distinct phases [see Fig. 2(a)]. There is a switching time τ_1 such that for $0 \leqslant t \leqslant \tau_1$ (phase I), $u_2(t) = 1$ and $u_1(t)$ is increased gradually from a value $u_1(0) < 1$ to $u_1(\tau_1) = 1$. Then, for time $\tau_1 \leqslant t \leqslant T$ (phase II), the optimal controls are $u_1(t) = u_2(t) = 1$.

(3) $T > T_B$ (case B2): Here the optimal pulse sequence has three distinct phases [see Fig. 3(a)]. There are two switching times τ_1 and $T - \tau_2$. Phases I and II are the same as above: For $0 \leqslant t \leqslant \tau_1$ (phase I), $u_2(t) = 1$ and $u_1(t)$ is increased gradually from a value $u_1(0) < 1$ to $u_1(\tau_1) = 1$. For time $\tau_1 \leqslant t \leqslant T - \tau_2$ (phase II), the optimal controls are $u_1(t) = u_2(t) = 1$. Finally, for $T - \tau_2 \leqslant t \leqslant T$ (phase III), we have $u_1(t) = 1$ and $u_2(t)$ is decreased from $u_2(T - \tau_2) = 1$ to $u_2(T) < 1$.

We now give physical explanation for the existence of these three cases. For small enough T, the major limitation for the transfer $r_1(0) \rightarrow r_2(T)$ is not the relaxation, but the limited available time. The optimal choice $u_1 = u_2 = 1$ maximizes (absolute value) the off-diagonal elements $\pm u_1 u_2$, which accomplish the transfer $r_1(t) \rightarrow r_2(t)$, as can be seen from the system equation (28). It also maximizes the diagonal elements, i.e., the relaxation rates of $r_1(t), r_2(t)$. But for small available time T, the gain that we get by maximizing the desired transfer at each moment t is more important than the (small) relaxation losses. As time T increases, the relaxation degrades more the performance and the choice $u_1 = u_2 = 1$ ceases to be optimal. With $u_1 < 1$ or $u_2 < 1$ we may reduce the transfer rate of $r_1(t) \rightarrow r_2(t)$, but at the same time we decrease also the instantaneous relaxation rates $\xi_i u_i^2 + \overline{\xi_i}, i = 1,2$. Since for large enough T the relaxation dominates, we conclude that by an appropriate choice of $u_1 \leqslant 1$ or $u_2 \leqslant 1$ we can get a better efficiency for the transfer $r_1(0) \rightarrow r_2(T)$. This appropriate choice corresponds to the cases B1 and B2. Note that for $k_1 < k_2$, the system in case B2 spends more time in phase I ($u_1 < 1, u_2 = 1$) than in phase III ($u_1 = 1, u_2 < 1$), see Fig. 3(a). This happens because for $k_1 < k_2$ and $u_1 = u_2 = u < 1$, the relaxation rate $\xi_1 u_1^2 + \overline{\xi_1}$ is lower than the rate $\xi_2 u_2^2 + \overline{\xi_2}$ [note $\xi_1 u_1^2 + \overline{\xi_1} - \xi_2 u_2^2 - \overline{\xi_2} = (\xi_1 - \xi_2) u^2 + \overline{\xi_1} - \overline{\xi_2} < \xi_1 - \xi_2 + \overline{\xi_1} - \overline{\xi_2} = 0$, since $\xi_1 + \overline{\xi_1} = \xi_2 + \overline{\xi_2} = k/J$]. Based on the above observation about the duration of phases I and III, we expect that as we increase T, from values where case A holds to values where case B2 is the optimal, there must be an intermediate range of values of T where the optimal pulse sequence has no phase III at all. This is the case B1.

The duration T_A above which the optimal pulse sequence is different than INEPT is $T_A = \cot^{-1}(2\xi_1)/\pi J$, for $\xi_1 > \xi_2$. We can explain the dependence of this quantity on the parameters k, k_1. Note that $\xi_1 = (k - k_1)/J$, so T_A is a decreasing function of k and an increasing function of k_1. For larger k (larger transverse relaxation) it is more costly to have the vectors $\boldsymbol{r}_1, \boldsymbol{r}_2$ parallel to the xy plane, i.e., it is more costly to have $u_1 = u_2 = 1$ (see Fig. 1). This explains why T_A, which determines the range of values of T where the INEPT pulse sequence is optimal, is decreased. Now for larger k_1 (larger longitudinal relaxation) it is more costly to have the vector $\boldsymbol{r}_1$ parallel to the z axis, i.e., to have $u_1 < 1$. This explains why T_A, and with it the range of optimality of INEPT, is increased.

The switching time τ_1 for case B1 is calculated using the following equation:

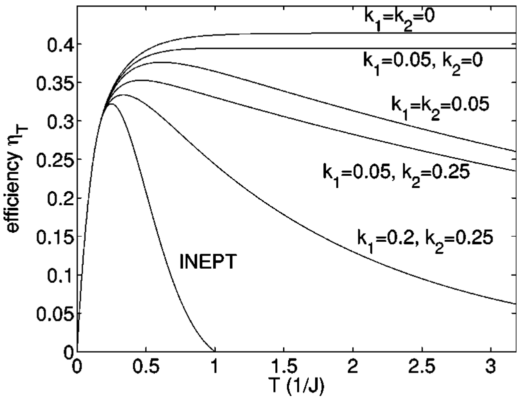


FIG. 5. Optimal transfer efficiency η_T as a function of the total transfer time T for $k=J$ and various values of k_1, k_2 (normalized with respect to J). Observe that for $k_1, k_2 \neq 0$ there is an optimal transfer time T_{opt}.

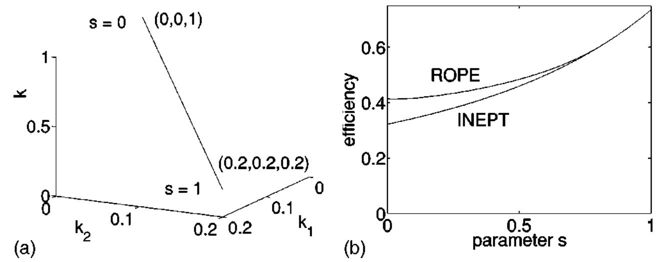


FIG. 6. (b) Maximum transfer efficiency η_T evaluated at T_{opt} for each point of the line in (k_1, k_2, k) space shown in (a). The line is parametrized by the parameter $0 \leqslant s \leqslant 1$ and has been chosen such that the increase of s from 0 to 1 simulates the transition from slow molecular motion, where $k \gg k_1 \simeq k_2$, to rapid molecular motion, where $k \simeq k_1 \sim k_2$. Note the superiority of the relaxation optimized pulse element (ROPE) compared to the INEPT pulse sequence for the case $k \gg k_1 \simeq k_2$.

''put'' much control to the system) and thus the maximum efficiency that we get is small. For large T the phenomenon of relaxation dominates, since there is no operator protected against it, and the maximum efficiency that we achieve is poor. So, there must be an intermediate time T such that η_T becomes maximum. This time is T_{opt}. In Fig. 6(b) we plot the maximum efficiency, calculated at T_{opt} for each choice of the parameters, along a specific line in (k_1, k_2, k) space. This line is shown in Fig. 6(a) and has been chosen to simulate the transition from the slow molecular motion (slowly tumbling regime), where $k \gg k_1 \simeq k_2$, to the rapid molecular motion, where $k \simeq k_1 \sim k_2$.

For $0 \leqslant t \leqslant \tau_1$ (phase I), the optimal control is given by

$$u_1(t) = \sqrt{\frac{\bar{\Lambda}_2^2[1+\cosh\phi_1(t)]}{2\bar{\Lambda}_1^2 \sinh^2\phi_1\left(\frac{\tau_1}{2}\right) + \bar{\Lambda}_2^2\cosh\phi_1(\tau_1) - \bar{\Lambda}_2^2\cosh\phi_1(t)}}, \tag{39}$$

where $\phi_1(t) = 2\pi J t\sqrt{1+\xi_1^2} + 2\sinh^{-1}\xi_1$ and

$$\bar{\Lambda}_1 = \frac{\eta_T}{\sqrt{1+\kappa_1(\tau_1)\tan^2\varphi_1}}, \quad \bar{\Lambda}_2 = \frac{\eta_T}{\sqrt{\kappa_1(\tau_1) + \frac{1}{\tan^2\varphi_1}}}. \tag{40}$$

For $T-\tau_2 \leqslant t \leqslant T$ (phase III), the optimal control is

$$u_2(t) = \sqrt{\frac{\bar{R}_1^2[1+\cosh\phi_2(T-t)]}{2\bar{R}_2^2 \sinh^2\phi_2\left(\frac{\tau_2}{2}\right) + \bar{R}_1^2\cosh\phi_2(\tau_2) - \bar{R}_1^2\cosh\phi_2(T-t)}}, \tag{41}$$

where $\phi_2(t) = 2\pi J t\sqrt{1+\xi_2^2} + 2\sinh^{-1}\xi_2$ and

$$\bar{R}_1 = \frac{\eta_T}{\sqrt{\kappa_2(\tau_2) + \tan^2\vartheta_2}}, \quad \bar{R}_2 = \frac{\eta_T}{\sqrt{1 + \frac{\kappa_2(\tau_2)}{\tan^2\vartheta_2}}}. \tag{42}$$

The corresponding rf amplitude for phase I is given by

$$\omega_y = \gamma_I B_y = 2\pi J \frac{u_1}{\sqrt{1-u_1^2}} \tanh\left(\frac{\phi_1}{2}\right)\sqrt{1+\xi_1^2} \tag{43}$$

and for phase III by

$$\omega_x = \gamma_I B_x = 2\pi J \frac{u_2^3}{\sqrt{1-u_2^2}} \tanh\left(\frac{\phi_2(T-t)}{2}\right)\sqrt{1+\xi_2^2}, \tag{44}$$

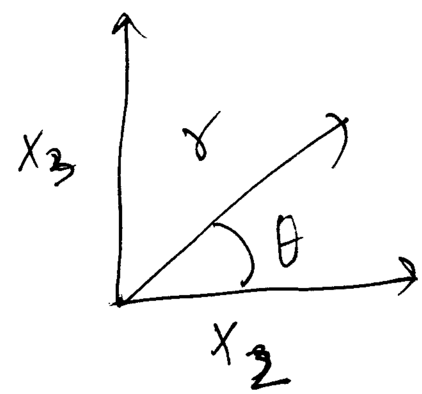
Example 3

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & -1 & & \\ 1 & 0 & -u & \\ & u & 0 & -1 \\ & & 1 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \to \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$ in minimum time

find $u^*(t)$

No apriori bounds on control



$x_2 = r\cos\theta$

$x_3 = r\sin\theta$

$y_1 = x_1$

$y_2 = r$

$y_3 = x_3$

$$\frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0 & -\cos\theta & 0 \\ \cos\theta & 0 & -\sin\theta \\ 0 & \sin\theta & 0 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

find $\theta(t)$ such that

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \to \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

in minimum time

Again let $\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix}$ be the adjoint variables then

$$H = \lambda_1 \dot{y}_1 + \lambda_2 \dot{y}_2 + \lambda_3 \dot{y}_3$$

$$\frac{d}{dt}\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & -\cos\theta & 0 \\ \cos\theta & 0 & -\sin\theta \\ 0 & \sin\theta & 0 \end{bmatrix}}_{\Omega(\theta)} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix}$$

$$H = \dot{\mathrm{Tr}}\left(\Omega(\theta)\, M\right)$$

where

$$M = \frac{y\lambda^T - \lambda y^T}{2}$$

$$\dot{M} = [\Omega(\theta), M] \quad — (**)$$

$$M = M_x \Omega_x + M_y \Omega_y + M_z \Omega_z$$

$$\Omega_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \Omega_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \Omega_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$H = Tr(\Omega(\theta) M)$$

$$= Tr(\Omega_x^2) M_x \sin\theta$$

$$+ M_z \cos\theta \, Tr(\Omega_z^2)$$

To minimize H, we allign $(\cos\theta, \sin\theta)$ along (M_x, M_z).

$$\Omega(\theta) = (M_x \Omega_x + M_z \Omega_z) \frac{1}{\sqrt{M_x^2 + M_z^2}}$$

If we look at the Equation

$$\dot{M} = -[M, \Omega(\theta)]$$ then. note

$$\dot{M}_y = 0 \Rightarrow M_y = \omega \text{ constant}$$

also $M_x^2 + M_z^2 + M_y^2 = \text{constant}$

$$\Rightarrow M_x^2 + M_z^2 = \text{constant}$$

so we just get from $**$ that

$$\dot{M}_x = -\omega_1 M_z$$
$$\dot{M}_z = \omega_1 M_x$$

$$M_x = A\cos(\omega_1 t + \theta_1)$$
$$M_z = A\sin(\omega_1 t + \theta_1)$$

$\Rightarrow$

$$\frac{dy}{dt} = \begin{pmatrix} 0 & -\cos\theta & 0 \\ \cos\theta & 0 & -\sin\theta \\ 0 & \sin\theta & 0 \end{pmatrix} y.$$

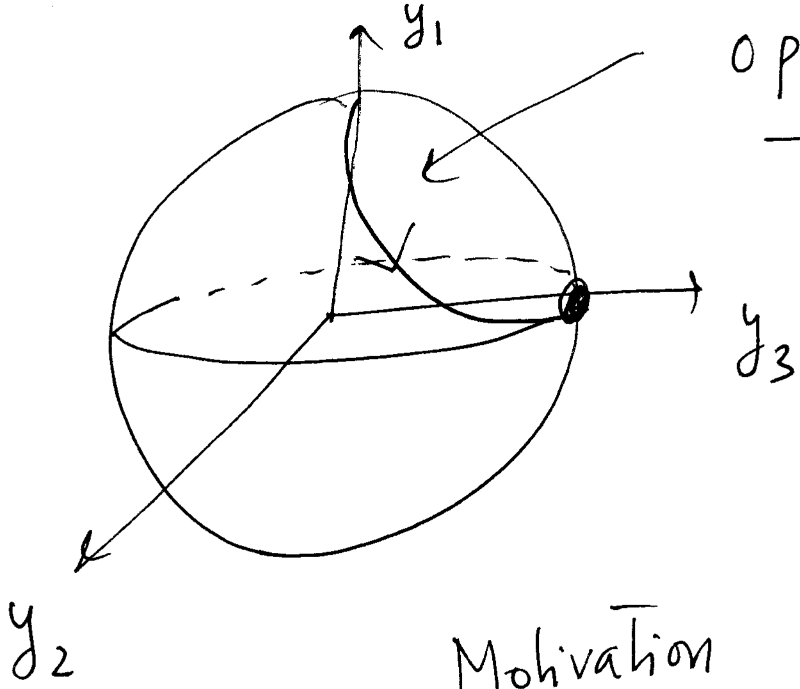
we have $\quad \dot{\theta} = \omega_1 t$

$$\theta(t) = \omega_1 t + \underbrace{\theta(0)}_{\theta_1}$$

Now we can find the right frequency ω_1 and the right phase $\theta(0)$.

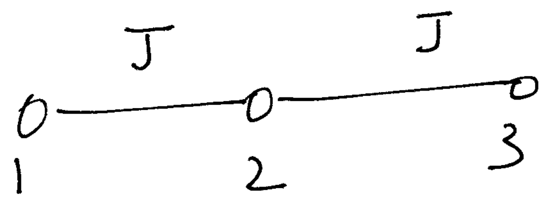
This means that

$u(t) = C_1$ constant.



optimal trajectory.

Motivation (Linear spin Chain)



$$\frac{d}{dt}\underbrace{\begin{pmatrix} \langle I_{1x} \rangle \\ \langle 2 I_{1y} I_{2z} \rangle \\ \langle 2 I_{1y} I_{2x} \rangle \\ \langle 4 I_{1y} I_{2y} I_{3z} \rangle \end{pmatrix}}_{X} = \begin{pmatrix} 0 & -J & & \\ J & 0 & -u & \\ & u & 0 & -J \\ & & J & \end{pmatrix} X$$

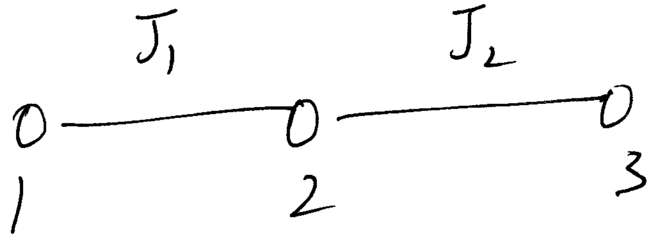
Find $u(t)$ to transfer.

$$\underset{= 1}{\langle I_{1x} \rangle} \longrightarrow \langle 4 I_{1y} I_{2y} I_{3z} \rangle$$

in minimum time

Example 4.

Linear Spin Chain with Unequal Couplings.

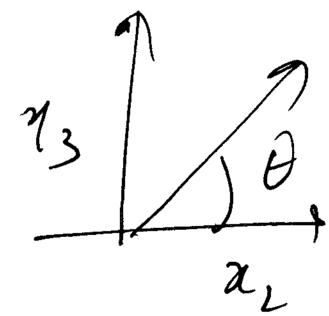


$$\frac{d}{dt}\underbrace{\begin{pmatrix} \langle I_{1x} \rangle \\ \langle 2I_{1y} I_{2z} \rangle \\ \langle 2I_{1y} I_{2x} \rangle \\ \langle 4 I_{1y} I_{2y} I_{3x} \rangle \end{pmatrix}}_{X} = \begin{pmatrix} 0 & -J_1 & & \\ J_1 & 0 & -u & \\ & u & 0 & -J_2 \\ & & J_2 & 0 \end{pmatrix} X$$

$$\frac{d}{dt}\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{pmatrix} = \begin{pmatrix} 0 & -1 & & \\ 1 & 0 & -u & \\ & u & 0 & -k \\ & & k & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}.$$

Find $u(t)$

Again $\quad y_1 = x_1 \quad y_2 = \sqrt{x_2^2 + x_3^2}\,, \; y_3 = x_4$



$\leftarrow$ Control Variable.

$$\frac{d}{dt}\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \underbrace{\underbrace{\begin{pmatrix} 0 & -\cos\theta & 0 \\ \cos\theta & 0 & -k\sin\theta \\ 0 & k\sin\theta & 0 \end{pmatrix}}_{\cos\theta\,\Omega_z + k\sin\theta\,\Omega_x}}_{\Omega(\theta).} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}.$$

$$\dot{\lambda} = \Omega(\theta)\,\lambda.$$

Again. $\quad M = \dfrac{x\lambda^T - \lambda x^T}{2}.$

$$H = \mathrm{tr}\left(\Omega(\theta)\, M\right).$$

$$\tan\theta = \frac{k M_x}{M_z}.$$

$$= -\left\{\cos\theta\, M_z + k\sin\theta\, M_x\right\} + 1$$

Along optimal trajectory H maximized $= 0$

$$\sin\theta = \frac{k M_x}{\sqrt{k^2 M_x^2 + M_z^2}} \quad ; \quad \cos\theta = \frac{M_z}{\sqrt{k^2 M_x^2 + M_z^2}}.$$

$$\Rightarrow \quad H = 1 - \sqrt{k^2 M_x^2 + M_z^2} = 0$$

$$\boxed{M_z^2 + k^2 M_x^2 = 1}$$

$$\tan\theta = \frac{k M_x}{M_z} \quad \Rightarrow \quad \sec^2\theta \, \dot\theta = \frac{k \dot M_x M_z - k M_x \dot M_z}{M_z^2}.$$

$$\dot M_x = -\cos\theta \, M_y$$

$$\dot M_y = \cos\theta \, M_x - k \sin\theta \, M_z$$

$$\dot M_z = k \sin\theta \, M_y.$$

$$\dot\theta = -k M_y$$

$$\ddot\theta = -k(1-k^2) M_x M_z$$

$$\boxed{\ddot\theta = \frac{(k^2-1)}{2} \sin 2\theta}$$

When $k=1$

$$\ddot\theta = 0$$

Elliptic functions

Example - 5.

Brockett (1981)

$$X \begin{cases} \dot{x} = u \\ \dot{y} = v \\ \dot{z} = xv - yu \end{cases}$$

Steer the system

$(0,0,0) \longrightarrow (0,0,1)$

$X(0) \rightarrow (X(1))$

minimize

$$\int_0^1 u^2 + v^2 \, dt$$

$$H = \lambda_1 \dot{x} + \lambda_2 \dot{y} + \lambda_3 \dot{z} + (u^2+v^2)\lambda_4$$

$\dot{\lambda}_4 = 0 \qquad \lambda_4(1) = 1$

$$H = \lambda_1 \dot{x} + \lambda_2 \dot{y} + \lambda_3 (xv - yu) + u^2 + v^2$$

$\dot{\lambda}_3 = 0 \qquad \dot{\lambda}_1 = -\lambda_1 - \lambda_3 v$

$\dot{\lambda}_2 = -\lambda_2 + \lambda_3 u$

$(u, v) = \text{argmin } H$

$u = \lambda_3 y/2 \; ; \; v = -\lambda_3 x/2$

$\dot{u} = \frac{\lambda_3}{2} v \qquad \dot{v} = -\lambda_3 u/2$

$$\frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & \lambda_3/2 \\ -\lambda_3/2 & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

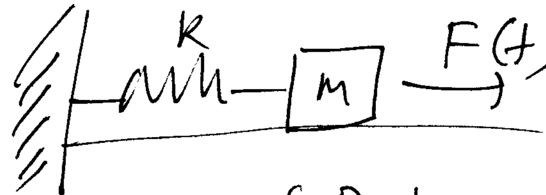
Constant Amplitude

$$(u, v) = \left(A \cos(\omega t + \phi),\ A \sin(\omega t + \phi)\right).$$

Again Sinusoids ! Wow !!

Example. 6

$$\underbrace{\ddot{X} + X = u}_{\text{Driven Harmonic Oscillator}}$$



(Pontryagin's Book)

Starting from $(X(0), \dot{X}(0)) \rightarrow (0,0)$

$x_1 = X$ in minimum time

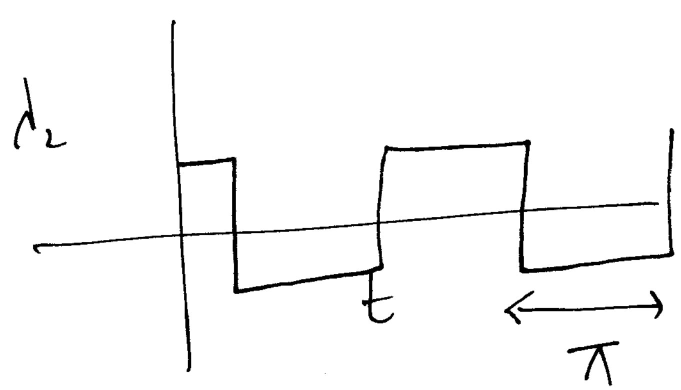
$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = -x_1 + u$$

$$H = \lambda_1 x_2 + \lambda_2(-x_1 + u)$$

$$\dot{\lambda}_1 = \lambda_2 \qquad \lambda_1 = A \sin(t + \phi)$$
$$\dot{\lambda}_2 = -\lambda_1 \qquad \lambda_2 = A \cos(t + \phi).$$

$$u = -\operatorname{sgn}(\lambda_2).$$

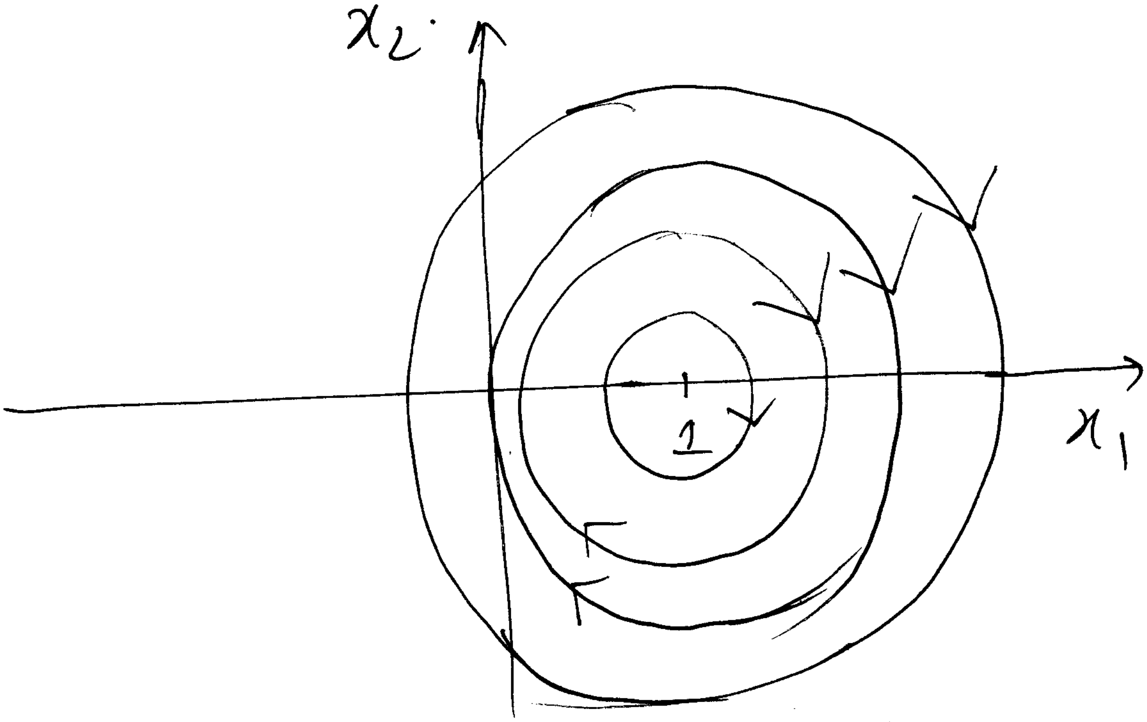
λ_2 switches sign every π units



$$y = +1 \quad \text{if} \quad \lambda_2 < 0$$
$$= -1 \quad \text{if} \quad \lambda_2 > 0$$

When $y = +1$ then

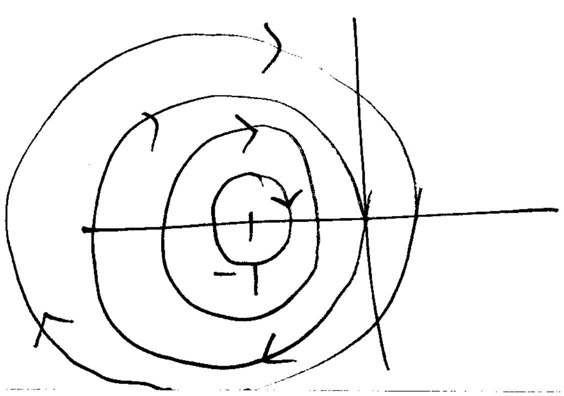
$$\dot{x}_1 = x_2 \qquad \Rightarrow \qquad (x_1 - 1)^2 + x_2^2 = C$$
$$\dot{x}_2 = -x_1 + 1$$



A

When $u = -1$ then

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = -(x_1 + 1)$$
$$(x_1 + 1)^2 + x_2^2 = C$$

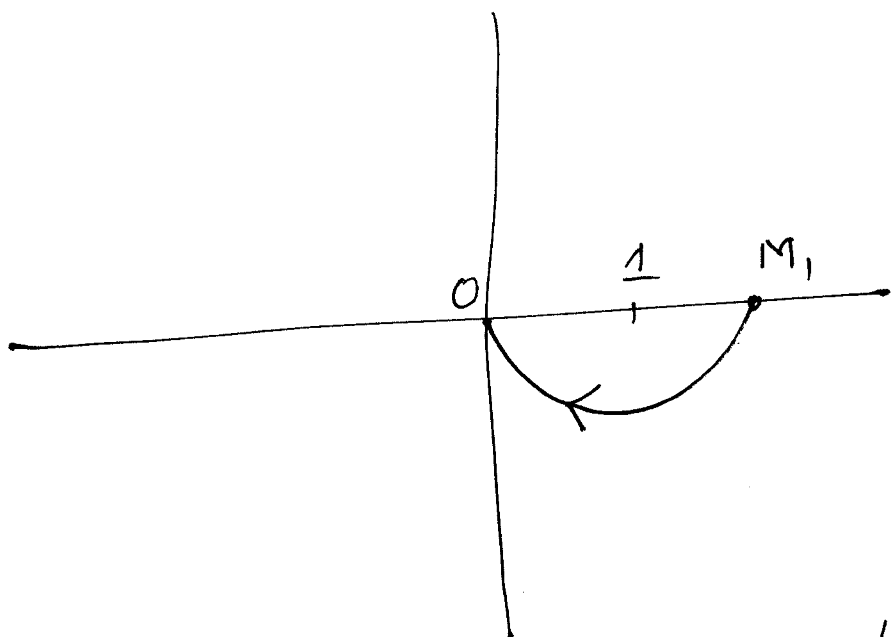


B

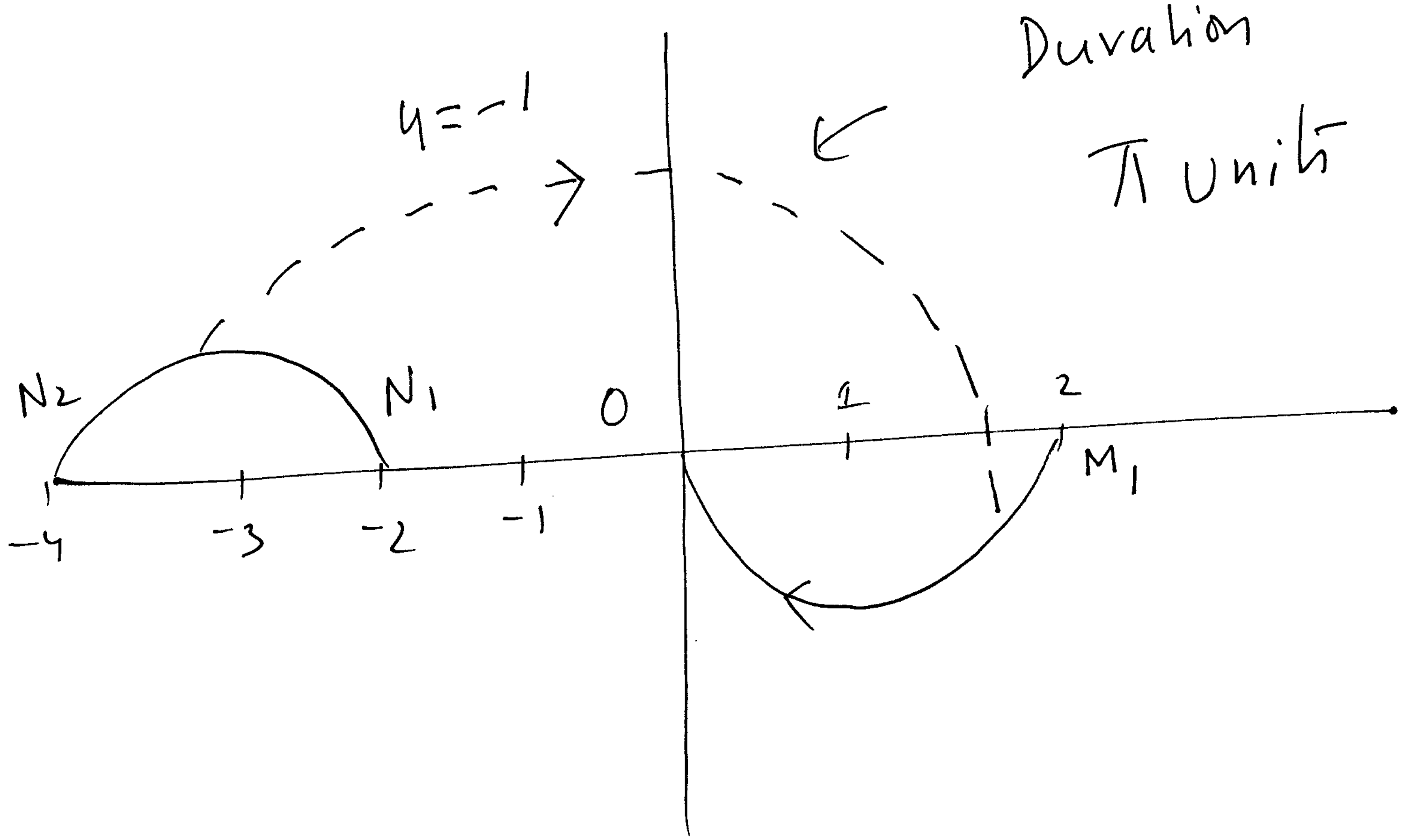
Suppose at T (final time)

λ_2 is negative, $u = +1$ then.

we come to the origin the following way.



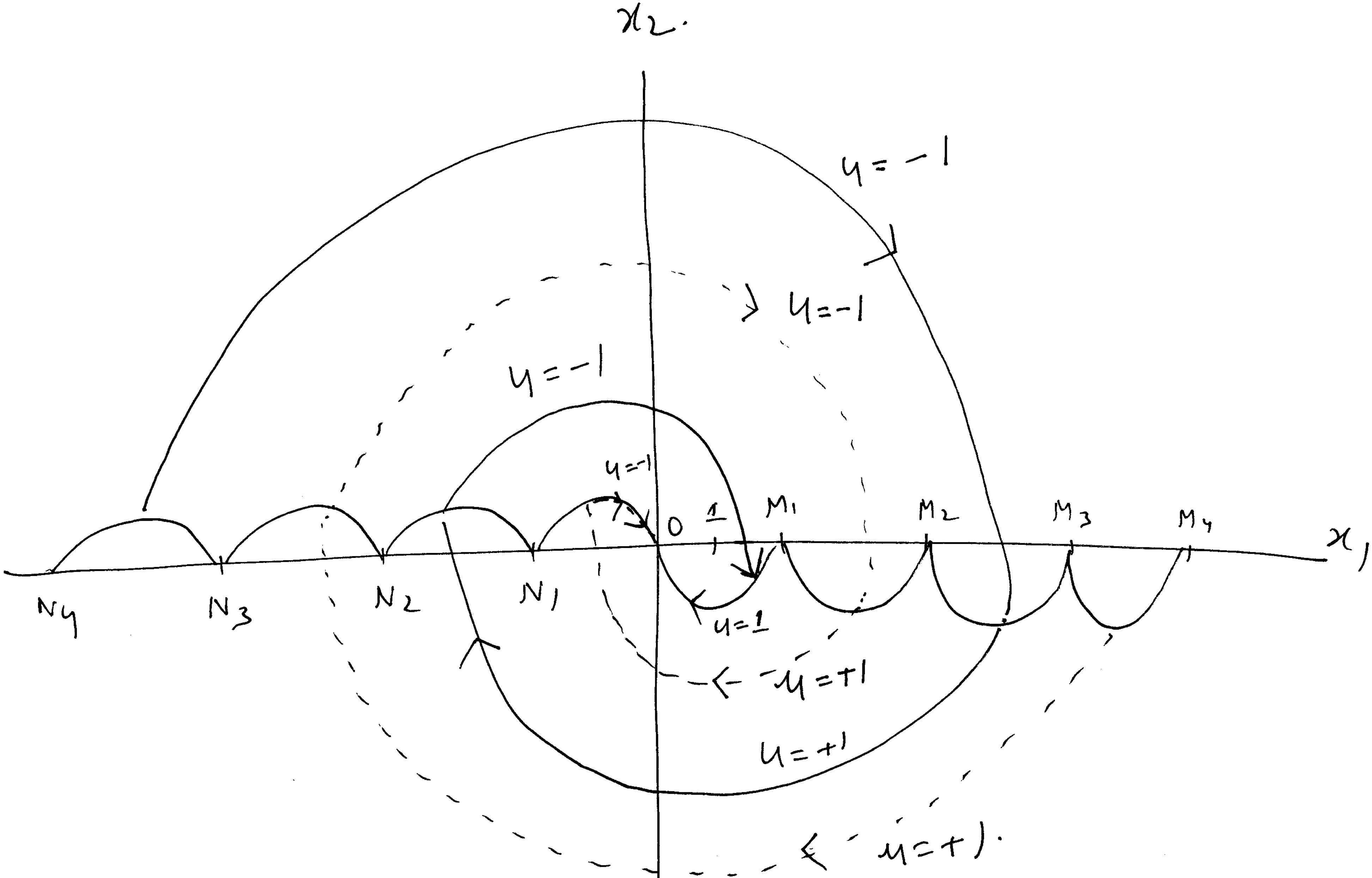
Clearly now when we proceed backwards in time then we must switch to $u=-1$ before or at point M_1 and we are in case B.



Semicircle N_1N_2 is obtained by reflecting OM_1 around point $(-1,0)$

Going backwards in time at N_1N_2 we switch again to $u=+1$.

We can now draw a full phase picture



— Solid lines shows possible trajectories when $u=+1$ at origin

--- dotted lines shows possible trajectories when $u=-1$ at origin.

Optimal Control is now Clear.

$$u(x) = \begin{cases} +1 & \text{below the curve} \\ & M_3 M_2 M_1 O N_1 N_2 N_3 \cdots \\ & \text{and on the arc } M_3 M_2 M_1 O; \\ -1 & \text{above the curve} \\ & \cdots M_3 M_2 M_1 O N_1 N_2 N_3 \cdots \\ & \text{and on the arc } O N_1 N_2 \cdots \end{cases}$$

(Again a feedback control law).