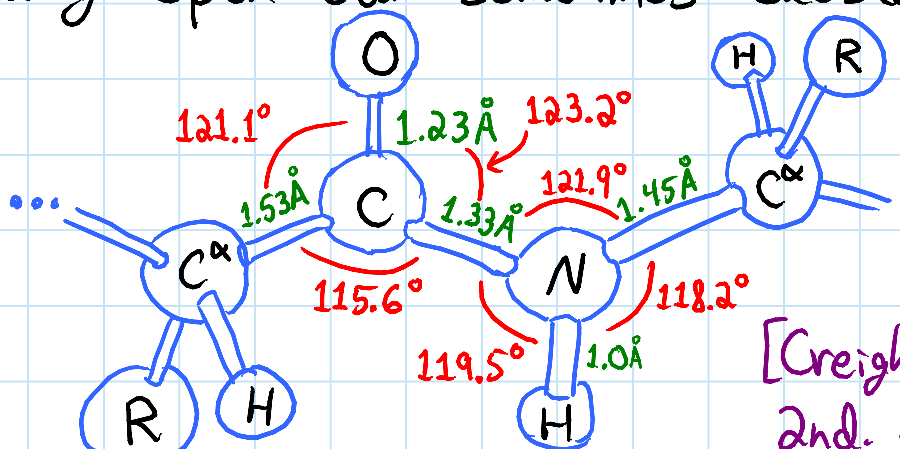
6.849	Lecture 18	Nov. 14, 2010

Fixed-angle linkages: fix angles between incident bars

- roughly the mechanics of a protein
  (ignore energy/actuation until next lecture)
- in fact, roughly fixed-angle tree
- protein backbone is roughly fixed-angle chain
  (usually open but sometimes closed)



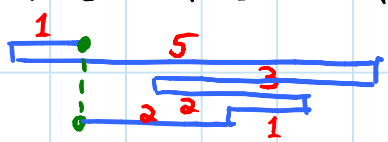
[Creighton: PROTEINS, 2nd. ed., p. 5]

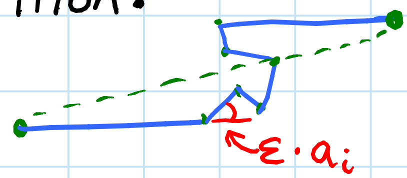
- usually focus on backbone, ignoring amino-acid "side chains" ~ reasonable approximation
- basic move: edge spin / local dihedral motion:

Major problems in fixed-angle linkages (esp. chains)

1. span = max/min distance between endpoints
2. flattening = motion to flat state
3. flat-state connectivity = motions between flat states
4. (un)locked = motion between any two states

<u>Span</u> of chain configuration = distance between endpoints
- distribution of span over configuration space heavily studied in e.g. polymer physics [>20 papers]
- weakly NP-hard to find <u>flat</u> state with min or max span (among flat states) [Soss 2001]
  - easy reductions from Partition:

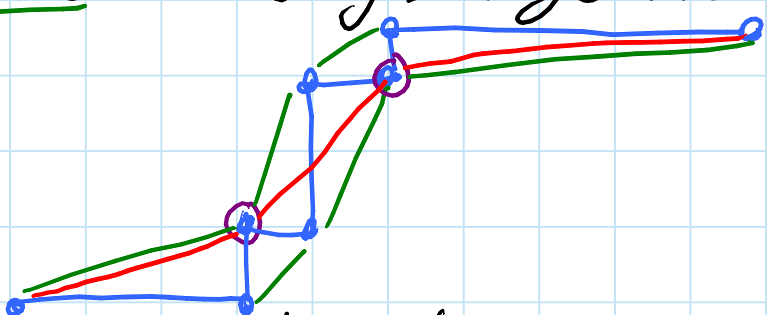
min: 

max: 

- $\boxed{\text{OPEN}}$: pseudopoly. alg. for flat min/max. span?
- $\boxed{\text{OPEN}}$: complexity of <u>3D</u> min/max span?

<u>3D max span:</u> structural characterization & poly. time for orthogonal (90°)
[Benbernou & O'Rourke 2006/2010; Borcea & Streinu 2010]

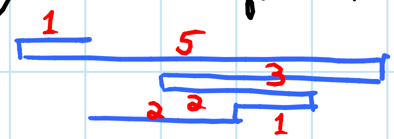
- <u>triangulate</u> into body & hinge assembly:



- <u>geodesic shortest path</u> = max span length
- each part stays planar & zigzag (this part gets hard for nonorthogonal)
- twist <u>connections</u> to align <u>path edges</u>

Flattening: weakly NP-hard [Soss & Toussaint 2000]

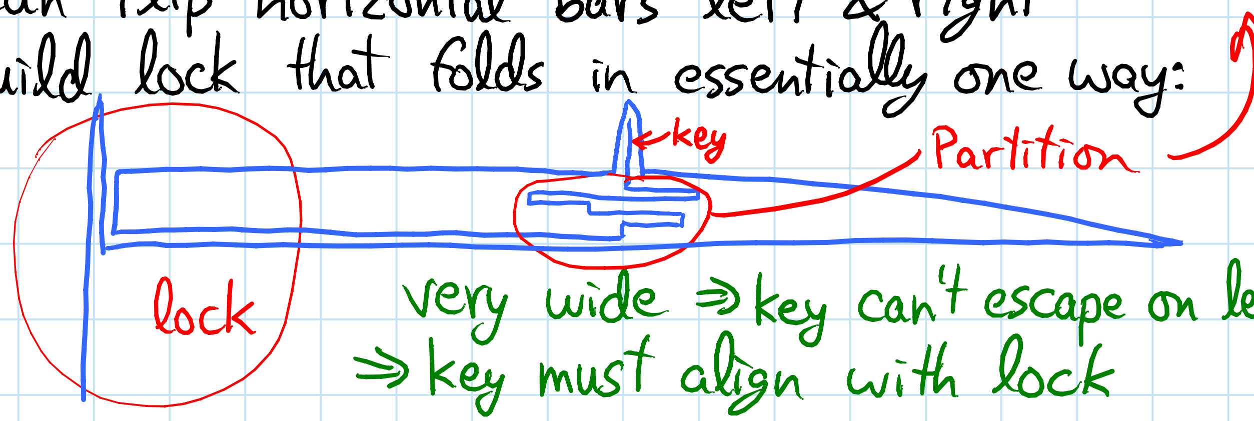
- reduction from <u>Partition</u>: divide n integers into 2 equal sums
- horizontal bars for integers



- vertical bars in between, length $< \frac{1}{n}$

$\Rightarrow$ can flip horizontal bars left & right

- build lock that folds in essentially one way:



very wide $\Rightarrow$ key can't escape on left

$\Rightarrow$ key must align with lock

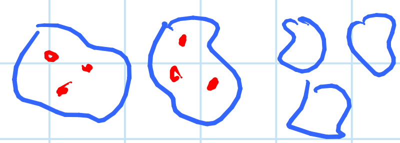
$\boxed{\text{OPEN}}$: pseudopolynomial-time algorithm?

Flat-state connectivity: [Aloupis et al. 2002 & 2002]

- <u>connected</u> if there's a motion between any two non-self-intersecting flat configurations
  - weaker form of connected config. space

  $\Rightarrow$ flat states are "canonical" for C

- <u>disconnected</u> otherwise
  - stronger notion of locked

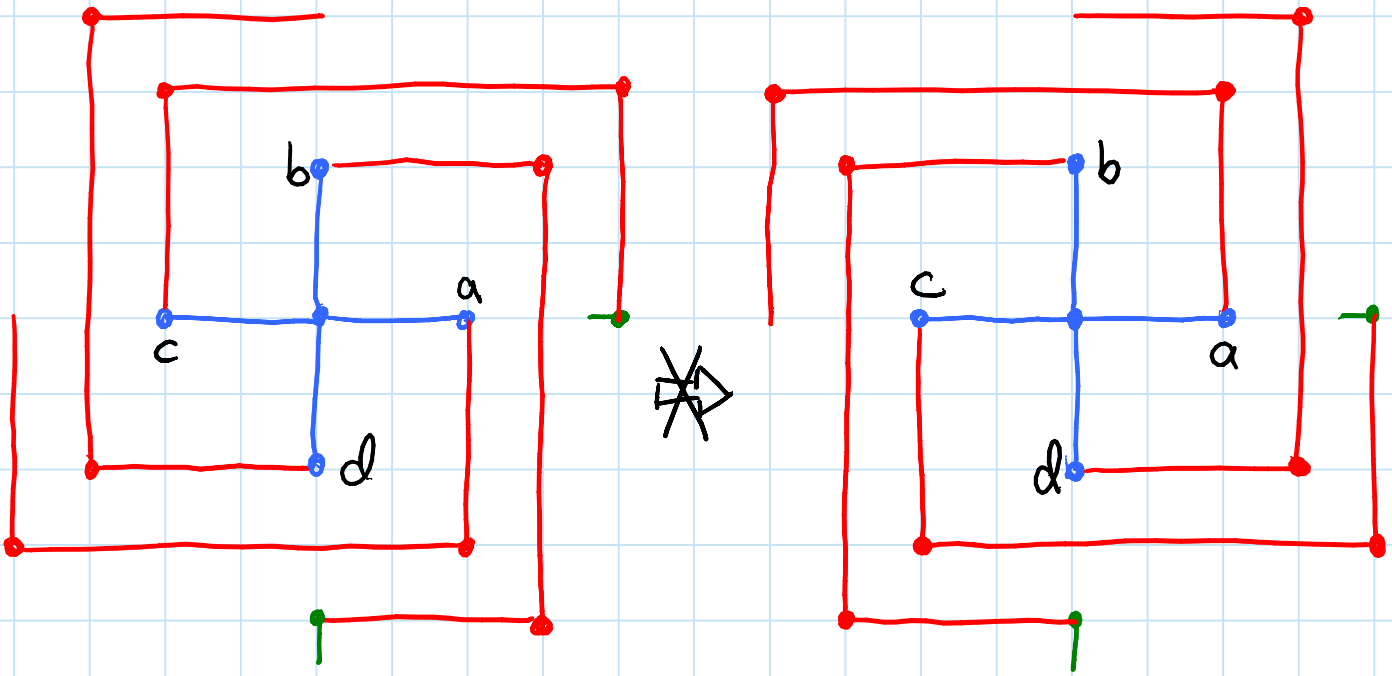


- fixed-angle chain might have <u>no</u> flat states (even NP-hard to know which) but proteins <u>do</u>, and seems important

Summary of results: [Aloupis et al. 2002 & 2002]

open chain	OPEN
– nonacute angles	connected
– equal acute angles	connected
– angles strictly between 60° & 90° & unit edge lengths	connected
– has a monotone state	connected
– angles strictly between 60° & 150° & unit edge lengths	connected [Aloupis & Meijer 2006]
– using 180° edge spins	disconnected
– orthogonal & using 180° edge spins	connected
set of open chains, pinned at one end	
– orthogonal	connected
– orthogonal & $\underbrace{\text{partially rigid}}_{\text{some edges can't spin}}$	disconnected
closed chain	OPEN
– nonacute	OPEN
– orthogonal	OPEN
– orthogonal & unit edge lengths	connected
tree	OPEN
– orthogonal	OPEN
– orthogonal & partially rigid	disconnected
graph – orthogonal	disconnected

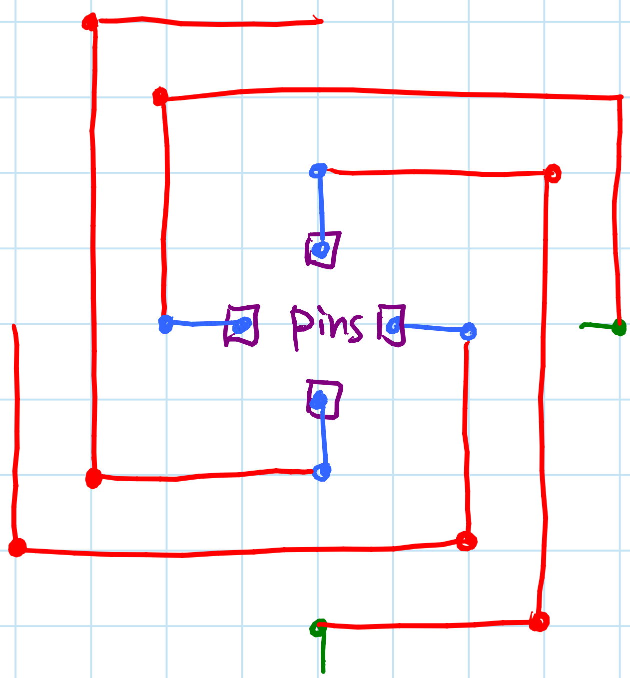
Flat-state disconnected partially rigid tree:

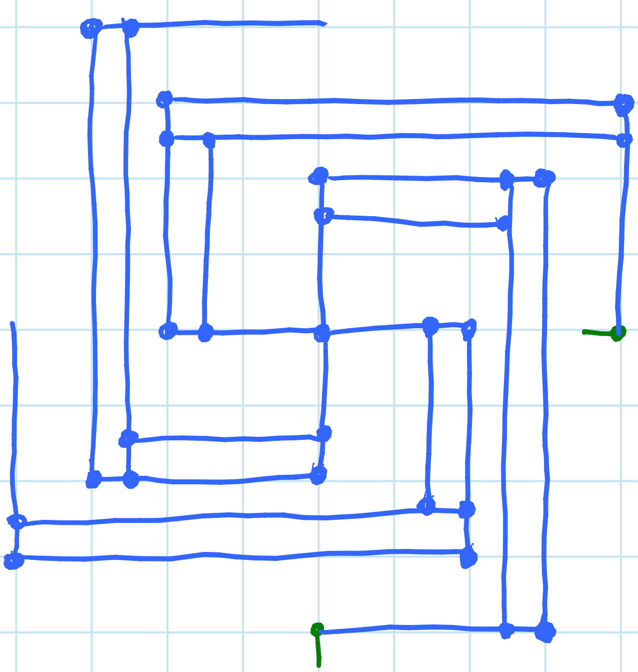


- inner edges flexible; rest rigid
- pins to remove reflectional symmetry

Variations:

① four pinned chains, partially rigid





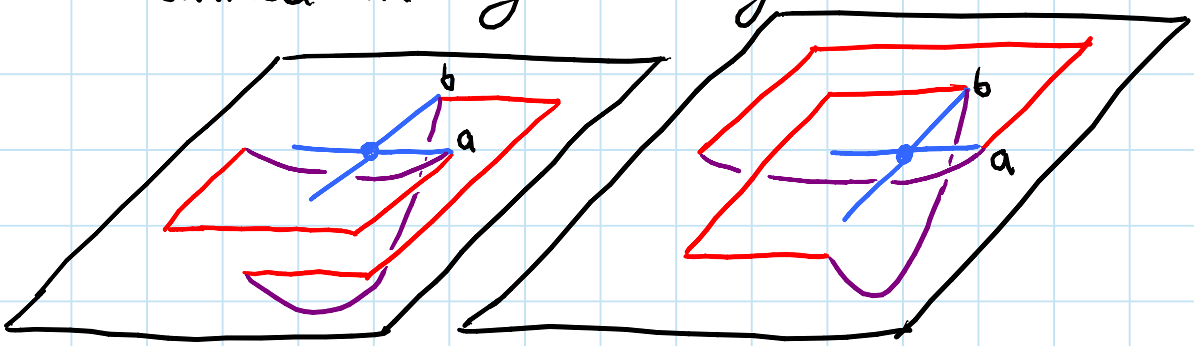
② orthogonal graph

Flat-state disconnected partially rigid tree: (cont'd)

Claim: these two flat states are disconnected

Proof: view plane abcd as stationary
- four branches & two sides of plane

$\Rightarrow$ ≥ 2 branches must flip through same side
- opposite branches (ac or bd) can't share:
  - geometric argument
  - links parallel to axis of rotation hit exactly
  - can shrink a & b edges for proper collision
- adjacent branches (say, ab) can't share:
  - topological argument
  - connect shallow rope a → end of a branch
  - connect deeper rope b → end of b branch
  - unlinked in left config.
  - linked in right config



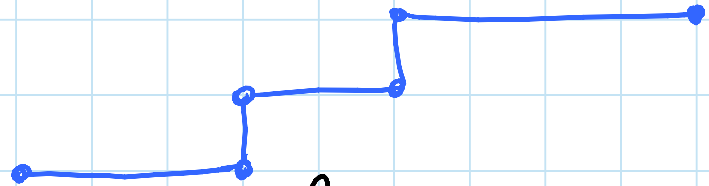
- ropes stay as-is during motion above plane

$\Rightarrow$ a & b branches intersect $\square$

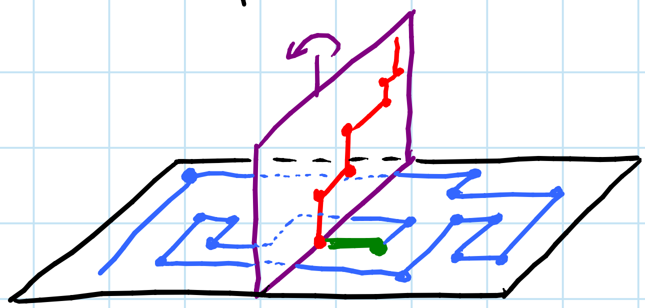
$\boxed{\text{OPEN}}$: flexible tree? orthogonal tree?

Orthogonal open chains are flat-state connected:

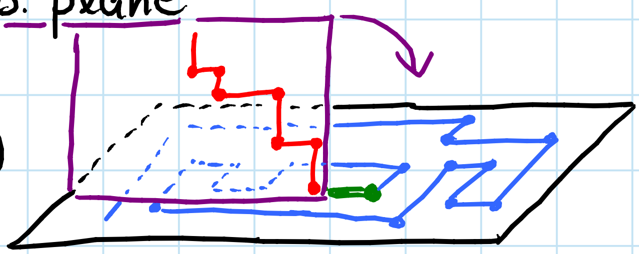
- canonical form: staircase (trans config. from L16)
  (alternate $\pm 90^\circ$ turns)



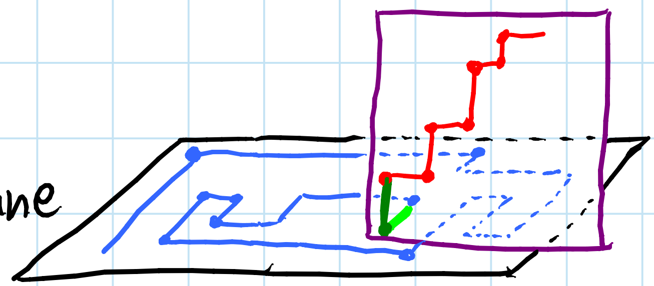
- lift a flat state into canonical form:
  Ⓞ induction hypothesis:
    - half of chain remains in plane
    - half of chain in canonical form in perp. plane



  ① rotate canonical half (and its containing plane) so that next edge makes a larger staircase

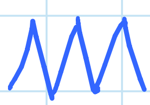


  ② rotate larger staircase (around following edge) to lift into staircase plane



  ③ repeat
- FedEx via canonical form

Nonacute open chains: similar
- canonical state = z-monotone ($\Rightarrow$ never hit $z=0$)

Equal acute chains: similar
- canonical state = zig-zag  ($\Rightarrow$ lifting harder)

$\boxed{\text{OPEN}}$: general chains?

Locked proteins:

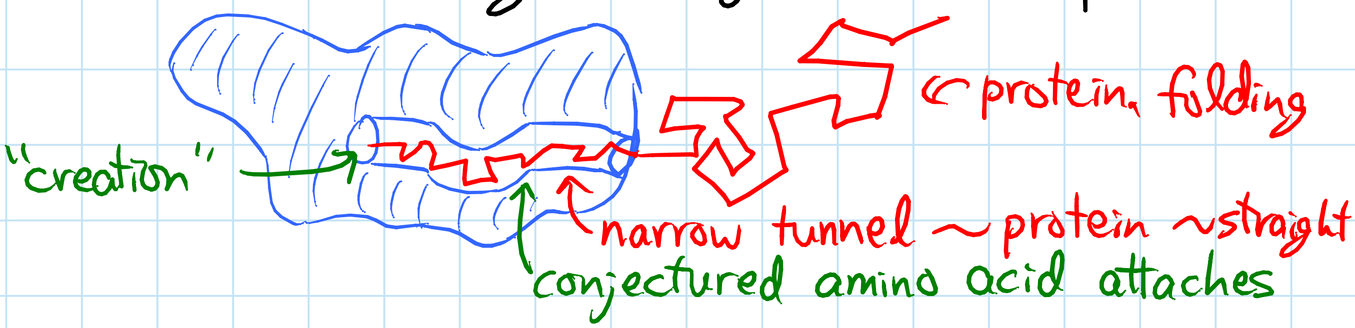
- locked universal-joint chains are locked fixed-angle too
  - even simpler, 4-link "crossed-legs": [Langerman 2002]

- existence of locked chains suggests config. space is hard to navigate ~ yet nature does it well
- Conjecture: additional constraints in nature prevent existence of locked chains
  - bond lengths all roughly equal (1-1.53Å)
  - bond angles all obtuse & roughly equal (115.6-123.2°)
  - $\boxed{\text{OPEN}}$: is there a locked fixed-angle chain that's equilateral, equiangular, & obtuse
    - crossed legs satisfies all but obtuse
    - subdivided knitting needles all but equi-ang.
  - proteins also produced sequentially by ribosome:

Producible protein (fixed-angle) chains:

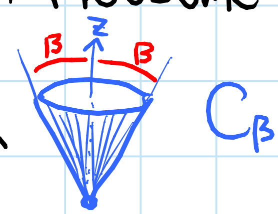
[Demaine, Langerman, O'Rourke 2003/6]

Ribosome = "machine" built from proteins & RNA translating messenger RNA into proteins



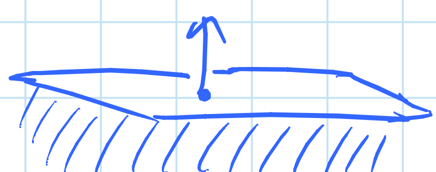
β-producible chain = simple geometric model of chains & configurations resulting from ribosome

- cone C_β of half-angle β
- chain produced in cone, link by link
- latest link passes through cone apex
- when latest vertex v_i reaches cone apex, next link (v_i, v_{i+1}) is instantly created in cone & v_i can never re-enter cone



Reality: $\beta = 90°$ (halfspace) is the closest model

(somewhat local model though ~ really long protein might reach around ribosome)

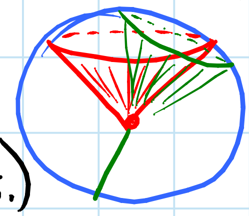


$(\leq\alpha)$-chain = chain of max. turn angle $\leq \alpha$

- β-producible $\Rightarrow \alpha/2 \leq \beta \leq 180° - \alpha/2$
- we'll assume $\alpha = \beta$

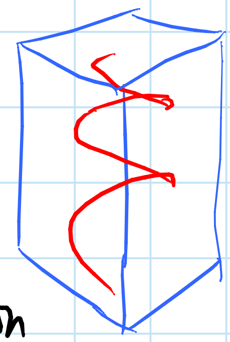
Canonical configuration for ($\le\alpha$)-chains:

- put $v_\emptyset$ at origin $(\emptyset, \emptyset, \emptyset)$
- put v_{i+1} on cone $C_{\alpha/2}$ centered at v_i
- v_1 chosen to maximize x coordinate
- v_{i+1} chosen to get correct turn angle at v_i:
  - view on sphere centered at v_i & radius $\alpha/2$
  - $C_{\alpha/2}$ intersects along circle around north pole
  - turn-angle cone intersects along tilted circle of radius τ_i

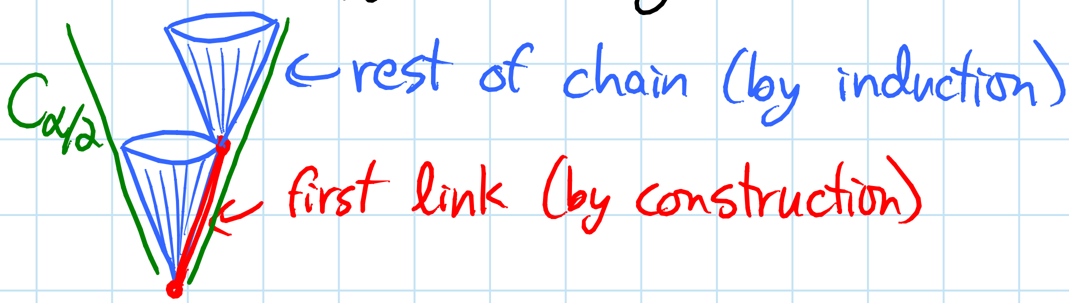


  - intersections overlap (at 1 or 2 pts.) because center of turn-angle circle is on $C_{\alpha/2}$ circle & $\tau_i \le \alpha$
  - take counterclockwise-most intersection for v_{i+1}
    - relative to origin

- kind of spiral
  ~ similar to nature's α-helix



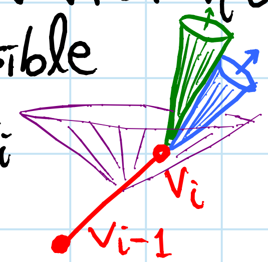
- contained in $C_{\alpha/2}$ cone: by induction



  - in fact, strictly inside cone $C_{\alpha/2}$ except for first link because $(v_\emptyset, v_1)$ & (v_1, v_2) not parallel

Canonicalizing $(\geq\alpha)$-producible $(\leq\alpha)$-chains:

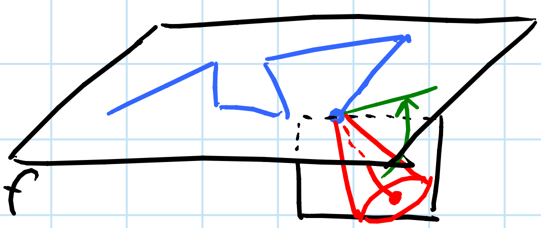
- main idea: play production movie backwards
  $\Rightarrow$ as links enter the cone, they disappear
- maintain these links in canonical configuration, translated to start at last existing vertex v_i & rotated to make cone as vertical as possible while satisfying turn angle at v_i



- viewed on sphere centered at v_i:
  put canonical cone axis $2\tau_i$ up from previous edge direction toward north pole (maxing out at north pole)
  $\Rightarrow$ canonical configuration is in $C_{\beta(\geq\alpha)}$ because (v_{i-1}, v_i) is too (by production)
- if (v_{i-1}, v_i) is vertical, then orientation of first link is not determined
  - choices for smaller & larger times may differ
  - freeze movie & continuously spin (v_{i-1}, v_i) to switch from previous choice to next
- when v_i reaches cone apex, need to extend canonical configuration & maintain invariant
  - spin (v_{i-1}, v_i) to make (v_i, v_{i+1}) as vertical as possible $\Rightarrow$ new canon. config. rotation
  - spin (v_i, v_{i+1}) to bring (v_i, v_{i+1}) into canonical configuration
  - note: already canonical $\Rightarrow$ rigid $\square$

What is producible?

- α-canonical configuration is β-producible for $\alpha/2 \le \beta \le 180° - \alpha/2$ (full range)
  - keep canonical configuration in complementary cone B_β
  - $\Rightarrow$ produces "rigidly" (no spinning required)
- $(\le\alpha)$-chain $(\ge\alpha)$-producible
  - $\Rightarrow$ β-producible for $\alpha/2 \le \beta \le 180° - \alpha/2$
  - β-produce α-canonical configuration
  - reverse canonicalization procedure far away from production cone C_β
- flat states of $(\le\alpha)$-chains are β-producible for $\alpha \le \beta \le 90°$
  - imagine moving cone instead of chain
  - create next link in vertical plane
  - slide up to plane of flat configuration with cone just touching plane
  - repeat



$\Rightarrow$ flat-state connected
  - canonicalize both, combine motions

$\Rightarrow$ for $(\le\alpha)$-chains & $\alpha \le \beta \le 90°$, configuration is flattenable $\Leftrightarrow$ it is β-producible