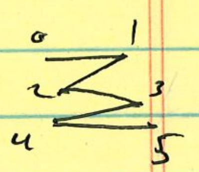
SCRATCH
(1)

$\boxed{\text{Normal mode analysis of N-linked chains}}$ → $\boxed{\text{-COMPLETELY SCREWED UP. -SOLVED (mostly) IN "SCRATCH 4" NOTES}}$ ☆

OPEN CHAIN



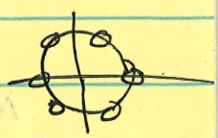
$$E = \frac{1}{\delta\sigma^2}\left[(x_0 - x_1)^2 + (x_1 - x_2)^2 + \cdots (x_5 - x_4)^2\right]$$

$x_0 \ldots x_5$ = displacements from ideal

$$= \frac{1}{2\sigma^2}[x_0\ x_1 \ldots x_5]\overbrace{\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}}^{A_{OPEN}}\begin{bmatrix} x_0 \\ \vdots \\ x_5 \end{bmatrix}$$

one eigvector: $x_0 \ldots x_5 = \frac{1}{\sqrt{6}}[1,1,1,1,1,1]$ ⇒ eigenvalue = 0.

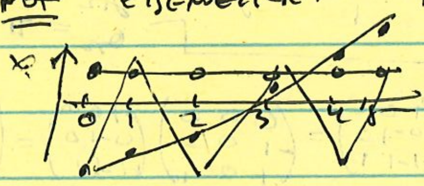
$$x_0, \ldots x_5 = \frac{1}{\sqrt{6}}\left[e^{-2\pi i \cancel{0} k/6}, \ldots\right] = \frac{1}{\sqrt{6}}\left[1, e^{-2\pi i k/6}, \ldots e^{-2\pi \cdot 5 ik/6}\right]$$



$$x_m = \frac{1}{\sqrt{6}} e^{-2\pi i m k/6}$$

$$\begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}\begin{bmatrix} e^{-2\pi i k/6} \\ \vdots \\ e^{-2\pi \cdot 5k/6} \end{bmatrix} = \begin{bmatrix} \cancel{\phi}\, 1 - e^{2\pi i k/6} \\ \underline{\left(-e^{2\pi i k/6} + 2 - e^{-2\pi i k/6}\right)} e^{2\pi i k/6} \\ = \cancel{0}. \\ \left(e^{2\pi i k/6} + 1\right) e^{-2\pi \cdot 5 i/6} \end{bmatrix}$$

NOT EIGENVECTOR? Try:



$x = \cos\left(2\pi i k m/6\right)$ (OPEN)

$$Ax = \begin{bmatrix} \cancel{0}\, 1 - \cos\left(\frac{2\pi i k}{6}\right) \\ 2\cos\left(\frac{2\pi i k}{6}\right) - \cancel{0}\, 1 - \cos\left(\frac{2\pi i k}{6}\right)^2 \end{bmatrix}$$

Set equal?

$$\cancel{\left[1 - \cos\left(\frac{2\pi i k}{6}\right)\right]^2 = 2\cos\left(\frac{2\pi i k}{6}\right)}$$

$$1 - \cancel{e^{-2\pi i k/6}} \overset{?}{=} 2 - e^{2\pi i k/6} - \cancel{e^{-2\pi i k/6}}$$

$$e^{2\pi i k/6} = 1 \quad ?$$

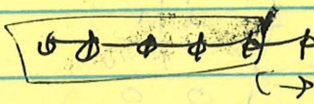
$k = 0$

To get to a quick answer, calc det of A_{OPEN} and det of A_{CLOSED} ⇒ $\begin{bmatrix} 2 & -1 & & & & -1 \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & -1 & 2 & -1 \\ -1 & & & & -1 & 2 \end{bmatrix}$

[in FACT, just get eigenvectors + eigenvalues?]

SCRATCH ②

$$\begin{pmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} \cancel{x} \\ \cancel{x} \\ \cancel{x} \\ \cancel{x} \\ \cancel{x} \\ \cancel{x} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \end{pmatrix}$$



$(x_0-x_1)^2 + (x_1-x_2)^2 + \dots (x_4-x_5)^2$

$= d_1^2 + d_2^2 + \dots d_5^2$

rel. separation

center of mass

with
$$\boxed{\begin{aligned} d_1 &= x_0 - x_1 & d_4 &= x_4 - x_3 & & \\ d_2 &= x_1 - x_2 & d_5 &= x_5 - x_4 & d_0 &= \frac{x_0 + x_1 + x_2 + \dots + x_5}{6} \\ d_3 &= x_3 - x_2 & & & & \end{aligned}}$$

$$\begin{pmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & \\ & & -1 & 1 \end{pmatrix}$$

THIS IS THE NATURAL BASIS FOR OPEN CHAIN.

$x_1 = x_0 - d_1$

$x_2 = x_1 - d_2 = x_0 - d_1 - d_2$

$\vdots$

$x_5 = x_0 - d_1 - d_2 - \dots d_4 - d_5$

So:

$6 d_0 = 6x_0 - 5d_1 - 4d_2 - 3d_3 - 2d_4 - d_5$

$x_0 = d_0 + \frac{5}{6}d_1 + \frac{4}{6}d_2 + \frac{3}{6}d_3 + \frac{2}{6}d_4 + \frac{1}{6}d_5.$

$x_1 = x_0 - d_1 = d_0 - \frac{1}{6}d_1 + \frac{4}{6}d_2 + \frac{3}{6}d_3 + \frac{2}{6}d_4 + \frac{1}{6}d_5$

$\vdots$

$\left(\frac{5}{6}, -\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6}\right)$ ← EIGENVECTOR?

$\Downarrow$

SCRATCH ③

$$\begin{pmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & \ddots & -1 & & \\ & & & & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ e^{ik} \\ e^{i2k} \\ e^{i3k} \\ \vdots \\ e^{i(N-1)k} \\ \end{pmatrix} = \begin{pmatrix} 1 - e^{ik} \\ e^{ik}[2-e^{ik}-e^{-ik}] \\ e^{2ik}[2-e^{ik}-e^{-ik}] \\ \vdots \\ e^{iNk}[2-e^{ik}-e^{-ik}] \\ a-e^{i(N-1)k} \end{pmatrix}$$

WANT $e^{ik} = e^{i(N-1)k}$

$$e^{i(N-2)k} = 1$$

$[N-2]k = 2\pi q$ $q \in$ integer

$$k = \frac{2\pi q}{N-2}$$

check that we can solve for a...

$$\left[a - e^{\frac{2\pi i q}{(N-2)}}\right] = a\left[2 - e^{ik} - e^{-ik}\right]$$

$$a - e^{\frac{2\pi i q}{N-2}} = a\left[2 - e^{\frac{2\pi q i}{N-2}} - e^{-\frac{i2\pi q}{N-2}}\right]$$

$$a\left[e^{\frac{2\pi q i}{N-2}} + e^{-\frac{2\pi q i}{N-2}} - 1\right] = e^{\frac{2\pi i q}{N-2}}$$

$$a = \frac{e^{2\pi i q/N-2}}{e^{\frac{2\pi q i}{N-2}} + e^{-\frac{2\pi q i}{N-2}} - 1}.$$

yup - solvable.

Eigenvals are...
$2\left[1-\cos\left(\frac{2\pi}{N-2}\right)\right]$, $2\left[1-\cos\left(\frac{2\pi}{N-2}\cdot 2\right)\right]$, ... $2\left[1-\cos\left(\frac{2\pi}{N-2}(N-1)\right)\right]$
[N-1 values]

<u>good?</u>

How to compute product?

$$\prod_{m=1}^{N-1} 2\left[1-\cos\left(\frac{2\pi m}{N-2}\right)\right]$$

$$= 2^{N-1}\prod_{m=1}^{N-1}\left[1 - e^{\frac{2\pi}{N-2}m} - e^{-\frac{2\pi}{N-2}m}\right]$$

$$= 2^{N-1}$$

$1 - e^{ik} = 2 - e^{ik} - e^{-ik}$

$e^{-ik} = 1$

$k = \frac{2\pi}{N}$?

?

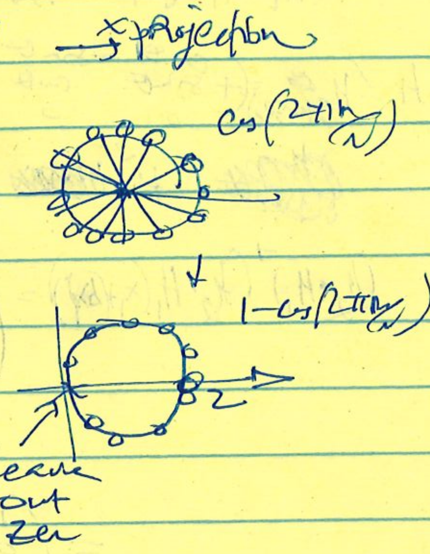
SCRATCH ④

CLOSED LINK:

$$\boxed{\text{Eigenvals are } 2 - e^{-i2\pi m/N} - e^{i2\pi m/N}, \quad m = 1, \dots, N-1}$$

$$= 2\left(1 - \cos 2\pi m/N\right)$$

$$= -\left[e^{\frac{i2\pi m}{2N}} - e^{-\frac{i2\pi m}{2N}}\right]^2$$



$$\prod_{m=1}^{N-1} -\left[e^{\frac{i2\pi m}{2N}} - e^{-\frac{i2\pi m}{2N}}\right]^2$$

$$4\prod_{m=1}^{N-1} \sin^2\left(\frac{\pi m}{N}\right)$$

$$= \left[\prod_{m=1}^{N-1} \sin\left(\frac{\pi m}{N}\right)\right]^2$$

$$\sin\left(\frac{\pi}{N}\right)\sin\left(\frac{2\pi}{N}\right) \cdots \underbrace{\sin\left(\frac{(N-1)\pi}{N}\right)}_{\sin\left(\pi - \frac{\pi}{N}\right)}$$

merge

$$\sin(x)\sin(\pi - x) = \cos\left[x + (\pi - x)\right] - \cos\left[x - (\pi - x)\right]$$

$$= \underbrace{\cos\pi}_{-1} - \cos(2x - \pi)$$

$$= -1 + \cos(2x)$$

$$\stackrel{?}{=} 2\sin x.$$

$$\sin^2\frac{x}{2} = \frac{1-\cos x}{2}$$

$$\left[e^{i\frac{\pi}{N}} - e^{-i\frac{\pi}{N}}\right]\left[e^{\frac{i2\pi}{N}} - e^{-\frac{i2\pi}{N}}\right] \cdots \left[e^{i\frac{\pi}{N}(N-1)} - e^{-i\frac{\pi}{N}(N-1)}\right]$$

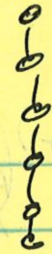
DIDN'T WORK...

$$1 + 2 + \dots N-1 = \frac{(N-1)N}{2}$$

so 1st term $\rightarrow$ $e^{i\frac{\pi}{\cancel{N}}\frac{(N-1)\cancel{N}}{2}} = e^{i\frac{\pi(N-1)}{2}}$

SCRATCH (5)

$$\begin{pmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ c\, e^{2\pi i k} \\ e^{2\pi i k \cdot 2} \\ \vdots \end{pmatrix}$$



OPEN CHAIN Revisited.

Eigenvalue [BASED on "middle" values
$$\lambda = 2 - e^{2\pi i k} - e^{-2\pi i k}$$

- $\boxed{\text{set } c = 1}$ wlog
- What do a & b have to be?

$$\begin{pmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ 1 \\ e^{2\pi i k} \\ e^{2\pi i k \cdot 2} \\ \vdots \end{pmatrix} = \lambda$$

(1) $a - b = \left[2 - e^{2\pi i k} - e^{2\pi i k}\right] a$

(2) $-a + \cancel{2}b - 1 = b\left(\cancel{2} - e^{2\pi i k} - e^{-2\pi i k}\right)$

(2) $\Rightarrow$ $a = -1 + b\left(e^{2\pi i k} + e^{-2\pi i k}\right)$ (3)

(1) $\Rightarrow$ $b = -a\left[1 - e^{2\pi i k} - e^{-2\pi i k}\right]$

Sub into (3):

$$a = -1 - a\left[1 - e^{2\pi i k} - e^{-2\pi i k}\right]\left[e^{2\pi i k} + e^{-2\pi i k}\right]$$

$$a = -1 - a\left[e^{2\pi i k} + e^{-2\pi i k} - e^{4\pi i k} - 1 - 1 - e^{-4\pi i k}\right]$$

$$-1 = a\left[e^{2\pi i k} + e^{-2\pi i k} - e^{4\pi i k} - e^{-4\pi i k} - 1\right]$$

$$a = \frac{1}{1 - e^{2\pi i k} - e^{-2\pi i k} + e^{4\pi i k} + e^{-4\pi i k}} \quad (4)$$

$$b = \frac{e^{2\pi i k} + e^{-2\pi i k} - 1}{1 - e^{2\pi i k} - e^{-2\pi i k} + e^{4\pi i k} + e^{-4\pi i k}} \quad (8)$$

SCRATCH ⑧

- what sets allowed wavemodes?

o- p. ③ I made the mistake of enforcing symmetry

I know the answer ("semi-empirically" from eigensystem analysis, MATLAB)...

$k =$ half integers... $= j/2N$ $(j = 0, \ldots N-1)$

OK

$$a = \cancel{\frac{1}{1 - e^{\pi i j} - e^{-\pi i j} + e^{2\pi i j} + e^{-2\pi i j}}}$$

$$= \cancel{\begin{cases} 1 & (j \text{ even}) \\ \frac{1}{5} & (j \text{ odd}) \end{cases}}$$

$$b = \cancel{\frac{e^{\pi i j} + e^{-\pi i j} - 1}{1 - e^{\pi i j} - e^{-\pi i j} + e^{2\pi i j} + e^{-2\pi i j}}}$$

$$= \cancel{\begin{cases} 1 & (j \text{ even}) \\ -\frac{3}{5} & (j \text{ odd}) \end{cases}}$$

Hmm, what about ~~s~~ centroid must remain at zero?

$$\underset{1}{a} + \underset{2}{b} + \underset{3}{1} + \underset{4}{e^{2\pi i k}} + \ldots \underset{N-2}{e^{2\pi i k(N-5)}} \quad \underset{N-1}{e^{2\pi i k(N-5)} \times b} \quad \underset{N}{e^{2\pi i k(N-5)} \times a}$$

$$\text{Sum} = \underbrace{(a+b)(1 + e^{2\pi i k(N-5)})}_{} + \underbrace{1 + e^{2\pi i k} + \ldots e^{2\pi i k(N-5)}}_{S}$$

$$\frac{(e^{2\pi i k} + e^{-2\pi i k})}{1 - e^{2\pi i k} - e^{-2\pi i k} + e^{4\pi i k} + e^{-4\pi i k}} \left(1 + e^{2\pi i k(N-5)}\right) \qquad S = \frac{e^{2\pi i k(N-4)} - 1}{e^{2\pi i k} - 1}$$

define $q = e^{2\pi i k}$

$$\text{Sum} = \frac{(q + q^{-1})(1 + q^{N-5})}{1 - q - q^{-1} + q^2 + q^{-2}} + \frac{q^{N-4} - 1}{q - 1} \stackrel{?}{=} 0$$

$$(q + q^{-1})(1 + q^{N-5})(q-1) = -(q^{N-4} - 1)(1 - q - q^{-1} + q^2 + q^{-2})$$

$$\cancel{q^2} - \cancel{q} + \cancel{q^{N-3}} - \cancel{q^{N-4}} + \cancel{1} - \cancel{q^{-1}} + \cancel{q^{N-5}} - \cancel{q^{N-6}} = \cancel{-q^{N-4}} + \cancel{q^{N-3}} + \cancel{q^{N-5}} - q^{N-2} - \cancel{q^{N-6}} \quad \cancel{+1} \; \cancel{-q} \; \cancel{-q^{-1}} + \cancel{q^2} + q^{-2}$$

SCRATCH ⑦

Zero centroid constraint

$\Rightarrow \quad 0 = -q_j^{N-2} + q_j^{-2}$

$q_j^N = 1$

$\Rightarrow \quad q_j = e^{2\pi i j/N}$, with j integer.

Not quite the right constraint – only picks out even.

what if we enforce REAL values ?!?

$\lambda = 2 - e^{2\pi i k} - e^{-2\pi i k} = 2[1 - \cos(2\pi k)]$

So k & $-k$ are both bona fide.

If we sum $\{ v_k + v_{-k}$ ← eigenvectors

First node position $= a(k) + a(-k)$

$=$ REAL VALUE since a is Real.

Ditto for second position.

How about $N-1$-th position?

$b(k)\, e^{2\pi i (N-5)} + b(k)\, e^{-2\pi i (N-5)}$

Yeah that will also come out as Real →

so REALITY is not A STRONG constraint.

$(x\ y)\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}$ SCRATCH-8

Simple test CASE → single link, two beads.

Try $\begin{pmatrix}1\\ e^{ik}\end{pmatrix} \to \begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\begin{pmatrix}1\\ e^{ik}\end{pmatrix} = \begin{pmatrix}1-e^{ik}\\ -1+e^{ik}\end{pmatrix}$

require: $\cancel{1}-e^{ik} = (-1+e^{ik})/e^{ik} = -e^{-ik}\cancel{+1}$

$$e^{ik}-e^{-ik}=0$$

$$k=\pi, 2\pi.$$

Need to be smarter about end of chain...

$$\begin{pmatrix}1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1\end{pmatrix}\begin{pmatrix}a\\ b\\ c\\ e^{i2\pi k(N-5)}\\ d\\ f\end{pmatrix}$$

wLOG, $c=1$ ...

$$\cancel{2d} - f - e^{i2\pi k(N-5)} = [\cancel{2} - e^{i\pi k} - e^{-i\pi k}]d \quad (4)$$

$$-d + f = [2 - e^{i\pi k} - e^{-i\pi k}]f \quad (5)$$

$$\Downarrow$$

$$d = -[1 - e^{i\pi k} - e^{-i\pi k}]f \quad (6)$$

Sub (6) into (4):

$$-f - e^{i2\pi k(N-5)} = [-e^{i\pi k} - e^{-i\pi k}]d$$

$$-f = e^{2\pi ik(N-5)} + f[e^{-i\pi k} + e^{-i\pi k}][1 - e^{i\pi k} - e^{-i\pi k}]$$

$$-e^{2\pi ik(N-5)} = f[-1 + e^{-i\pi k} + e^{i\pi k} - e^{-2i\pi k} - e^{2i\pi k}]$$

$$f = \frac{e^{2\pi ik(N-5)}}{1 - e^{-i\pi k} - e^{i\pi k} + e^{2\pi ik} + e^{2\pi ik}}$$

$$d = \frac{[e^{i\pi k} + e^{-i\pi k} - 1]\, e^{2\pi ik(N-5)}}{1 - e^{-i\pi k} - e^{i\pi k} + e^{2\pi ik} + e^{2\pi ik}}$$

SCRATCH-(9)

$$-c\cancel{e^{2\pi i k(N-6)}} + 2\cancel{ce^{2\pi i k(N-5)}} - d = \left[\cancel{2} - \cancel{e^{i\pi k}} - e^{-i\pi k}\right] c e^{2\pi i k(N-p)}$$

$$d \stackrel{?}{=} c e^{2\pi i k(N-p)}$$

$$\Downarrow$$

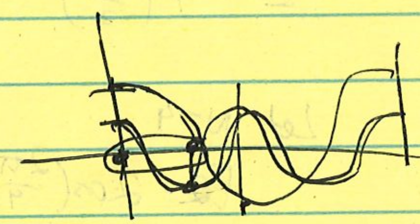
$$\frac{e^{i\pi k} + e^{-i\pi k} - 1}{1 - e^{-i\pi k} - e^{i\pi k} + e^{2\pi i k} + e^{-2\pi i k}} = 1$$

$$\Rightarrow \quad e^{i\pi k} + e^{-i\pi k} - 1 = 1 - e^{-i\pi k} - e^{i\pi k} + e^{2\pi i k} + e^{-2\pi i k}$$

$$2 = 2\left(e^{-i\pi k} + e^{i\pi k}\right) - e^{-2\pi i k} - e^{+2\pi i k}$$

~~$1 = \cos($~~

$$1 = 2\cos(\pi k) - \cos(2\pi k)$$



$$1 = 2\cos x - \cos x$$

$\cos 2x = \cos(x + x)$

$=$

$$k = 0, \tfrac{1}{2}, ?, \tfrac{3}{2}$$

SPARTH - 8 (1'')

Need one more equation...

$$\begin{pmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{pmatrix} \begin{pmatrix} a \\ b \\ 1 \\ e^{2\pi i k} \\ \vdots \end{pmatrix}$$

$$-b + 2 - e^{2\pi i k} = \left[e^{2\pi i k} + 2 - e^{2\pi i k} \right]$$

$$\Rightarrow b = +e^{2\pi i k}$$

Use (5):

$$+e^{2\pi i k} = \frac{e^{2\pi i k} + e^{-2\pi i k} - 1}{1 - e^{2\pi i k} - e^{-2\pi i k} + e^{4\pi i k} + e^{-4\pi i k}}$$

$$+\cancel{e^{-2\pi i k}} - 1 - e^{-4\pi i k} + \cancel{e} + e^{-6\pi i k} = -\cancel{e^{2\pi i k}} + \cancel{e^{-2\pi i k}} - 1$$

$$e^{2\pi i k} = 1$$

So k is integer?

Ugh...

$$\begin{pmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & \end{pmatrix} \begin{pmatrix} a \\ e^{i\pi k} \\ e^{2 i \pi k} \\ e^{3 i \pi k} \\ \vdots \end{pmatrix} \Rightarrow \cancel{a} - e^{i\pi k} = a\left[\cancel{2} - e^{i\pi k} - e^{-i\pi k}\right]$$

$$a = \frac{-e^{i\pi k}}{[1 - e^{i\pi k} - e^{-i\pi k}]}$$

AND...

$a = 1$ (?)

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

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

$$\boxed{e^{i\pi k} = 1} \text{ (?)}$$