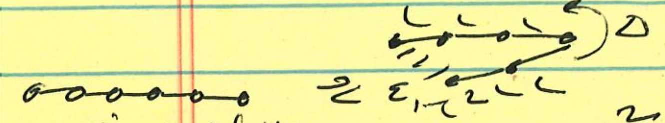
SCRATCH *** — 1

HAIRPIN CLOSURE "with strain"




gaussian convolution

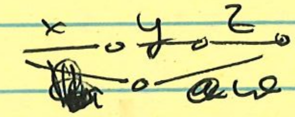
$$K = e^{-\epsilon}\, e^{-\Delta}\, \frac{e^{-\frac{1}{2}\frac{\gamma^2}{\delta\sigma^2}}}{\sqrt{2\pi}\sqrt{\delta\sigma}} \cdot \frac{1}{K_d} = e^{-\left(\epsilon+\gamma+\frac{L^2}{\sqrt{\sigma}}\right)}\left(\frac{\tau}{\sqrt{\delta\sigma}}\right)$$

$$\frac{\sqrt{\delta}}{\sqrt{2\pi}\,\tau}$$

Normal modes

Does this work with normal modes?

First, find minimum of closed chain




$(x+y+z-w)$

$$E = \frac{1}{2}\left\{ (x+y+z-w-1)^2 + (x-1)^2 + (y-1)^2 + (z-1)^2 + (w-1)^2 \right\}$$

$$0 = \frac{\partial E}{\partial x} = [(x+y+z-w)-1] + (x-1)$$

$$0 = \frac{\partial E}{\partial y} = [x+y+z-w-1] + (y-1)$$

$$0 = \frac{\partial E}{\partial z} = [x+y+z-w-1](z-1)$$

$$\Bigg\} \; x = y = z$$

$$0 = \frac{\partial E}{\partial w} = -[x+y+z-w-\cancel{1}] + (w-\cancel{1})$$

$$3x = 2w \qquad w = \frac{3}{2}x$$

and $3x - w - 1 + x - 1 = 0$

$$4x - 2 - w = 0$$

$$\left[4 - \frac{3}{2}\right]x = 2$$

$$\frac{5}{2}x = 2$$

$$\boxed{x = \frac{4}{5} \qquad w = \frac{6}{5}}$$

SCRATCH *** (2)

$$E\Big|_{\substack{t=2/5\\ s=\frac{1}{5}t\\ \omega=\frac{?}{}t}} = \frac{1}{2}\left\{3\cdot\left(\frac{1}{5}\right)^2 + \left(\frac{1}{5}\right)^2 + 2\right\}\frac{L^2}{\sigma^2}$$

$$= \frac{L^2}{2\cdot 5\sigma^2} \quad \boxed{\text{O.K.?}}$$

$$E(\Delta x,\Delta y,\Delta z,\Delta\omega) = \left\{(\Delta x+\Delta y+\Delta z+\Delta\omega)^2 + \Delta x^2 + \Delta y^2 + \Delta z^2 + \Delta\omega^2\right\}\frac{1}{2\sigma^2} + E_0$$

where $\omega = \omega_0 + \Delta\omega$, $x = x_0 + \Delta x$, $y = y_0 + \Delta y$, $z = z_0 + \Delta z$

(First derivs must cancel)

$$= \frac{1}{2\sigma^2}(\Delta x, \Delta y, \Delta z, \Delta\omega)\underbrace{\begin{pmatrix}2&1&1&1\\1&2&1&1\\1&1&2&1\\1&1&1&2\end{pmatrix}}_{A}\begin{pmatrix}\Delta x\\ \Delta y\\ \Delta z\\ \Delta\omega\end{pmatrix} + E_0.$$

Need determinant...

$\det\begin{pmatrix}2&1\\1&2\end{pmatrix} \to 3$

$\det\begin{pmatrix}2&1&1\\1&2&1\\1&1&2\end{pmatrix} \to 6 + (-1) + (-1) = 4.$

- $\det \Sigma = 5$ (I think)
- Would be cool to compute eigenvals, eigenvectors
- so

$$Z_{closed} = \frac{e^{-\varepsilon-\Delta}\, e^{-L^2/2\cdot 5\cdot\sigma^2}}{(\sqrt{2\pi})^4\sqrt{5}\,\sigma^4}\;\frac{1}{\sqrt{2\pi}\,\tau}$$

$$Z_{open} = \frac{1}{(\sqrt{2\pi})^5\sigma^5}$$

$$K = Z_{closed}/Z_{open} = e^{-(\varepsilon+\Delta+\frac{L^2}{10\sigma^2})}\frac{\sigma}{\sqrt{5}\,\tau}$$

yes?

Eigenvectors?

$(1, e^{ik}, e^{2ik}, e^{3ik})$ $\quad e^{4ik} = 1 \Rightarrow k = \frac{2\pi}{4}m,\ m = 0,1,2,3$

Eigenvalues

$2 + e^{ik} + e^{2ik} + e^{3ik}$

$k=0 \to 5$
$k=\pi/2 \to 2 + 0 - 1 + 0 = 1$
$k=\pi \to 2 - 1 + 1 - 1 = 1$
$k=3\pi/2 \to 2 + 0 - 1 + 0 = 1$

$\det A = 5.$