① DERIVS OF POTENTIAL !

24 JAN 2017

$\vec{v} = v\,\hat{v}$ ← axis-angle / rotation vector

$q_v = \left(\sin\left(\frac{v}{2}\right)\hat{v},\ \cos\left(\frac{v}{2}\right)\right)$ ← quaternion.

Can compute: $\nabla_v E = \left(\frac{\partial E}{\partial v_x}, \frac{\partial E}{\partial v_y}, \frac{\partial E}{\partial v_z}\right)$ ← stored on disk

- Have to convert to lab frame → $\frac{\partial E}{\partial \omega} = \vec{\omega} \cdot f\left(\frac{\partial E}{\partial v}\right)$ ← hopefully?

Rotate by ω around $\vec{v}$

I.e. want: $\boxed{\frac{\partial E}{\partial \omega_x}, \frac{\partial E}{\partial \omega_y}, \frac{\partial E}{\partial \omega_z}}$

- Imagine rotation by $\omega\hat{\omega}$, $\omega \ll 1$: How much does $\vec{v}$ change?

$$\left(\sin\left(\tfrac{v}{2}\right)\hat{v},\ \cos\left(\tfrac{v}{2}\right)\right) \cdot \left(\sin\tfrac{\omega}{2}\hat{\omega},\ \cos\tfrac{\omega}{2}\right)$$

$$\approx \left(\sin\left(\tfrac{v}{2}\right)\hat{v},\ \cos\left(\tfrac{v}{2}\right)\right) \cdot \left(\left(\tfrac{\omega}{2}\right)\hat{\omega},\ 1\right)$$

$$= \left(\cos\left(\tfrac{v}{2}\right)\left(\tfrac{\omega}{2}\right)\hat{\omega} + \sin\left(\tfrac{v}{2}\right)\hat{v} + \tfrac{\omega}{2}\sin\left(\tfrac{v}{2}\right)\hat{v}\times\hat{\omega},\ \ \underline{\cos\tfrac{v}{2} - \tfrac{\omega}{2}\sin\left(\tfrac{v}{2}\right)\hat{v}\cdot\hat{\omega}}\right)$$

← Hmm... order matters...

Set this equal to:

$$\frac{\partial q_v}{\partial \omega} = \left(\left[\sin\left(\tfrac{v}{2}\right)\left(\frac{\partial \hat{v}}{\partial \omega}\right) + \frac{1}{2}\cos\left(\tfrac{v}{2}\right)\frac{\partial v}{\partial \omega}\hat{v}\right]\omega + \sin\left(\tfrac{v}{2}\right)\hat{v},\ \ \underline{-\frac{1}{2}\sin\frac{v}{2}\frac{\partial v}{\partial \omega}\omega + \cos\frac{v}{2}}\right)$$

$\Rightarrow$ $\boxed{\frac{\partial v}{\partial \omega} = \hat{v}\cdot\hat{\omega}}$ (scalar term) and

$$\cos\left(\tfrac{v}{2}\right)\left(\tfrac{\cancel{\omega}}{2}\right)\hat{\omega} + \left(\tfrac{\cancel{\omega}}{2}\right)\sin\left(\tfrac{v}{2}\right)\left[\hat{v}\times\hat{\omega}\right] = \left[\sin\tfrac{v}{2}\left(\frac{\partial \hat{v}}{\partial \omega}\right) + \frac{1}{2}\cos\frac{v}{2}\,(\hat{v}\cdot\hat{\omega})\,\hat{v}\right]\cancel{\omega}$$

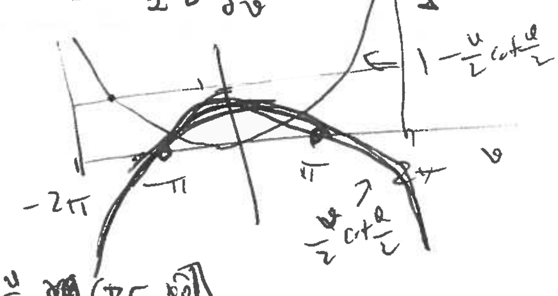
$$\frac{\partial \hat{v}}{\partial \omega} = \frac{\frac{1}{2}\cos\left(\frac{v}{2}\right)}{\sin\left(\frac{v}{2}\right)}\left[\hat{\omega} - (\hat{v}\cdot\hat{\omega})\hat{v}\right] - \frac{1}{2}\left[\hat{v}\times\hat{\omega}\right].$$

~~Now we identify~~

$$\frac{\partial E}{\partial \omega} = \frac{\partial E}{\partial \vec{v}}\cdot\frac{\partial \vec{v}}{\partial \omega} = \frac{\partial E}{\partial \vec{v}}\cdot\left[\frac{\partial}{\partial \omega}(v\hat{v})\right] = \frac{\partial E}{\partial \vec{v}}\cdot\left[\frac{\partial v}{\partial \omega}\hat{v} + v\left(\frac{\partial \hat{v}}{\partial \omega}\right)\right]$$

$$= \frac{\partial E}{\partial \vec{v}}\cdot\left[\underline{(\hat{v}\cdot\hat{\omega})}\hat{v} + \frac{v}{2}\cot\left(\tfrac{v}{2}\right)\left[\hat{\omega} - \underline{(\hat{v}\cdot\hat{\omega})\hat{v}}\right] - \frac{v}{2}\left[\hat{v}\times\hat{\omega}\right]\right]$$

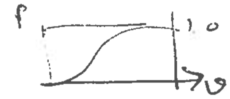
$$= \hat{\omega}\cdot\left[\underbrace{\left(\frac{\partial E}{\partial \vec{v}}\cdot\hat{v}\right)\hat{v}\times\left[1 - \frac{v}{2}\cot\frac{v}{2}\right]}_{\text{suppressed to 0 at } v=0 \text{, scaled to 1 at } v=1} + \underbrace{\frac{v}{2}\cot\frac{v}{2}\left(\frac{\partial E}{\partial \vec{v}}\right)}_{1 \text{ at } v=0 \text{, reduced to at } v=1.} - \frac{v}{2}\left[\frac{\partial E}{\partial \vec{v}}\times\hat{v}\right]\right]$$



$$= \hat{\omega}\cdot\left[(\nabla_v E\cdot\hat{v})\hat{v} + \frac{v}{2}\cot\frac{v}{2}\underbrace{\left(\nabla_v E - \hat{v}\cdot\nabla_v E\,\hat{v}\right)}_{\text{PERPENDICULAR TO } \hat{v}} - \frac{v}{2}\underbrace{\left(\nabla_v E\times\hat{v}\right)}_{\text{PERPENDICULAR TO } \hat{v}}\right]$$

SANITY CHECK

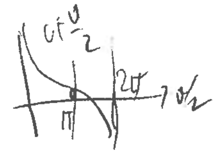
? Suppose ~~$\frac{\partial E}{\partial v} = \log[\sin^2(v/2)]$~~ i.e. Flat PROBABILITY distribution?



$\frac{\partial p_{dim}}{\partial v} \propto \sin^2\frac{v}{2}$

~~$E = \log p + \text{const},$~~

~~$\frac{\partial E}{\partial v} = \frac{1}{p}\frac{\partial p}{\partial v} = \frac{2\cdot\frac{1}{2}\sin\frac{v}{2}\cos\frac{v}{2}}{\sin^2\frac{v}{2}} = \cot\frac{v}{2}.$~~



~~$\frac{\partial E}{\partial w} = \hat{v}\cdot\left[\frac{1}{2}\cot\frac{v}{2}\,\hat{v}\right]$~~

$\boxed{\text{CRAP}}$

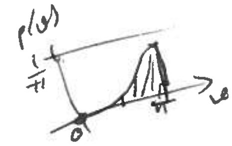
No,... need to define $E = \log(p/p_{ref})$

Flat distribution!

p of $\ldots = \frac{1}{\pi}[v - \sin v]$, i.e.,

$p(v) = \frac{\partial p_{dim}}{\partial v} = \frac{1}{\pi}[1-\cos v]$

$= \frac{2}{\pi}\sin^2\left(\frac{v}{2}\right)$



$\int p(v)\,dv = 1$

Need to divide by $4\pi v^2$

$$\frac{p(\vec{v})}{p_{REF}} = \frac{1}{2\pi^2 v^2}\sin^2\frac{v}{2} = \frac{1\sin^2(v/2)}{8\pi^2 (v/2)^2}$$

$$\int_{v=0}^{\pi} p_{REF}(\vec{v})\,d^3v = \int \frac{1}{8\pi^2}\frac{\sin^2(v/2)}{(v/2)^2}\,4\pi v^2\,dv = \int_0^{\pi}\frac{2}{\pi}\sin^2\frac{v}{2}\,dv = \int_0^{\pi}\frac{1}{\pi}[1-\cos v]\,dv = \frac{1}{\pi}[v - \sin v]_0^{\pi} = 1.$$

$$\boxed{p(\vec{v}) = \frac{1}{8\pi^2}\frac{\sin^2(v/2)}{(v/2)^2}}$$

$p(0) = \frac{1}{8\pi^2}$ → BEAUTIFUL!