Ware function of the from first principles:

24th June 2018

~) Starting point as in Bergstrom:

$$\phi_A = C \cdot \exp\left(-\frac{1}{2} \upsilon_A \cdot \sum_{i=1}^4 (\vec{x}_i - \vec{R})^2\right)$$

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I we transform into the cons system 2=0

~) Then we apply the Jacob: variables:

$$\vec{R} = \frac{1}{4} (\vec{x}_1 + \vec{x}_2 + \vec{x}_3 + \vec{x}_4)$$

$$\vec{\Gamma}_1 = \vec{x}_2 - \vec{x}_1$$

$$\vec{\Gamma}_2 = \vec{x}_3 - \frac{1}{2} (\vec{x}_2 + \vec{x}_4)$$

$$\vec{\Gamma}_3 = \vec{x}_4 - \frac{1}{3} (\vec{x}_3 + \vec{x}_4 + \vec{x}_4)$$

~ As derived in Morceynski, we can verify with Mathematica;

For the Jacobian, we obtain:

$$\frac{1}{2}(\vec{k}_1 - \vec{k}_2)^2 = \frac{1}{4}(2\vec{k}_1^2 + 2\vec{k}_2^2 + 2\vec{k}_3^2) \quad \text{The rest of the definition during definition denting} \\
d\vec{k} d\vec{k}_1 d\vec{k}_2 d\vec{k}_3 = \left| \det \frac{\partial (\vec{k}_1 + \vec{k}_1 + \vec{k}_3 + \vec{k}_3)}{\partial (\vec{k}_1 + \vec{k}_2 + \vec{k}_3 + \vec{k}_3)} \right| d\vec{k}_1 d\vec{k}_2 d\vec{k}_3 d\vec{k}_4 \quad \text{valid!}$$

and thus
$$\begin{vmatrix}
\frac{\partial R}{\partial x_1} & \cdots & \frac{\partial r_3}{\partial x_4} \\
\vdots & \vdots & \vdots \\
\frac{\partial R}{\partial x_4} & \cdots & \frac{\partial r_3}{\partial x_4}
\end{vmatrix} = \begin{vmatrix}
\frac{1}{2} & -1 & -\frac{1}{2} & -\frac{1}{2} \\
\frac{1}{2} & 0 & 1 & -\frac{1}{2} \\
\frac{1}{2} & 0 & 0 & 1
\end{vmatrix} = 7.$$

-> For the normal-sation constant, we thus get: = [ | that dx, ... dx, = [ exp (-70, (252+352+75)) dr, dr2dr3 1) = (4) 3 / 52. exp(- 2524)d57. [52. exp(- 352) d5. [53. exp(- 352) d5 43.0912 (1)312 => C2= (2, 2. 3)312 4 (250) 312 4 (240) 312 4.13 MZAKI S470/

we obtain accordingly: 12 ft (x; -R)2. log2 de de de des des 1 = 1 (x; -R) (cee first page)

- 2 = 1 (x2 + x2 + x2 + x2 + x2). |φ<sub>A</sub>|<sup>2</sup> dx, dx<sub>2</sub> dx<sub>3</sub> dx<sub>4</sub> = 1/2. ( 1 ( 1/2 exp(- 1/2 v4 r2) · exp(- 3/2 v4 r2) · exp(- 3/4 r2) dr dr dr dr dr 1 because mg describes the + \frac{2}{2} \left( \tau\_2^2 \cdot \texp(...) \cdot \texp(...) \cdot \texp(...) \cdot \dr\_2 dr\_2 dr\_3 = (47)3. -2. -2. -2 obtain for 6: 2 (4 13) · [ 52 exp(- 2 UA 52) dry · [ 52 exp(- 3 0, 52) drz · [ 52 exp(- 3 132) drz  $= \left( 4\pi \right)^{3} \cdot \frac{1}{2} \cdot \frac{3\sqrt{4}}{8} \cdot \frac{1}{\left( \frac{1}{2} v_{\Delta} \right)^{5/2}} \cdot \frac{\sqrt{\pi}}{4} \cdot \frac{1}{\left( \frac{1}{2} v_{\Delta} \right)^{3/2}} \cdot \frac{\sqrt{\pi}}{4} \cdot \frac{1}{\left( \frac{3}{2} v_{\Delta} \right)^{3/2}}$ => -2 = (2 (0 + 0 + 0) + 2/3 + \frac{\langle \langle \langl  $= \frac{1}{v_{A}} \cdot \frac{1}{4} \cdot \frac{4 \cdot 5}{2^{3}} = \frac{9}{8v_{A}}$