Wave function of ^4He from first principles:

24th June 2018

$$\phi_A = C \cdot \exp\left(-\frac{1}{4} \upsilon_A \cdot \sum_{i=0}^{A} \sum_{j=i+1}^{A} (\vec{x}_i - \vec{x}_j)^2\right)$$

→ fix mistake in current version of paper equation (25)

with $\vec{x}_{ij} = \vec{x}_i - \vec{x}_j$ we obtain for $A=4$:

$$\phi_A = C \cdot \exp\left(-\frac{1}{4} \upsilon_A \left(\vec{x}_{12}^{\,2} + \vec{x}_{13}^{\,2} + \vec{x}_{14}^{\,2} + \vec{x}_{23}^{\,2} + \vec{x}_{24}^{\,2} + \vec{x}_{34}^{\,2}\right)\right)$$

We then transform the variables as: (Jacobi coordinates)

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

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

$$\vec{r}_2 = \vec{x}_3 - \frac{1}{2}(\vec{x}_2 + \vec{x}_1)$$

$$\vec{r}_3 = \vec{x}_4 - \frac{1}{3}(\vec{x}_1 + \vec{x}_2 + \vec{x}_3)$$

As also outlined in Mrowczynski, one then obtains

$$\vec{x}_1^{\,2} + \vec{x}_2^{\,2} + \vec{x}_3^{\,2} + \vec{x}_4^{\,2} = 4\vec{R}^2 + \frac{1}{2}\vec{r}_1^{\,2} + \frac{2}{3}\vec{r}_2^{\,2} + \frac{3}{4}\vec{r}_2^{\,2}$$

and $$\vec{x}_{12}^{\,2} + \vec{x}_{13}^{\,2} + \ldots + \vec{x}_{34}^{\,2} = 2\vec{r}_1^{\,2} + \frac{8}{3}\vec{r}_2^{\,2} + 3\vec{r}_3^{\,2}$$

⇝ We need the wave-function normalised:

$$d\vec{R}\, d\vec{r}_2\, d\vec{r}_3\, d\vec{r}_3 = \left|\det \frac{\partial(\vec{r}_1, \ldots \vec{r}_4)}{\partial(\vec{x}_1, \ldots, \vec{x}_4)}\right| d\vec{x}_1\, d\vec{x}_2\, d\vec{x}_3\, d\vec{x}_4$$

and thus:
$$\begin{vmatrix} \frac{\partial \vec{R}}{\partial x_1} & \cdots & \frac{\partial r_3}{\partial x_1} \\ \vdots & & \\ \frac{\partial R}{\partial x_4} & \cdots & \frac{\partial r_3}{\partial x_4} \end{vmatrix} = \begin{vmatrix} \frac{1}{4} & -1 & -\frac{1}{2} & -\frac{1}{3} \\ \frac{1}{4} & 1 & -\frac{1}{2} & -\frac{1}{3} \\ \frac{1}{4} & 0 & 1 & -\frac{1}{3} \\ \frac{1}{4} & 0 & 0 & 1 \end{vmatrix} = 1 \checkmark$$

(as expected as the transformation to the Jacobi variables keeps the volume constant.)

For the normalisation constant we thus obtain:

$$\int |\phi_A|^2 \, d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 d\vec{x}_4 \overset{!}{=} 1$$

$$\Rightarrow \frac{1}{C^2} = \int \exp\left(-\frac{v_A}{2\cancel{4}}\left(2\vec{r}_1^{\,2} + \frac{8}{3}\vec{r}_2^{\,2} + 3\vec{r}_3^{\,2}\right)\right) \underbrace{d\vec{r}_1}_{4\pi r_1^2 dr_1} \underbrace{d\vec{r}_2}_{4\pi r_2^2 dr_2} \underbrace{d\vec{r}_3}_{4\pi r_3^2 dr_3}$$ with $V=1$ (integration over R)

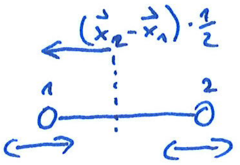
↑ from the square

$$= (4\pi)^3 \cdot \underbrace{\int r_1^2 \cdot e^{-v_A r_1^2} dr_1}_{\frac{\sqrt{\pi}}{4} \cdot \frac{1}{v_A^{3/2}}} \cdot \underbrace{\int r_2^2 e^{-v_A \cdot \frac{4}{3} r_2^2} dr_2}_{\frac{\sqrt{\pi}}{4} \cdot \frac{1}{(\frac{4}{3} v_A)^{3/2}}} \cdot \underbrace{\int r_3^2 \cdot e^{-v_A \cdot \frac{3}{2} r_3^2} dr_3}_{\frac{\sqrt{\pi}}{4} \cdot \frac{1}{(\frac{3}{2} v_A)^{3/2}}}$$

$$= \frac{\cancel{4^3} \cdot \pi^{9/2}}{\cancel{4^3} \cdot v_A^{9/2} \cdot \left(1 \cdot \frac{4}{\cancel{3}}^2 \cdot \frac{\cancel{3}}{2}\right)^{3/2}} = \left(\frac{\pi}{v_A}\right)^{9/2} \cdot \frac{1}{2^{3/2}}$$

← consistent mit Mrowczynski for $\alpha = \frac{v_A}{2}$

For the RMS the calculation is slightly more complicated:



$$\cancel{r_{rms}^2 = \int \sum_{i=1}^{4} (\vec{x}_i - \vec{R})}$$

$$\cancel{r_{rms}^2 = \int \sum_{i=0}^{4} \sum_{j=i+1}^{4} \vec{x}_{ij}^2 \cdot |\phi_A|^2 \, d\vec{x}_1 \dots d\vec{x}_4} \qquad r_{rms}^2 = \int \sum_{i=0}^{4} \sum_{j=i+1}^{4} \left(\frac{\vec{x}_i - \vec{x}_j}{2}\right)^2 \cdot |\phi_A|^2 \cdot d\vec{x}_1 \dots d\vec{x}_4$$

$$= C^2 \cdot \frac{1}{4} \int \left(2r_1^2 + \frac{8}{3} r_2^2 + 3 r_3^2\right) \cdot \exp\left(-\frac{v_A}{2}\left(2r_1^2 + \frac{8}{3}r_2^2 + 3r_3^2\right)\right) d\vec{r}_1 \, d\vec{r}_2 \, d\vec{r}_3$$

$$= C^2 \frac{1}{4} \Bigg(\underbrace{\int 2r_1^2 \cdot \exp\left(-\frac{v_A}{2}\left(2r_1^2 + \frac{8}{3}r_2^2 + 3r_3^2\right)\right) \cdot (4\pi)^3 \cdot r_1^2 \cdot r_2^2 \cdot r_3^2 \, dr_1 \, dr_2 \, dr_3}_{1}$$

$$+ \int \frac{8}{3} r_2^2 \cdot \exp(\dots) \cdot (4\pi)^3 \cdot r_1^2 \cdot r_2^2 \cdot r_3^2 \, dr_1 \, dr_2 \, dr_3$$

$$+ \int 3 r_3^2 \cdot \exp(\dots) \cdot (4\pi)^3 \cdot r_1^2 \cdot r_2^2 \cdot r_3^2 \, dr_1 \, dr_2 \, dr_3 \Bigg)$$

Evaluation of 1

$$\int 2r_1^2 \cdot \exp\left(-\frac{v_A}{2} \cdot 2r_1^2 \dots\right) \cdot r_1^2 \cdot r_2^2 \cdot r_3^2 \, dr_1 \, dr_2 \, dr_3 \cdot (4\pi)^3$$

$$= \underbrace{\int 2r_1^4 \exp\left(-\frac{v_A}{2} \cdot 2r_1^2\right) dr_1 \cdot (4\pi)^3}_{2 \cdot \frac{3\sqrt{\pi}}{8} \cdot \frac{1}{v_A^{5/2}}} \cdot \underbrace{\int r_2^2 \cdot \exp\left(-v_A \cdot \frac{4}{3} r_2^2\right) dr_2}_{\frac{\sqrt{\pi}}{4} \cdot \frac{1}{\left(\frac{4}{3} v_A\right)^{3/2}}} \cdot \underbrace{\int r_3^3 \cdot \exp\left(-\frac{3}{2} v_A \cdot r_3^2\right) dr_3}_{\frac{\sqrt{\pi}}{4} \cdot \frac{1}{\left(\frac{3}{2} v_A\right)^{3/2}}}$$

$$\Rightarrow r_{rms}^2 = (4\pi)^3 \cdot C^2 \cdot \frac{1}{4} \left(\frac{2 \cdot 3 \, \pi^{3/2}}{8 \cdot 4^2 \cdot v_A^{11/2} \cdot \left(\frac{4}{3} \cdot \frac{3}{2}\right)^{3/2}} + \frac{\frac{8}{3} \cdot 3 \cdot \pi^{3/2}}{8 \cdot 4^2 \cdot v_A^{11/2} \cdot \left(\frac{4}{3}\right)^{5/2} \cdot \left(1 \cdot \frac{3}{2}\right)^{3/2}} \right.$$

$$\left. + \frac{3 \cdot 3 \cdot \pi^{3/2}}{8 \cdot 4^2 \cdot v_A^{11/2} \left(\frac{3}{2}\right)^{5/2} \cdot \left(1 \cdot \frac{4}{3}\right)^{3/2}} \right)$$

$$= \frac{4^{\cancel{3}} \cdot \pi^3 \cdot C^2 \, 3 \cdot \pi^{3/2}}{8 \cdot 4^{\cancel{2}} \cdot v_A^{11/2}} \cdot \frac{1}{4} \left(\frac{2}{\left(\frac{4}{\cancel{3}} \cdot \frac{\cancel{3}}{2}\right)^{3/2}} + \frac{8/3}{\left(\frac{4}{3}\right)^{5/2} \cdot \left(1 \cdot \frac{3}{2}\right)^{3/2}} + \frac{3}{\left(\frac{3}{2}\right)^{5/2} \cdot \left(1 \cdot \frac{4}{3}\right)^{3/2}} \right)$$

which simplifies to:

$$r_{rms}^2 = \frac{2^{3/2} \cdot \cancel{v_A^{9/2}}}{\cancel{\pi^{9/2}}} \cdot \frac{1}{2} \cdot \frac{\cancel{\pi^{9/2}} \cdot 3}{v_A^{\cancel{11/2}}} \cdot \frac{1}{4} \underbrace{\left(\frac{2}{2^{3/2}} + \frac{8/3}{\left(\frac{4}{3}\right)^{5/2} \cdot \left(\frac{3}{2}\right)^{3/2}} + \frac{3}{\left(\frac{3}{2}\right)^{5/2} \cdot \left(\frac{4}{3}\right)^{3/2}} \right)}_{= \frac{3}{\sqrt{2}}}$$

$$= \frac{1 \cdot 3}{\sqrt{2}\, v_A} \cdot \frac{1}{4} \cdot \frac{3}{\sqrt{2}} \cancel{= \frac{9}{4 v_A}}$$

$$\cancel{= \frac{9}{2 v_A}}$$

$$\cancel{= \frac{9}{8 v_A}}$$

$$\Rightarrow \quad r_{rms}^2 = \frac{9}{8 v_A}.$$