

Show that

$$\int \frac{\psi_1^2 \psi_2^2}{r_{12}} dV_1 dV_2 = \frac{5}{8} \alpha$$

where

$$\psi_j = \sqrt{\frac{\alpha^3}{\pi}} \exp(-\alpha r_j)$$

and

$$r_{12} = \sqrt{r_1^2 + r_2^2 - r_1 r_2 \cos \theta_{12}}$$

Symbol θ_{12} is angular separation.

Let $I(r_1)$ be the following integral over V_2 .

$$I(r_1) = \int \frac{\psi_2^2}{r_{12}} dV_2$$

The measure dV_2 is a volume element in spherical coordinates.

$$dV_2 = r_2^2 \sin \theta_2 dr_2 d\theta_2 d\phi_2$$

Write out the full integral and make $\theta_2 = \theta_{12}$ by independence of the coordinate system.

$$I(r_1) = \frac{\alpha^3}{\pi} \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{\exp(-2\alpha r_2)}{\sqrt{r_1^2 + r_2^2 - r_1 r_2 \cos \theta_2}} r_2^2 \sin \theta_2 dr_2 d\theta_2 d\phi_2$$

Integrate over ϕ_2 .

$$I(r_1) = 2\alpha^3 \int_0^\pi \int_0^\infty \frac{\exp(-2\alpha r_2)}{\sqrt{r_1^2 + r_2^2 - r_1 r_2 \cos \theta_2}} r_2^2 \sin \theta_2 dr_2 d\theta_2$$

Expand $1/r_{12}$ in Legendre polynomials. The first integral is over $r_2 < r_1$ and the second is over $r_2 > r_1$.

$$\begin{aligned} I(r_1) = 2\alpha^3 \int_0^\pi \int_0^{r_1} \exp(-2\alpha r_2) \left(\sum_{k=0}^\infty \frac{r_2^k}{r_1^{k+1}} P_k(\cos \theta_2) \right) r_2^2 \sin \theta_2 dr_2 d\theta_2 \\ + 2\alpha^3 \int_0^\pi \int_{r_1}^\infty \exp(-2\alpha r_2) \left(\sum_{k=0}^\infty \frac{r_1^k}{r_2^{k+1}} P_k(\cos \theta_2) \right) r_2^2 \sin \theta_2 dr_2 d\theta_2 \end{aligned}$$

It turns out that

$$\int_0^\pi P_k(\cos \theta_2) \sin \theta_2 d\theta_2 = \begin{cases} 2, & k = 0 \\ 0, & k > 0 \end{cases}$$

Hence

$$I(r_1) = \frac{4\alpha^3}{r_1} \int_0^{r_1} \exp(-2\alpha r_2) r_2^2 dr_2 + 4\alpha^3 \int_{r_1}^\infty \exp(-2\alpha r_2) r_2 dr_2$$

Solve the integrals.

$$I(r_1) = \frac{4\alpha^3}{r_1} \exp(-2\alpha r_2) \left(-\frac{r_2^2}{2\alpha} - \frac{r_2}{2\alpha^2} - \frac{1}{4\alpha^3} \right) \Big|_0^{r_1} + 4\alpha^3 \exp(-2\alpha r_2) \left(-\frac{r_2}{2\alpha} - \frac{1}{4\alpha^2} \right) \Big|_{r_1}^{\infty}$$

Evaluate per limits.

$$I(r_1) = \frac{1}{r_1} - \frac{1}{r_1} \exp(-2\alpha r_1) - \alpha \exp(-2\alpha r_1)$$

Having obtained $I(r_1)$ we can now evaluate the integral over V_1 .

$$I = \frac{\alpha^3}{\pi} \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \exp(-2\alpha r_1) I(r_1) r_1^2 \sin \theta_1 dr_1 d\theta_1 d\phi_1$$

Integrate over θ_1 and ϕ_1 .

$$I = 4\alpha^3 \int_0^{\infty} \exp(-2\alpha r_1) I(r_1) r_1^2 dr_1$$

Expand the integrand.

$$I = 4\alpha^3 \int_0^{\infty} \exp(-2\alpha r_1) r_1 dr_1 - 4\alpha^3 \int_0^{\infty} \exp(-4\alpha r_1) r_1 dr_1 - 4\alpha^4 \int_0^{\infty} \exp(-4\alpha r_1) r_1^2 dr_1$$

Solve the integrals.

$$I = \exp(-2\alpha r_1) \left(-2\alpha^2 r_1 - \alpha \right) \Big|_0^{\infty} - \exp(-4\alpha r_1) \left(-\alpha^2 r_1 - \frac{1}{4}\alpha \right) \Big|_0^{\infty} - \exp(-4\alpha r_1) \left(-\alpha^3 r_1^2 - \frac{1}{2}\alpha^2 r_1 - \frac{1}{8}\alpha \right) \Big|_0^{\infty}$$

The result vanishes for $r_1 = \infty$ hence

$$I = 0 - \left(-\alpha + \frac{1}{4}\alpha + \frac{1}{8}\alpha \right) = \frac{5}{8}\alpha$$