86(12): Direct Analytical Solution of the Schrödinger Equation of Helium.

In general:
$$H\psi = E\psi \qquad -(1)$$
where
$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{2e^2}{4\pi\epsilon_0 r_1} - \frac{2e^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0 r_{12}}$$
$$-(2)$$

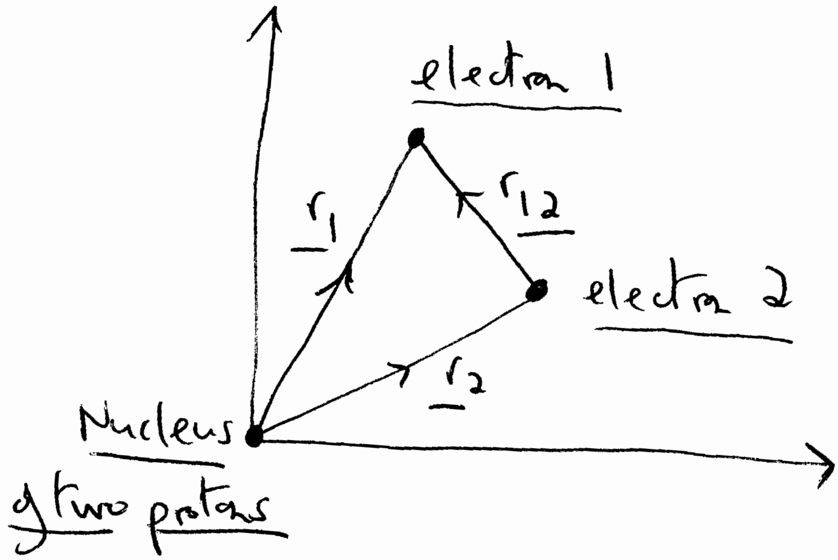
where:
$$\frac{1}{r_{12}} = \frac{1}{r_1}\sum_{l=0}^{\infty}\sum_{m_l=1}^{l}\left(\frac{4\pi}{2l+1}\right)\left(\frac{r_2}{r_1}\right)^l Y_{lm_l}(\theta_1,\phi_1)\,Y_{lm_l}(\theta_2,\phi_2) \qquad -(3)$$

if $r_1 > r_2$, and interchange r_1 and r_2 when $r_2 > r_1$. Eq (3) is an expansion in terms of spherical harmonics.

The mathematical problem is to solve a second order differential equation for two variables:
$$\underline{r_1} = \underline{r}_1(r_1, \theta_1, \phi_1) \qquad -(4)$$
$$\underline{r_2} = \underline{r}_2(r_2, \theta_2, \phi_2). \qquad -(5)$$

because $\underline{r_{12}}$ is expressed as a function of $\underline{r_1}$ and $\underline{r_2}$ in eq. (3). The vectors are related as in the following diagram.

2)



So:
$$\underline{r}_1 = \underline{r}_2 + \underline{r}_{12} \quad - (6)$$

i.e.
$$\underline{r}_{12} = \underline{r}_1 - \underline{r}_2 . \quad - (7)$$

and
$$r_{12} = |\underline{r}_{12}| = |\underline{r}_1 - \underline{r}_2| . \quad - (8)$$
$$= \left(r_{12x}^2 + r_{12y}^2 + r_{12z}^2\right)^{1/2}$$

in Cartesian coordinates. Thus:
$$r_{12} = \left((r_{1x} - r_{2x})^2 + (r_{1y} - r_{2y})^2 + (r_{1z} - r_{2z})^2\right)^{1/2}$$

and
$$\boxed{\frac{1}{r_{12}} = \left((r_{1x} - r_{2x})^2 + (r_{1y} - r_{2y})^2 + (r_{1z} - r_{2z})^2\right)^{-1/2}} \quad - (9)$$

Next consider:
$$\boxed{\frac{1}{r_1} = \left(r_{1x}^2 + r_{1y}^2 + r_{1z}^2\right)^{-1/2}} \quad - (10)$$

3)

$$\boxed{\frac{1}{r_2} = \left(r_{2x}^2 + r_{2y}^2 + r_{2z}^2\right)^{-1/2}} \quad -(11)$$

$$\boxed{\nabla_1^2 + \nabla_2^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2}} \quad -(12)$$

These equations are rewritten as:

$$\frac{1}{r_{12}} = \left((x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2\right)^{-1/2} \quad -(13)$$

$$\frac{1}{r_1} = \left(x_1^2 + y_1^2 + z_1^2\right)^{-1/2} \quad -(14)$$

$$\frac{1}{r_2} = \left(x_2^2 + y_2^2 + z_2^2\right)^{-1/2} \quad -(15)$$

Computer Algebra Task

This is to solve equation (1) using eqs. (13) to (15), using eq. (8).

Radiative Correction

Eq. (1) becomes defined by:

$$\boxed{\nabla_1^2 + \nabla_2^2 \to \left(1 + \frac{\alpha}{4\pi}\right)^2 \left(\nabla_1^2 + \nabla_2^2\right)} \quad -(16)$$

and proceed as per previous notes