

## Sketch of Paper 86

In note 86(b) it was shown that the basic equation is:

$$-\frac{\hbar^2}{2m} \left(1 + \frac{d}{4\pi}\right)^2 \frac{d^2 P}{dr^2} - V_{\text{eff}}^{(0)} P = EP \quad (1)$$

and this is equivalent by hypothesis to:

$$-\frac{\hbar^2}{2m} \frac{d^2 P}{dr^2} - V_{\text{eff}} P = EP \quad (2)$$

where:

$$V_{\text{eff}} = \frac{e^2}{4\pi\epsilon_0(r+r_{\text{vac}})} - \frac{l(l+1)\hbar^2}{2m(r+r_{\text{vac}})^2} \quad (3)$$

Therefore to first order in  $d$ :

$$\boxed{-\frac{\hbar^2 d}{4\pi m} \frac{d^2 P_0}{dr^2} = \left(V_{\text{eff}}^{(0)} - V_{\text{eff}}\right) P_0} \quad (4)$$

where we have assumed:

$$P = P_0 \quad (5)$$

Here:

$$P_0 = rR(r) \quad (6)$$

where  $R(r)$  is the H atom radial wavefunction.

Here also:

$$V_{\text{eff}}^{(0)} = \frac{e^2}{4\pi\epsilon_0 r} - \frac{l(l+1)\hbar^2}{2m r^2}, \quad - (7)$$

So:

$$V_{\text{eff}}^{(0)} - \bar{V}_{\text{eff}} = \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{r} - \frac{1}{r + r_{\text{vac}}} \right) - \frac{l(l+1)\hbar^2}{2m} \left( \frac{1}{r^2} - \frac{1}{(r + r_{\text{vac}})^2} \right) \quad - (8)$$

## Computer Algebra

This should be used to solve eq. (4) for  $l$  Land shift using eq. (8). This method introduces the centrifugal repulsion, giving a Lennard-Jones type potential.

- 1) Land shift for  $2s$  and  $\langle 2p \rangle$ .
- 2) Perhaps higher orbital Land shifts.

IN THIS METHOD THE ANGULAR DEPENDENCE IS INCORPORATED IN THE CENTRIFUGAL TERM, SO WE ONLY HAVE TO USE  $l(l+1)$ .