



$$\left\{ \sum \Delta_i + \frac{8\pi^2 m}{h^2} \left[E - e^2 \left(\frac{Z_a Z_b}{R} - \sum_{i=1}^{Z_a} \frac{Z_a}{y_{ai}} - \sum_{k=1}^{Z_b} \frac{Z_b}{y_{bk}} + \sum_{i,k} \frac{1}{y_{ik}} \right) \right] \right\}$$

$$x \Psi = 0$$

$$\begin{cases} \alpha \Psi_{\ell'}(1, 2, \dots, Z_a) \\ \beta \varphi_{\ell''}(Z_a+1, \dots, Z_a+Z_b) \end{cases}$$

$$\alpha \Psi_{\ell'} \cdot \beta \varphi_{\ell''} = u_{\ell}(I)$$

$$\Psi = \sum_R^{(nm)!} C_R u_{R\ell}(R)$$

$$\Psi = \Psi_0 + \Psi_1 + \dots$$

$$H_0 \Psi_0 = \left[\sum \Delta_i + \frac{8\pi^2 m}{h^2} \left\{ E_0 + e^2 \left(\frac{Z_a}{y_{ai}} + \sum_{k=Z_a+1}^{Z_a+Z_b} \frac{Z_b}{y_{bk}} \right) \right\} \right] \Psi_0 = 0$$

$$H_1 \Psi_1 = \left[\sum \Delta_i + \frac{8\pi^2 m}{h^2} \left\{ E_1 + e^2 \left(\sum_{k=Z_a+1}^{Z_a+Z_b} \frac{Z_a}{y_{ak}} + \sum_{i=1}^{Z_a} \frac{Z_b}{y_{bi}} - \frac{Z_a Z_b}{R} + \sum_{i,k} \frac{1}{y_{ik}} \right) \right\} \right] \Psi_1 + \dots \Psi_0 = 0$$

$$\Psi_0^r = \sum_{s=1}^{\infty} a_s \Psi_0^s$$

$$\frac{8\pi^2 m}{h^2} (E_{0s} - E_{0r}) a_s + \frac{8\pi^2 m}{h^2} (E_{1r} + V_1^{rs}) a_s = 0$$

$$a_r = 0, \quad V_1 \Psi_0^r = V_1^{rs} \Psi_0^s$$

$$a_s = \frac{V_1^{rs}}{E_{0r} - E_{0s}}$$

$$E_{1r} = V_1^{rr} = e^2 \left(\Psi_0^r \left(\sum \frac{Z_a}{y_{ak}} + \sum \frac{Z_b}{y_{bi}} - \frac{Z_a Z_b}{R} + \sum \frac{1}{y_{ik}} \right) \Psi_0^r \right)$$

$$n = \frac{n(n-1)}{2} = \frac{1}{2} n^2 - \frac{1}{2} n$$

$$\frac{1}{y_{ak}} = \frac{1}{\left(R^2 + y_{bk}^2 + 2Ry_{bk} \cos \theta_{bk} \right)^{-\frac{1}{2}}} = \frac{1}{R} \left(1 + \frac{y_{bk} \cos \theta_{bk}}{R} + \frac{y_{bk}^2 - 3y_{bk}^2 \cos^2 \theta_{bk}}{2R^2} + \dots \right)$$

$$\frac{1}{y_{bi}} = \frac{1}{\left(R^2 + y_{ai}^2 - 2Ry_{ai} \cos \theta_{ai} \right)^{-\frac{1}{2}}} = \frac{1}{R} \left(1 + \frac{y_{ai} \cos \theta_{ai}}{R} + \frac{y_{ai}^2 (2 - 3 \cos^2 \theta_{ai})}{2R^2} + \dots \right)$$

$$\frac{1}{y_{ik}} = \frac{1}{\left(y_{bk}^2 + y_{bi}^2 - 2y_{bk}y_{bi} \cos \theta_{bik} \right)^{-\frac{1}{2}}} = \frac{1}{\left(y_{bk}^2 + y_{bi}^2 R^2 + y_{ai}^2 - 2Ry_{ai} \cos \theta_{ai} - 2y_{bk}R \left(1 + \frac{y_{ai} \cos \theta_{ai}}{R} \right) \right)^{-\frac{1}{2}}}$$

$$= \frac{1}{R} \left\{ 1 + \frac{r_{ai} \cos \theta_{ai}}{R} - \frac{r_{bk} \cos \theta_{bk}}{R} - \frac{1}{2} \frac{r_{ai}^2 + r_{bk}^2}{R^2} \right.$$

$$\begin{aligned} \cos \theta_{bik} &= \cos \theta_{bk} \cos \theta_{bi} + \sin \theta_{bk} \sin \theta_{bi} \cos(\varphi_{bk} - \varphi_{bi}) \\ &= \cos \theta_{bk} - 1 + \sin \theta_{bk} \sin \theta_{bi} \frac{r_{ai}}{R} \cos(\varphi_{bk} - \varphi_{bi}) \end{aligned}$$

$$- 2 r_{bk} R + 2 r_{bk} r_{ai} (\cos \theta_{ai} -$$

$$\begin{aligned} r_{bi} \cos \theta_{bik} &= r_{bi} \cos \theta_{bk} + r_{bi} \sin \theta_{bk} \sin \theta_{bi} \cos(\varphi_{bk} - \varphi_{bi}) \\ &= (-R + \frac{r_{ai} \cos \theta_{ai}}{R}) \cos \theta_{bk} + r_{ai} \sin \theta_{ai} \sin \theta_{bk} \cos(\varphi_{bk} - \varphi_{ai}) \\ &= -R \cos \theta_{bk} + \frac{r_{ai}}{R} (\cos \theta_{ai} \cos \theta_{bk} + \sin \theta_{ai} \sin \theta_{bk} \cos(\varphi_{bk} - \varphi_{ai})) \end{aligned}$$

$$\begin{aligned} \frac{1}{r_{ik}} &= \left(R^2 - 2R (r_{ai} \cos \theta_{ai} - r_{bk} \cos \theta_{bk}) \right. \\ &\quad \left. + r_{ai}^2 + r_{bk}^2 - 2 r_{ai} r_{bk} (\cos \theta_{ai} \cos \theta_{bk} + \sin \theta_{ai} \sin \theta_{bk} \cos(\varphi_{bk} - \varphi_{ai})) \right)^{-1/2} \end{aligned}$$

$$= \frac{1}{R} \left\{ 1 + \frac{r_{ai} \cos \theta_{ai} - r_{bk} \cos \theta_{bk}}{R} - \frac{1}{2R^2} (r_{ai}^2 + r_{bk}^2) \right.$$

$$\left. - 2 r_{ai} r_{bk} (\cos \theta_{ai} \cos \theta_{bk} + \sin \theta_{ai} \sin \theta_{bk} \cos(\varphi_{bk} - \varphi_{ai})) \right\}$$

$$- 4 \cdot \frac{3}{8} (2 r_{ai} \cos \theta_{ai} r_{bk} \cos \theta_{bk})$$

$$\sum \frac{r_{ai}}{r_{ak}} + \sum \frac{r_{bk}}{r_{bi}} - \sum \frac{1}{r_{ik}} - \frac{r_{ai} r_{bk}}{R} = \frac{1}{R^3} \sum_{ik} r_{ai} r_{bk} \{ 2 \cos \theta_{ai} \cos \theta_{bk} - \sin \theta_{bk} \sin \theta_{ai} \cos(\varphi_{bk} - \varphi_{ai}) \}$$