Let us show rigorously that there is no net overlap between the H 1s and the F $2p_x$ orbitals.

i.e. prove that $\int \psi^*_{1s,H} \psi_{2p_x,F}\, d\tau = 0$

Earlier in the semester, we proved that

$$\psi_{2p_x} = +\frac{1}{\sqrt{2}}\psi_{21+1} - \frac{1}{\sqrt{2}}\psi_{21-1}$$

Thus, we need to show that

$$+\frac{1}{\sqrt{2}}\int \psi^*_{1s,H}\psi_{21+1,F}\, d\tau - \frac{1}{\sqrt{2}}\int \psi^*_{1s,H}\psi_{21-1,F} = 0$$

$$\psi^*_{1s,H} = \psi_{1s,H} = R_{10}Y_{00} = \left[2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}\right]\left[\frac{1}{\sqrt{4\pi}}\right]$$

$$\left(\text{since } \rho = \frac{2Z}{na_0}r = \frac{2(1)}{(1)\,a_0}r = \frac{2}{a_0}r\right)$$

$$\psi_{21+1,F} = R_{21,F}Y_{1+1} = \left[\frac{1}{\sqrt{24}}\left(\frac{9}{a_0}\right)^{3/2}\left(\frac{9}{a_0}\right) r\, e^{-9r/2a_0}\right]\left[-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}\right]$$

$$\left(\text{since } \rho = \frac{2Z}{na_0}r = \frac{2(9)}{2a_0}r = \frac{9}{a_0}r\right)$$

$$\text{so} \int \psi^*_{1s,H}\psi_{21+1,F}\, d\tau = 2\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{1}{\sqrt{4\pi}}\right)\left(\frac{1}{\sqrt{24}}\right)\left(\frac{9}{a_0}\right)^{5/2}\left(-\sqrt{\frac{3}{8\pi}}\right)$$

$$\int_0^\infty r^3 e^{-11r/2a_0}\, dr \int_0^\pi \sin^2\theta\, d\theta$$

$$\int_0^{2\pi} e^{i\phi}\, d\phi$$

but $\int_0^{2\pi} e^{i\phi} d\phi = \frac{1}{i} e^{i\phi} \Big]_0^{2\pi} = \frac{1}{i}\left[e^{i2\pi} - e^{0}\right]$

and $e^0 = 1$ and $e^{i2\pi} = \cos 2\pi + i \sin 2\pi = 1$

so $\int_0^{2\pi} e^{i\phi} d\phi = 0 \Rightarrow \int \psi^*_{1s,H} \psi_{21+1,F}\, d\tau = 0$

Likewise, $\int \psi^*_{1s,H} \psi_{21-1,F}\, d\tau$ depends on the integral $\int_0^{2\pi} e^{-i\phi} d\phi$, which also equals zero.

Thus, $\int \psi^*_{1s,H} \psi_{2p_x,F}\, d\tau$

$$= +\frac{1}{\sqrt{2}} \int \psi^*_{1s,H} \psi_{21+1,F}\, d\tau - \frac{1}{\sqrt{2}} \int \psi^*_{1s,H} \psi_{21-1,F}\, d\tau$$

$$= +\frac{1}{\sqrt{2}}(0) - \frac{1}{\sqrt{2}}(0)$$

$$= 0$$

$\therefore$ $\psi_{1s,H}$ and $\psi_{2p_x,F}$ are <u>orthogonal</u> (no net overlap).

- One can show the same for $\psi_{1s,H}$ and $\psi_{2p_y,F}$
- Seniors know how to prove these results simply and elegantly using <u>group theory</u>