1) a) $f(1)\, g(2)\, \alpha(1)\alpha(2) \equiv \Psi$

$\downarrow$

$f(2)\, g(1)\, \alpha(2)\alpha(1)$ this is neither Ψ or $-\Psi$

b) $f(1)\, f(2)\, [\alpha(1)\, \beta(2) - \beta(1)\,\alpha(2)] \equiv \Psi$

$\downarrow$

$f(2)\, f(1)[\alpha(2)\, \beta(1) - \beta(2)\,\alpha(1)] = f(1)f(2)[-(\beta(2)\alpha(1) - \alpha(2)\beta(1))] = -\Psi$

antisymmetric

c) $f(1)\, f(2)\, f(3)\; \beta(1)\,\beta(2)\,\beta(3) \equiv \Psi$

$\downarrow$

$f(2)\, f(1)\, f(3)\; \beta(2)\,\beta(1)\,\beta(3) = \Psi$

any switch will return Ψ, symmetric

d) $[f(1)g(2) - g(1)f(2)][\alpha(1)\,\beta(2) - \alpha(2)\,\beta(1)] \equiv \Psi$

$\downarrow$

$[f(2)\,g(1) - g(2)\,f(1)]\,[\alpha(2)\,\beta(1) - \alpha(1)\,\beta(2)] = [-(g(2)\,f(1) - f(2)g(1))][-(\alpha(1)\,\beta(2) - \alpha(2)\,\beta(1))]$

$= +[f(1)g(2) - g(1)\,f(2)][\alpha(1)\beta(2) - \alpha(2)\,\beta(1)] = \Psi$, symmetric

2) a) $P_{1,0}(r) = R_{10}^2(r) \cdot r^2$ find $\left.\frac{dP(r)}{dr}\right|_{r=r_0} = 0$

$$R_{10} = 2\left(\frac{z}{a_0^3}\right)^{1/2} e^{-zr/a_0}$$

$$\frac{dP_{10}(r)}{dr} = \frac{4z}{a_0^3}\frac{d}{dr}\left(e^{-2zr/a_0} \cdot r^2\right) = \frac{4z}{a_0^3}\left(r^2\left(\frac{-2z}{a_0}\right)e^{-2zr/a_0} + 2re^{-2zr/a_0}\right) = 0$$

$$\cancel{2}r\cancel{e^{-2zr/a_0}} = \frac{\cancel{2}zr^2}{a_0}\cancel{e^{-2zr/a_0}}$$

$$r = \frac{zr^2}{a_0} \quad ; z=1 \text{ for H} \qquad r = a_0$$

we should prove that $\left.\frac{d^2P}{dr^2}\right|_{r=a_0}$ is <0 for maximum, but we know what this function looks like, and that it has only one extremum

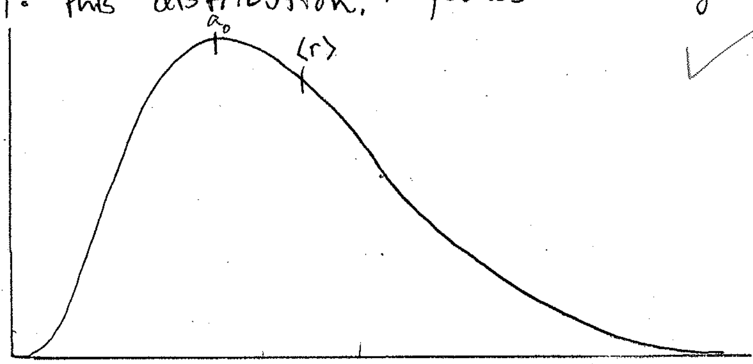
b) See example 3.2 in text

$$\langle r\rangle = \int \psi_{1s}^* r \psi_{1s}\, d\tau \quad \text{, by definition}$$

$$\langle r\rangle = \frac{4}{a_0^3}\int_{r=0}^{\infty} e^{-r/a_0}\, r\, e^{-r/a_0}\, r^2 dr = \frac{4}{a_0^3}\int_0^{\infty} r^3 e^{-2r/a_0} dr \quad \text{(using integral table)}$$

$$= \frac{4}{a_0^3}\frac{3!}{(2/a_0)^4} = \frac{24}{a_0^3}\frac{a_0^4}{16} = \frac{3a_0}{2}$$

The average is greater than the most probable because of the tail to this distribution. It pushes the average to higher values.



3) a) $\hat{H} = \hat{E}_k + \hat{V}$

$$= \frac{-\hbar^2}{2m_H}\left(\nabla_A^2 + \nabla_B^2\right) + \frac{-\hbar^2}{2m_e}\nabla_1^2 + \frac{-e^2}{4\pi\varepsilon_0 r_{1A}} + \frac{-e^2}{4\pi\varepsilon_0 r_{1B}} + \frac{e^2}{4\pi\varepsilon_0 R}$$

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b) $$\hat{H}_{el} = \frac{-\hbar^2}{2m_e}\nabla_1^2 + \frac{e^2}{4\pi\varepsilon_0}\left(\frac{-1}{r_{1A}} + \frac{-1}{r_{1B}} + \frac{1}{R}\right) \equiv \hat{H}_{tot} - \hat{T}_{nuc}$$

c) $$\Psi(\vec{r}_1, \vec{R}_A, \vec{R}_B) = \psi_{el}(\vec{r}_1; R)\,\psi_{nuc}(\vec{R}_A, \vec{R}_B)$$

then

$$\hat{H}_{el}(\vec{r}_1; R)\,\psi_{el}(\vec{r}_1; R) = E_{el}(R)\,\psi_{el}(\vec{r}_1, R)$$

This is just like our normal SWE: $\hat{H}\psi = E\psi$, but we have parameterized the Hamiltonian, $\hat{H}_{el}$. That is, it is only valid for the particular value of R we have chosen, as it enters the functional form of $\hat{H}_{el}$ as a constant. Therefore the energies we get will be for a specific R, giving E_{el} as a function of R, i.e. $E = E(R)$.

d) The total $\hat{H}$ is

$$\hat{H}_{tot} = \hat{H}_{el} + \hat{T}_{nuc}$$

$$\underline{\underline{\hat{H}_{tot}\Psi_{tot} = E\,\Psi_{tot}}}$$

So sub. into SWE

) $\hat{H}_{tot}\Psi_{tot} = (\hat{H}_{el} + \hat{T}_{nuc})\Psi_{tot} = (\hat{H}_{el} + \hat{T}_{nuc})\psi_{el}\psi_{nuc}$

) $= \hat{H}_{el}\psi_{el}\psi_{nuc} + \hat{T}_{nuc}\psi_{el}\psi_{nuc}$ (expanding term)

) $= \psi_{nuc}\hat{H}_{el}\psi_{el} + \psi_{el}\hat{T}_{nuc}\psi_{nuc}$ (moving through operators, as we've built them to be independent)

) $= \psi_{nuc}E_{el}(R)\psi_{el} + \psi_{el}\hat{T}_{nuc}\psi_{nuc}$ $(\hat{H}_{el}\psi_{el} = E_{el}(R)\psi_{el})$

5) $= \underbrace{\psi_{el}(E_{el}(R) + \hat{T}_{nuc})\psi_{nuc}}$ $= \hat{H}_{tot}\Psi_{tot}$ (ψ_{el} can move to left, we are done operating on it. ψ_{nuc} cannot, we have not operated on it.)

) $\psi_{el}(\hat{T}_{nuc} + E_{el}(R))\psi_{nuc} = E\,\Psi_{tot}$ (using $H_t\psi_t = E\psi_t$ from top of page)

7) $\psi_{el}(\hat{T}_{nuc} + E_{el}(R))\psi_{nuc} = E\,\psi_{el}\psi_{nuc}$ (sub in for Ψ_{tot})

8) $(\hat{T}_{nuc} + E_{el}(R))\psi_{nuc} = E\,\psi_{nuc}$ (same logic as line 5)

9) $\left(\frac{-\hbar^2}{2m_H}(\nabla_A^2 + \nabla_B^2) + E_{el}(R)\right)\psi_{nuc} = E\,\psi_{nuc}$ (def for my operator $\hat{T}_{nuc}$)