(1) a Find the expectation value of total energy E for the ground state of hydrogen

$$\langle E \rangle = \frac{\int \Psi^* \hat{H} \Psi d\tau}{\int \Psi^* \Psi d\tau}$$

$$\int \Psi^* \hat{H} \Psi d\tau = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} e^{-\alpha r} \left[\frac{-1}{2} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{1}{r} \right] e^{-\alpha r} r^2 dr \sin\theta \, d\theta \, d\phi$$

$$= 4\pi \left(-\frac{1}{8\alpha} + \frac{1}{4\alpha} - \frac{1}{4\alpha^2} \right)$$

$$\int \Psi^* \Psi d\tau = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} e^{-\alpha r} e^{-\alpha r} r^2 dr \sin\theta \, d\theta \, d\phi$$

$$= 4\pi \left(\frac{1}{4\alpha^3} \right)$$

$$\therefore \langle E \rangle = \frac{\alpha^2}{2} - \alpha$$

b The condition for E to have its minimum value is:

$$\left. \frac{dE}{d\alpha} \right|_{\alpha = \alpha_{min}} = 0$$

$$\therefore \alpha_{min} - 1 = 0$$

$$\alpha_{min} = 1$$

$$E_{min} = -0.5 \; Hartree$$

(2)

$$\langle E \rangle = \frac{3}{2} \beta - 2\sqrt{\frac{2\beta}{\pi}}$$

$$\beta_{min} = \frac{8}{9\pi} \approx 0.28$$

$$E_{min} \approx -0.42 \; Hartree$$

The energy calculated using Gaussian function is higher than what I got using slater function (exact function), but slater function will bring integral difficulties to solve schrödinger equation. The linear combination of several number of Gaussians is instead of slaters to improve the accuracy.