Programme 4 (Python)

```
from math import exp
terms = 1000
beta = 1/100
S = 0.0
Z = 0.0
for n in range(terms):
    E = n + 0.5
    weight = exp(-beta*E)
    S += weight*E
    Z += weight
print(S/Z)
```

$$\langle r \rangle = \int_0^{+\infty}\int_0^{\pi}\int_0^{2\pi} \left(\frac{1}{\sqrt{\pi}}\right)\left(\frac{1}{a_0}\right)^{3/2} \cdot e^{-r/a_0} \cdot (r) \cdot \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \cdot e^{-r/a_0} \cdot r^2 \sin\theta \, dr\, d\theta\, d\varphi$$

$$= \frac{1}{\pi} \cdot \frac{1}{a_0^3} \int_0^{+\infty} r^3 e^{-2r/a_0} dr \int_0^{\pi} \sin\theta \, d\theta \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \underbrace{[\varphi]_0^{2\pi}}$$

$$= \frac{1}{\pi} \cdot \frac{1}{a_0^3} \cdot \left(\frac{a_0}{2}\right)^4 \cdot 3! \underbrace{[-\cos\theta]_0^{\pi}}_{2} \cdot 2\pi$$

$$= \frac{1}{\pi} \cdot \frac{1}{a_0^3} \cdot \frac{a_0^4}{4 \cdot 4_2} \cdot \frac{6}{3} \cdot 2 \cdot 2\pi$$

$$\langle r \rangle = \frac{3a_0}{2} \quad \checkmark \quad (02b)$$

$$\langle r^2 \rangle = \frac{1}{\pi} \cdot \frac{1}{a_0^3} \cdot \int_0^{+\infty} r^4 e^{-2r/a_0} dr \cdot 2 \cdot 2\pi$$

$$= \frac{1}{\pi} \cdot \frac{1}{a_0^3} \cdot \left(\frac{a_0}{2}\right)^5 \cdot 4! \cdot 2 \cdot 2\pi$$

$$= \frac{1}{\pi} \cdot \frac{1}{a_0^3} \cdot \frac{a_0^5}{2^5} \cdot 4 \cdot 3 \cdot 2 \cdot 2 \cdot 2\pi$$

$$= 3a_0^2 \quad (02b)$$