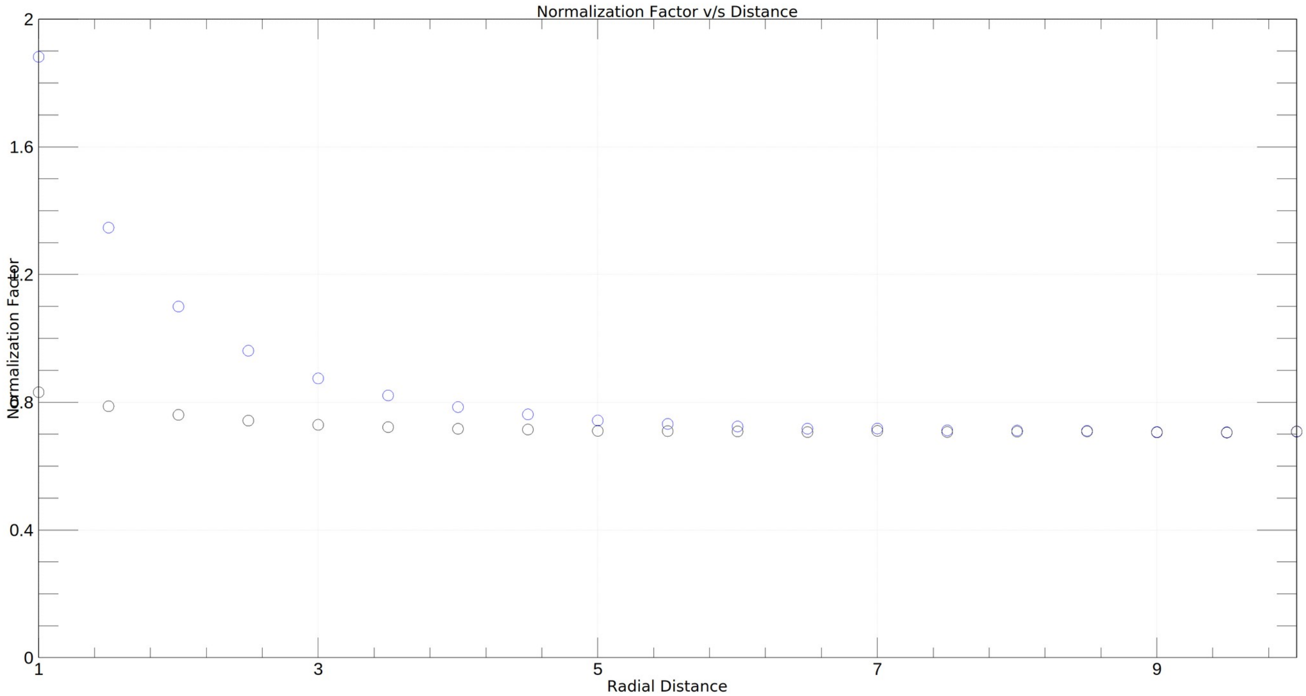
Assignment-8

8. (a) The analytical derivation can be found attached below.

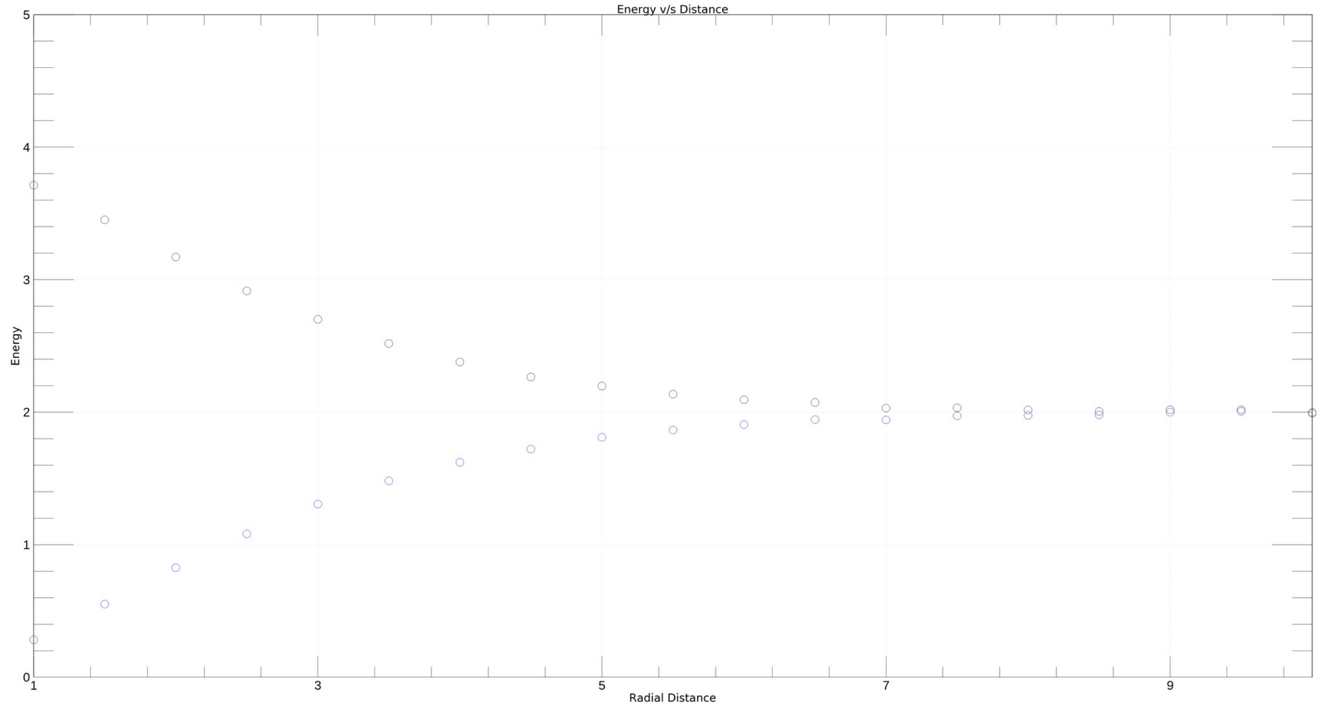
The normalization values versus distance over a range of 10 bohr radius units is shown below.



Blue circles indicate Na normalization factor and black circles indicate Ns normalization values.

(b)

The energy values versus radial distance is plotted below:



The black circles indicate energy of symmetric wave function (calculates from Na), the black circles indicate anti-symmetric wave function calculated from Ns.

15. (a) The integral is found to be 0.415825 with an error of 0.00286 for N=10000. This verifies the result.

The minimum number of points needed is 818 for 1% accuracy. The calculation is shown below.

(b) With the weight function x, the integral is found to be 0.497515 with an error of 0.00289 for N=10000, this does not verify the result.

The minimum number of points needed is 28 for 1% accuracy. The calculation is shown below.

(c) a=0.16, calculation is attached below.

Assignment - 8

8 (a) We have,

$$\Psi_{s,a}(\vec{r}) \equiv N_{s,a}(\phi_1(\vec{r}) \pm \phi_2(\vec{r}))$$

where $\phi_1 \equiv \frac{1}{\sqrt{\pi}} e^{-(|\vec{r} - \hat{z}\frac{d}{2})}$

$$\phi_2 \equiv \frac{1}{\sqrt{\pi}} e^{-(|\vec{r}+\hat{z}\frac{d}{2})}$$

$$\therefore \int_{-\infty}^{\infty} |\Psi(\vec{r})|^2 d^3r = \int_{-\infty}^{\infty} N_{s,a}^2 (\phi_1(\vec{r}) \pm \phi_2(\vec{r}))^2 d^3r$$

$$= \int_{-\infty}^{\infty} N_{s,a}^2 (\phi_1(\vec{r})^2 \pm 2\phi_1(\vec{r})\phi_2(\vec{r}) + \phi_2(\vec{r})^2) d^3r$$

$$= N_{s,a}^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y,z)\, e^{x+y+z}\, dx\,dy\,dz$$

$[f(x,y,z) = e^{x+y+z}(\phi_1(\vec{r})^2 \pm 2\phi_1(\vec{r})\phi_2(\vec{r}) + \phi_2(\vec{r})^2)]$

$$= 8N_{s,a}^2 \int_0^{\infty}\int_0^{\infty}\int_0^{\infty} f(x,y,z)\, e^{\cancel{x+y+z}}\, dx\,dy\,dz$$

[functions are even]

$$= 8 N_{s,a}^2 I_{s,a}$$

$\therefore$ Probability distribution chosen for ~~the~~ monte-carlo integration is $\rho = e^{-x-y-z}$

$$\therefore \; N_{s,\rho} = \sqrt{\frac{1}{8 I_{s,a}}}$$

ii) According to the Schroedinger equation,

$$H \Psi_{s,a} = E_{s,a} \Psi_{s,a}$$

$$= \left(-\frac{1}{2} \nabla^2 - \frac{1}{|\vec{r} + \hat{z}\frac{d}{2}|} - \frac{1}{|\vec{r} - \hat{z}\frac{d}{2}|} \right) \Psi_{s,a}$$

$$= N_{s,a}^2 \Psi_{s,a}$$

$$\therefore E_{s,a} = N_{s,a}^2$$

$\therefore$

18) a) Error (σ) $= \dfrac{0.286}{\sqrt{N}}$

for 1% accuracy,

$$\frac{0.286}{\sqrt{N}} \leq \frac{1}{100}$$

$$0.286 \times 100 \leq \sqrt{N}$$

$$\sqrt{N} \geq 28.6$$

$$N \geq 817.96$$

$\therefore$ N should be atleast 818 for 1% accuracy.

(b) $$\frac{0.0523}{\sqrt{N}} \leq \frac{1}{100}$$

$$\sqrt{N} \geq 0.0523 \times 100$$

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$$\sqrt{N} = 5.23$$

$$N = 27.36$$

Minimum 28 ~~values~~ points are needed for 1% accuracy

(c) The ratio of variances is given as:-

$$\frac{\sigma_1^2}{\sigma_2^2} = \frac{\bar{f_1}^2 - I^2}{f_2^2 - I^2} = \frac{\Pi \bar{f_1}^2(x_i) - \Pi I_i^2}{\Pi \bar{f_2}^2(x_i) - \Pi I_i^2}$$

If $D \to \infty$

$$\Pi_i = I_i^2 = 0$$

$$\therefore \frac{\sigma_1^2}{\sigma_2^2} = \frac{\Pi \bar{f_1}^2(x_i)}{f_2^2(x_i)} = \left(\frac{\bar{f_1}^2(x_i)}{\bar{f_2}^2(x_i)}\right)^D$$

$$= 1.4564^D$$

$$= 10^{0.161}$$

$$\therefore \boxed{a = 0.16}$$