

Assignment8

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October 2020

1 EX8

1.1 Normalization factor

We have

$$\begin{aligned} \int_{-\infty}^{\infty} |\psi(\vec{r})|^2 d^3r &= \int_{-\infty}^{\infty} N_{s,a}^2 (\phi_1(\vec{r}) \pm \phi_2(\vec{r}))^2 d^3r \\ &= \int_{-\infty}^{\infty} N_{s,a}^2 (\phi_1(\vec{r})^2 \pm 2\phi_1(\vec{r})\phi_2(\vec{r}) + \phi_2(\vec{r})^2) d^3r \\ &= N_{s,a}^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z) e^{x+y+z} dx dy dz \\ &= 8N_{s,a}^2 \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} f(x, y, z) e^{-x-y-z} dx dy dz \\ &= 8N_{s,a}^2 I_{s,a} \end{aligned}$$

where $f(x, y, z) = (\phi_1(\vec{r})^2 \pm 2\phi_1(\vec{r})\phi_2(\vec{r}) + \phi_2(\vec{r})^2)e^{x+y+z}$. So we can choose the probability distribution $\rho(x, y, z) = e^{-x-y-z}$, and then calculate the average value of $f(x, y, z)$. Therefore we can get the normalization factor $N_{s,a} = \sqrt{1/(8I_{s,a})}$. Then we can plot the normalization factors as the function of the distance d . The results are showed in follow:

When the distance to the infinity, the two atoms become independent, therefore, the normalization factor of symmetry and anti-symmetry wave functions approach to $1/\sqrt{2}$.

1.2 Energy

We have the Schrodinger equation:

$$\begin{aligned} H\psi_{s,a} &= E_{s,a}\psi_{s,a} \\ &= \left(-\frac{1}{2}\nabla^2 - \frac{1}{|\vec{r} + \hat{z}d/2|} - \frac{1}{|\vec{r} - \hat{z}d/2|}\right)\psi_{s,a} \\ &= N_{s,a}^2\psi_{s,a} \end{aligned}$$

Therefore we have $E_{s,a} = N_{s,a}^2$. And here the normalization factors can be obtained from previous subsection.

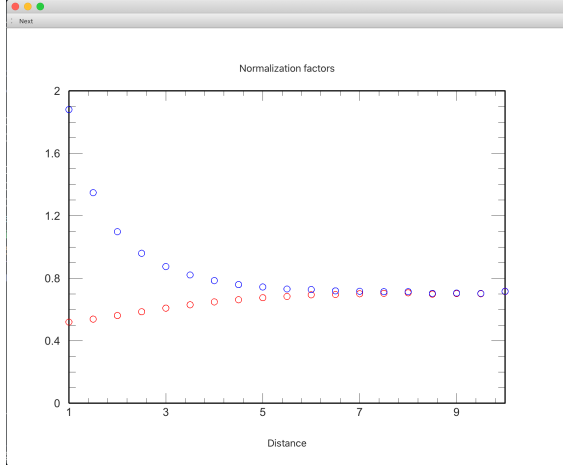


Figure 2: Normalization factors.

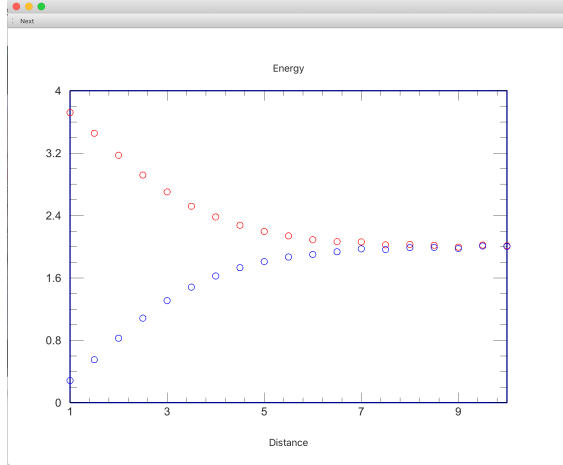


Figure 3: Energy of the system

The energy of symmetric wave function (red circle) decreases with the increase of distance d , while the energy of the anti-symmetric wave function (blue circle) increases with the increase of distance d . And as $d \rightarrow \infty$, the energy approach to 2, which is the energy for two isolated atom.

2 EX9

The probability of a gamma ray emitted from the depth z in a angle of θ to arrive the surface of the material is:

$$P = 1 - \int_0^z \frac{1}{\lambda} e^{-\frac{x}{\lambda}} = e^{-\frac{z}{\lambda}}$$

Since we can not simulate the infinity uniform distribution, we can start from the uniform distribution in the interval $[0, X]$. By letting $X \rightarrow \infty$, we can have the asymptotic result of P .

In my algorithm, I first generate three uniformly distributed random numbers $x \in [0, X]$, $th \in [0, \pi]$ and $a \in [0, 1]$. If $e^{-x/(\lambda \cos(th))} > a$, the photon from depth x in an angle th can reach the surface of granite. I repeated this process for 1000000 times for different X and the result are showed in follow:

As we can see from the diagram, the probability approach to $1/2$ as $X \rightarrow \infty$. And only the gamma ray travel upward can reach the surface, therefore the total probability is $1/4$, which consist with the result in EX5.12.

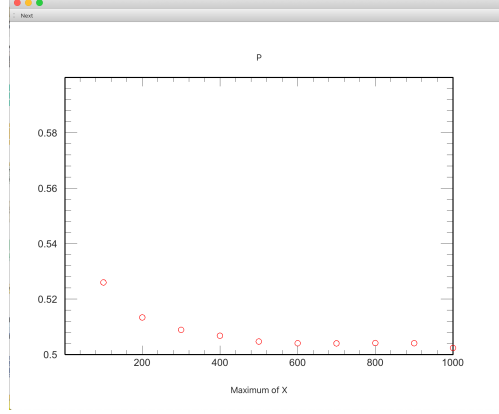


Figure 3: Probability for a photon to reach the surface

3 EX15

3.1

We have:

$$\begin{aligned}\sigma_1 &= \sqrt{\frac{\bar{f}^2 - \bar{f}^2}{N}} = \sqrt{\frac{\int_0^1 (e^x - 1)^2 / (e - 1)^2 dx - I^2}{N}} \\ &= \left(\sqrt{\frac{e^2 - 4e + 5}{2(e - 1)^2}} - I^2 \right) / \sqrt{N} = \frac{0.286}{\sqrt{N}}\end{aligned}$$

If we want to achieve 1% accuracy, we have $0.286/\sqrt{N} < 0.01 \Rightarrow N > 817$.

3.2

We can choose $\rho(x) = 2x$, then we have:

$$\bar{f}^2 = \int_0^1 \left(\frac{(e^x - 1)}{2x(e - 1)} \right)^2 2x dx = 0.1775$$

Therefore we have $\sigma_2 = \sqrt{0.177489 - 0.17474}/\sqrt{N} = 0.0524/\sqrt{N}$. If we want to achieve 1% accuracy, we have $0.0524/\sqrt{N} < 0.01 \Rightarrow N > 26$.

Here I calculated the integral by using two weight functions with different N for 50 times, and I plot the average error in the diagram below:

We can read from the diagram that the slop of the two line is around 1/2 which consist with the formula. When $N > 30$, the accuracy for the second weight function is smaller that 1%. And when $N > 800$, the accuracy for the first weight function is smaller that 1%.

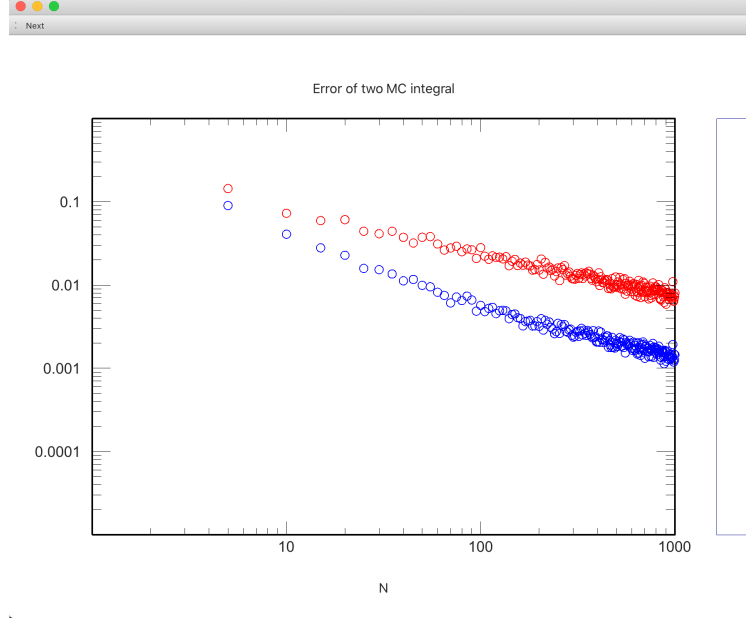


Figure 4: Error of two different weight functions: $w = 1$ (red circle) and $w = x$ (blue circle).

3.3

We have the ratio of variance:

$$\frac{\sigma_1^2}{\sigma_2^2} = \frac{\bar{f}_1^2 - I^2}{\bar{f}_2^2 - I^2} = \frac{\Pi \bar{f}_1^2(x_i) - \Pi I_i^2}{\Pi \bar{f}_2^2(x_i) - \Pi I_i^2}$$

In the limit of $D \rightarrow \infty$, we have $\Pi I_i = I_i^{2D} = 0$. Now we have:

$$\frac{\sigma_1^2}{\sigma_2^2} = \prod \frac{\bar{f}_1^2(x_i)}{\bar{f}_2^2(x_i)} = \left(\frac{\bar{f}_1^2(x_i)}{\bar{f}_2^2(x_i)} \right)^D = 1.4464^D = 10^{0.16D}$$