

Homework #1

1D Infinity potential well

EECS, GIST College

Seungcheol Han, 20165190

In 1 dimensional infinity potential well, and there is only 1 electron. Then the theoretical value of eigen energy is $1.26835101\text{e-}20\text{J}$.

When the number of mesh points is 5, the eigen energy is $1.20448\text{e-}20\text{J}$. Also in case of 50 and 500, the eigen energies are $1.26792\text{e-}20\text{J}$ and $1.26835\text{e-}20\text{J}$ each.

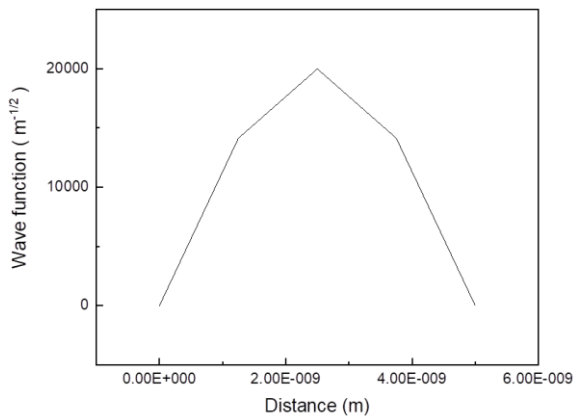


Figure 1. Wave function when the number of mesh points is 5. (Error is 5.039%)

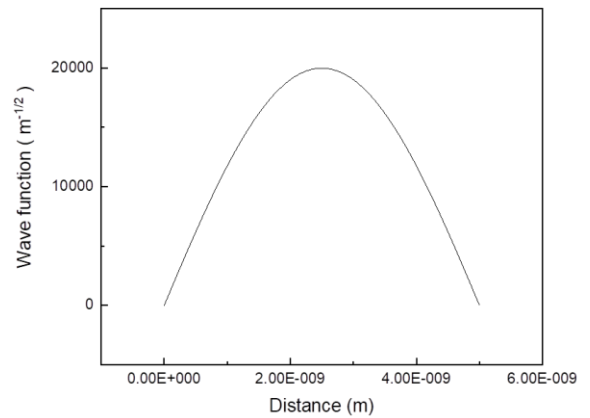


Figure 2. Wave function when the number of mesh points is 50. (Error is 0.3425%)

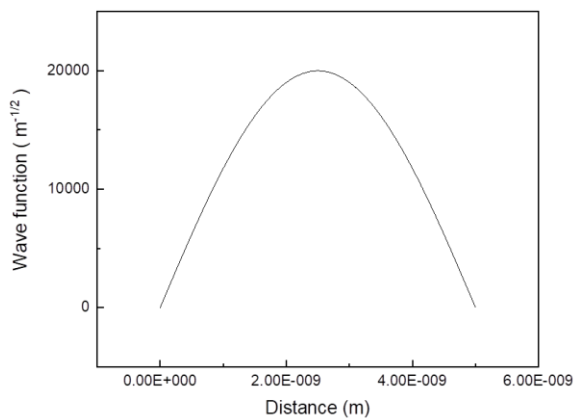


Figure 3. Wave function when the number of mesh points is 500. (Error is $3.3030 \times 10^4\%$)

When the number of mesh points is increases, the graph of eigen energy is shown below.

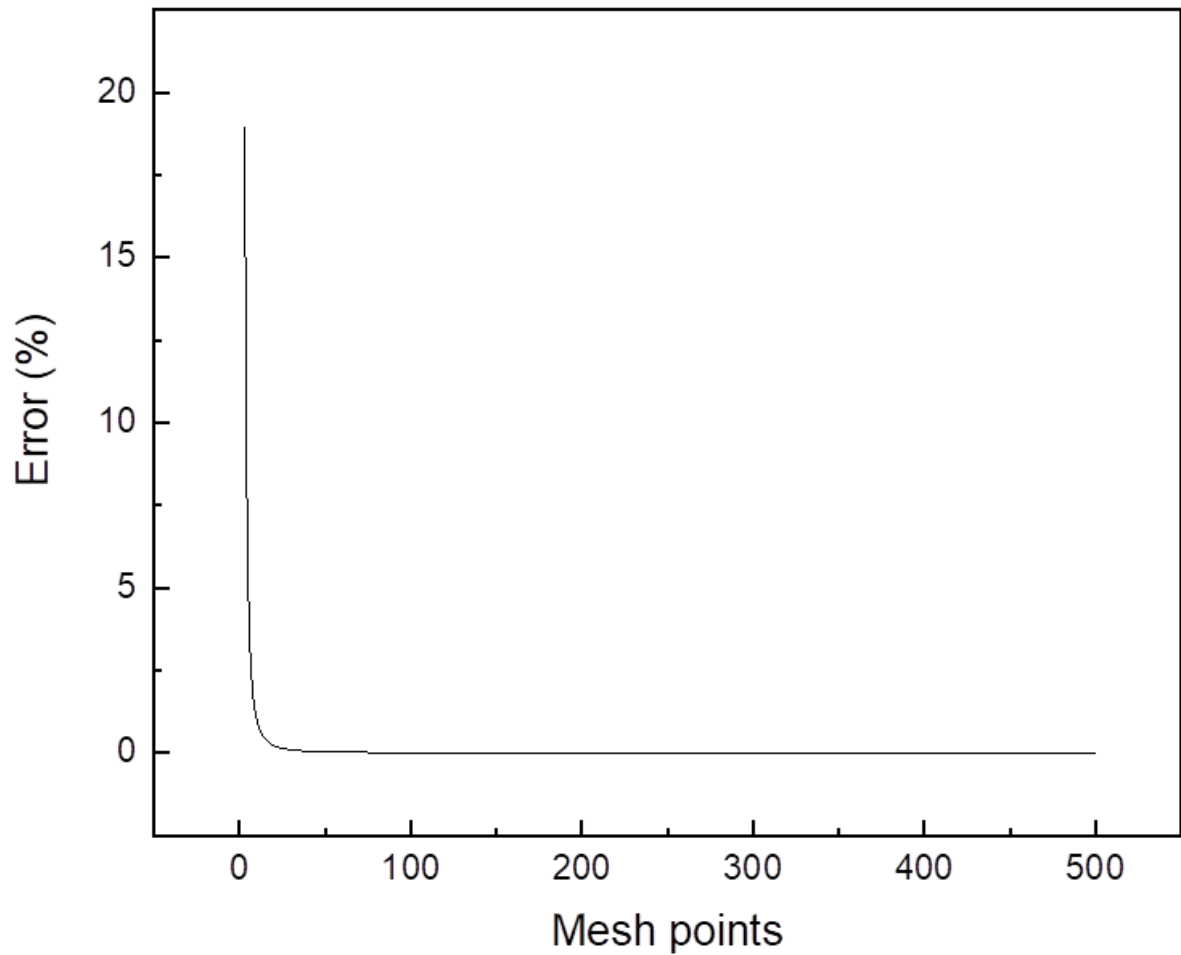


Figure 4. Error of eigen energy when the number of mesh points is from 3 to 500.

We can see the error of eigen energy is decreased when the number of mesh points is increased. Therefore we can get more accurate value when use more mesh points.