Summer Research Fellowship Programme 2020

Week 2

Assignment

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Basic – II

Electric Multipoles

Description of 'electric_mutipoles.py'

- Class 'Charge'
  - Has
    - a scalar Q corresponding to the electrostatic charge
    - a vector $\vec{r} = (x, y, z)$ corresponding to the position of the 'Charge'
  - Constructor
    - $Charge(Q, x, y, z)$
      - Returns a 'Charge' object with electrostatic charge equal to Q and position vector, $\vec{r} = (x, y, z)$
  - Methods
    - $\vec{E}(\vec{r})$
      - Returns electric field vector at a point with position vector $\vec{r}$ due to the 'Charge' object
    - $V(\vec{r})$
      - Returns the electrostatic potential at a point with position vector $\vec{r}$ due to the 'Charge' object
    - $PE(V)$
      - Returns the potential energy due to interaction of the potential field V (callable method) with the 'Charge' object
    - $\overrightarrow{P_e}(\overrightarrow{r_o})$
      - Returns the dipole moment due to the 'Charge' object measured about $\vec{r}_o$
      - $\overrightarrow{P_e} = Q \cdot (\vec{r} - \overrightarrow{r_o})$
      - Default value of $\overrightarrow{r_o} = (0,0,0)$
    - $\overline{\overline{q_e}}(\overrightarrow{r_o})$
      - Returns the second moment matrix due to the 'Charge' object measured about $\overrightarrow{r_o}$
      - $\overline{\overline{q_e}}_{3\times3} = \begin{bmatrix} (\vec{r} - \overrightarrow{r_o}) \cdot \hat{\imath} \\ (\vec{r} - \overrightarrow{r_o}) \cdot \hat{\jmath} \\ (\vec{r} - \overrightarrow{r_o}) \cdot \hat{k} \end{bmatrix}_{3\times1} \cdot \begin{bmatrix} \overrightarrow{P_e}(\overrightarrow{r_o}) \cdot \hat{\imath} & \overrightarrow{P_e}(\overrightarrow{r_o}) \cdot \hat{\jmath} & \overrightarrow{P_e}(\overrightarrow{r_o}) \cdot \hat{k} \end{bmatrix}_{1\times3}$
      - Default value of $\overrightarrow{r_o} = (0,0,0)$
    - $\overline{\overline{Q_e}}(\overrightarrow{r_o})$
      - Returns the quadrupole moment matrix due to the 'Charge' object measured about $\overrightarrow{r_o}$
      - $\overline{\overline{Q_e}}_{3\times3} = 3 \cdot \overline{\overline{q_e}}_{3\times3} - Q \cdot |\vec{r} - \overrightarrow{r_o}|^2 \cdot I_{3\times3}$
      - Default value of $\overrightarrow{r_o} = (0,0,0)$

- Class ‘ChargeDistribution’
  - Has
    - a list of ‘Charge’ objects name ‘Charges’ (to be generalized later)
  - Constructor
    - $ChargeDistribution(Q\_array, Coordinates\_array)$
      - Returns a ‘ChargeDistribution’ object with the ‘Charges’ list containing ‘Charge’ objects with electrostatic charge equal to Q_array_i positioned at $Coordinates\_array_i$
    - More to be added later
  - Methods
    - $\overrightarrow{meanPosition}()$
      - Returns the mean position of all the ‘Charge’ objects in the ‘Charges’ list (No weight is applied to the position of the ‘Charge’ objects)
    - $\vec{E}(\vec{r})$
      - Returns electric field vector at a point with position vector $\vec{r}$ due to each ‘Charge’ object in the ‘Charges’ list
      - Calculated using superimposition principle
    - $\overrightarrow{F_{internal}}(chargeIndex)$
      - Returns the force on ‘Charge’ object situated at $chargeIndex$ position of ‘Charges’ array due to other objects in the ‘Charges’ array
    - $V(\vec{r})$
      - Returns the electrostatic potential at a point with position vector $\vec{r}$ due to each ‘Charge’ object in the ‘Charges’ list
      - Calculated using superimposition principle
    - $PE_{internal}()$
      - Returns the potential energy due to interaction between each pair of ‘Charge’ objects in the ‘Charges’ list
    - $PE_{external}(V)$
      - Returns the potential energy due to interaction of the potential field V (callable method) with each ‘Charge’ object in the ‘Charges’ list
    - $\overrightarrow{P_e}(\overrightarrow{r_o})$
      - Returns the dipole moment vector of the ‘ChargeDistribution’ object about $\overrightarrow{r_o}$
      - $\overrightarrow{P_e} = \sum_i \overrightarrow{P_{e_i}}(\overrightarrow{r_o})$
      - Default value of $\overrightarrow{r_o} = (0,0,0)$
    - $\overline{\overline{q_e}}(\overrightarrow{r_o})$
      - Returns the second moment matrix of the ‘ChargeDistribution’ object about $\overrightarrow{r_o}$
      - $\overline{\overline{q_e}} = \sum_i \overline{\overline{q_{e_i}}}(\overrightarrow{r_o})$
      - Default value of $\overrightarrow{r_o} = (0,0,0)$
    - $\overline{\overline{Q_e}}(\overrightarrow{r_o})$

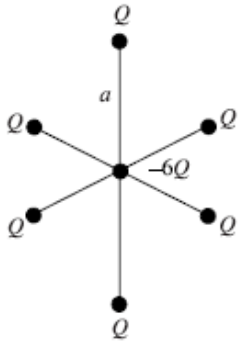
- Returns the quadrupole moment matrix of the 'ChargeDistribution' object about $\overrightarrow{r_o}$
- $\overline{\overline{Q_e}} = \sum_i \overline{\overline{Q_{e_i}}}(\overrightarrow{r_o})$
- Default value of $\overrightarrow{r_o} = (0,0,0)$

- Class 'Dipole'
  - Has
    - a vector $\vec{p}$ corresponding to the dipole moment of the 'Dipole'
    - a vector $\vec{r} = (x, y, z)$ corresponding to the position of the 'Dipole'
  - Constructor
    - $Dipole(\vec{p}, x, y, z)$
      - Returns a 'Dipole' object with dipole moment equal to $\vec{p}$ and position vector, $\vec{r} = (x, y, z)$
    - $Dipole.fromChargeDistro(chargeDistro)$
      - Returns a 'Dipole' object with dipole moment equal to $\overrightarrow{P_e}$ of the $chargeDistro$ (a 'ChargeDistribution' object) and position vector $\vec{r} = chargeDistro.\overrightarrow{meanPosition}()$
  - Methods
    - $V(\vec{r})$
      - Returns the electrostatic potential at a point with position vector $\vec{r}$ due to 'Dipole' object
      - Calculated assuming V falls with $\frac{1}{r^2}$
    - $\vec{E}(\vec{r})$
      - Returns electric field vector at a point with position vector $\vec{r}$ due to 'Dipole' object
      - Calculated using $\vec{E} = -\vec{\nabla}V$
    - $\overrightarrow{P_e}()$
      - Returns the dipole moment $\vec{p}$ of the 'Dipole' object
    - $PE(V)$
      - Returns the potential energy due to interaction of the potential field V (callable method) with the 'Dipole' object

Q1

Consider the following charge distribution of point charges in space and estimate the first and second moments of the distribution for at least three different values of a.

The charge Q has the same magnitude as charge on an electron.



Ans

Using electric_multipoles.py, first created a charge distribution corresponding to the above configuration – six charges with magnitude e at $(a, 0,0)$, $(-a, 0,0)$, $(0, a, 0)$, $(0, -a, 0)$, $(0,0, a)$ and $(0,0, -a)$, and, one charge with magnitude $-6e$ at $(0,0,0)$. Used the method $ChargeDistribution.\overrightarrow{P_e}$ and $ChargeDistribution.\overline{\overline{q_e}}$ to calculate the dipole moment and the second moment of the above charge distribution. Associated code can be found in the script assignment_2_q1.py. The output –

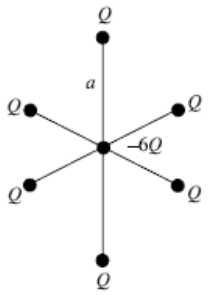
```
a =  1e-10  m
P_e :
[0. 0. 0.]
q_e :
[[3.20435297e-39 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 3.20435297e-39 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 3.20435297e-39]]

a =  5e-10  m
P_e :
[0. 0. 0.]
q_e :
[[8.01088244e-38 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 8.01088244e-38 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 8.01088244e-38]]

a =  2.4e-09  m
P_e :
[0. 0. 0.]
q_e :
[[1.84570731e-36 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 1.84570731e-36 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 1.84570731e-36]]
```

Q2

Take Octahedral charge distribution of point charges in space and estimate quadrupole moment of the distribution.



What will be quadrupole moment matrix if two charges above and below are 2Q and the Centre charge is -8Q?

Ans

Similar to Q1, the charge distribution for the above configuration was created for sub-problem 1. The quadrupole moment was calculated using the method $chargeDistribution.\overline{\overline{Q_e}}$. Associated code can be found in the script assignment_2_q2_subprob_1.py. The output –

```
a =  1e-10  m
Q_e :
[[0. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]]

a =  5e-10  m
Q_e :
[[4.17619486e-53 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 4.17619486e-53 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 4.17619486e-53]]

a =  2.4e-09  m
Q_e :
[[0. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]]
```

Even though the $\overline{\overline{Q_e}}$ for $a = 5 \times 10^{-10}\ m$ seems non-zero, it is extremely small. It can be assumed to be zero, attributing the non-zero values to computer's limitation to representing floating point numbers. Hence, we may infer that $\overline{\overline{Q_e}}$ for an octahedral charge distribution is $\overline{\overline{0}}$.

For sub-problem 2, instead of charges of magnitude e, e and $-6e$ at $(0,0,a)$, $(0,0,-a)$ and $(0,0,0)$ respectively, the charges of magnitude $2e$, $2e$ and $-8e$ were

used. Associated code can be found in the script assignment_2_q2_subprob_2.py. The output –

```
a =  1e-10  m
Q_e :
[[-3.20435297e-39  0.00000000e+00  0.00000000e+00]
 [ 0.00000000e+00 -3.20435297e-39  0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  6.40870595e-39]]

a =  5e-10  m
Q_e :
[[-8.01088243e-38  0.00000000e+00  0.00000000e+00]
 [ 0.00000000e+00 -8.01088243e-38  0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  1.60217649e-37]]

a =  2.4e-09  m
Q_e :
[[-1.84570731e-36  0.00000000e+00  0.00000000e+00]
 [ 0.00000000e+00 -1.84570731e-36  0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  3.69141463e-36]]
```

Q3

You can estimate the moment matrices for different charges, keeping the overall system electrically neutral.

Consider the tetrahedral arrangement of carbon atom with equally spaced 4 sp3 hybridized orbitals.

Assume 4Q+ charge at the centre, keeping it at origin and Q- charge at each vertex of the tetrahedron.

What will be moment matrices of the system.

Ans

Using electric_multipoles.py, first created a charge distribution corresponding to the above configuration – four charges with magnitude $-e$ at $(a, 0,0)$, $(a, 109.4^o, -60^o)$, $(a, 109.4^o, 60^o)$ and $(a, 109.4^o, 180^o)$, and, one charge with magnitude $4e$ at $(0,0,0)$ where a is the carbon atomic radius and the coordinates are in polar form (physics notation). Used the methods $ChargeDistribution.\overrightarrow{P_e}$, $ChargeDistribution.\overline{\overline{q_e}}$ and $chargeDistribution.\overline{\overline{Q_e}}$ to calculate the dipole moment, second moment and quadrupole moment of the above charge distribution. Associated code can be found in the script assignment_2_q3.py. The output –

```
P_e :
[-1.40129846e-45 -7.02956646e-46 -7.00649232e-46]
```

```
q_e :
[[-3.08472380e-40  2.51846475e-56  1.01957882e-56]
 [ 2.51846475e-56 -3.08472380e-40  8.90411751e-57]
 [-1.01957882e-56  8.90411751e-57 -3.08472380e-40]]

Q_e :
[[-8.15663058e-56  7.55539425e-56  0.00000000e+00]
 [ 7.55539425e-56  0.00000000e+00  2.67123525e-56]
 [-4.07831529e-56  2.67123525e-56  1.22349459e-55]]
```

Again, though the values appear to be non-zero, they are extremely small (compared to the order of $e \times a^2$). Hence, the values with order less than $e \times a^2$ may be assumed zero, attributing the non-zero values to computer's limitation to representing floating point numbers. Hence, we may infer that $\overrightarrow{P_e}$ and $\overline{\overline{Q_e}}$ for a tetrahedral charge distribution is $\vec{0}$ and $\bar{\bar{0}}$ respectively.

Q4

Estimate magnitude of electrostatic potential because of the octahedral charge distribution in space as a function of r from the centre.

Estimate magnitude of electrostatic potential because of the tetrahedral electric charge distribution in carbon atom as function of r, from central carbon kept at the origin

You may try to plot the potential in 3D diagram using MATLAB.

Ans

Using electric_multipoles.py, created octahedral charge distribution for sub-problem 1. Used the method $chargeDistribution.V$ to find the potential field from a range r_{min} to r_{max}.

In the script assignment_2_q4_subprob_1_2D.py, the variation of potential with r for n_{plots} different values of θ is plotted on a 2D plot for a particular ϕ, with ϕ varying with time.

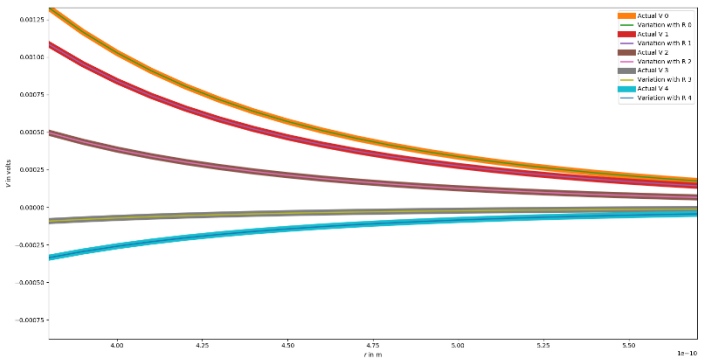


Figure 1: Variation of Potential with the power of r

In the script assignment_2_q4_subprob_1_3D.py, the potential as a function of r and θ for a particular ϕ is shown using a 3D plot, with ϕ varying with time.

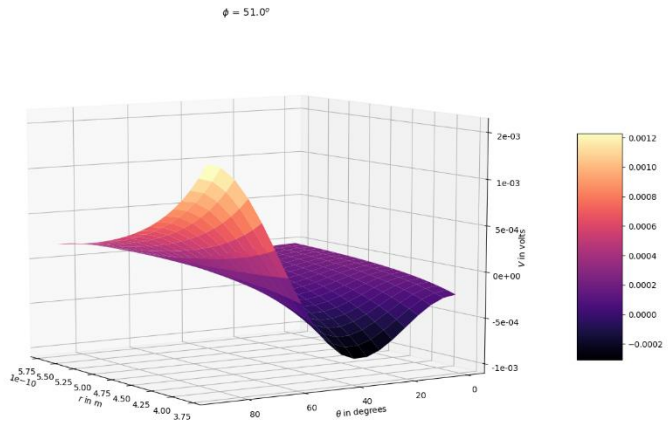


Figure 2: Variation of Potential for Octahedral Charge Distribution

In the script assignment_2_q4_subprob_1_equipot_surf.py, equipotential surface for the described charge distribution is plotted. Please note, the script requires the library Mayavi (Ramachandran and Varoquaux 2011).

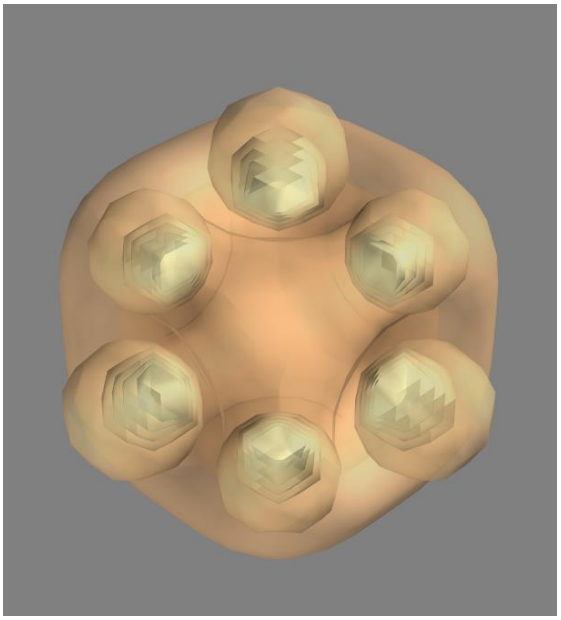


Figure 3: Equipotential surfaces for Octahedral charge distribution

From Figure 1 (kindly refer to the output from python script for better resolution), we observe potential falls with $\frac{1}{r^5}$, i.e., $V \propto \frac{1}{r^5}$. Hence, we infer the octahedral charge distribution is a multipole of order $n = 4$.

Again, using electric_multipoles.py simulated, the tetrahedral charge distribution for carbon atom is created. Used the method $chargeDistribution.V$ to find the potential field from a range r_{min} to r_{max}.

In the script assignment_2_q4_subprob_2_2D.py, the variation of potential with r for n_{plots} different values of θ is plotted on a 2D plot for a particular ϕ, with ϕ varying with time.

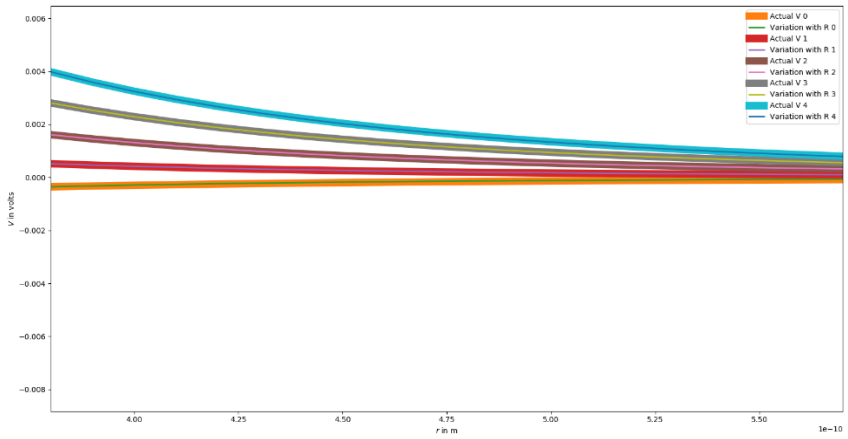


Figure 4: Variation of Potential with the power of r

In the script assignment_2_q4_subprob_2_3D.py, the potential as a function of r and θ for a particular ϕ is shown using a 3D plot, with ϕ varying with time.

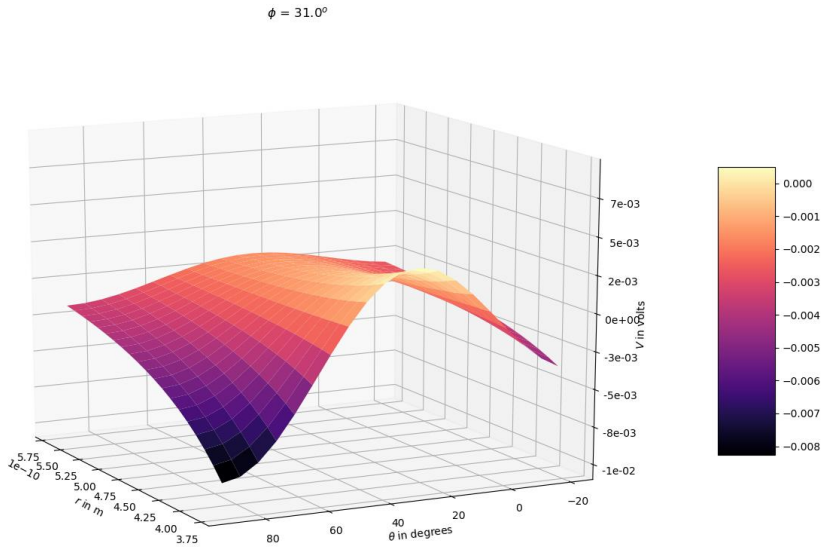


Figure 5: Variation of Potential for Tetrahedral Charge Distribution

In the script assignment_2_q4_subprob_2_equipot_surf.py, equipotential surface for the described charge distribution is plotted. Please note, the script requires the library Mayavi (Ramachandran and Varoquaux 2011).

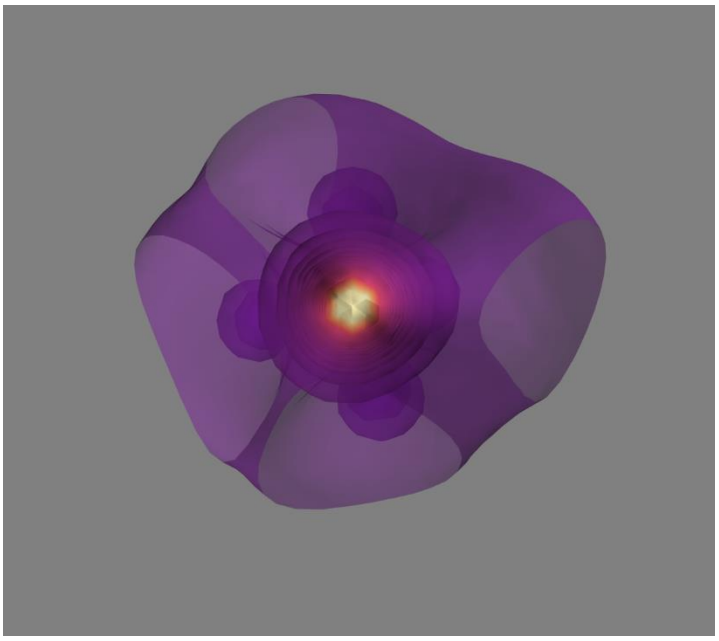


Figure 6: Equipotential surfaces for Tetrahedral charge distribution

In Figure 4 (kindly refer to the output from python script for better resolution), we observe the potential falls with $\frac{1}{r^4}$, i.e., $V \propto \frac{1}{r^4}$. From this we can infer that a tetrahedral distribution of charge acts as a multipole of order $n = 3$.

Q5

Consider a methane molecule, with central carbon atom and 4 hydrogens at apexes of a regular tetrahedron.

The central carbon is a multipole with +4Q charge at the origin, and –Q charge at four vertices of a tetragon whose dimensions are decided by atomic radius of carbon.

Four hydrogen atoms, in line with the tetrahedron's vertices, are at bond length of 0.16nm from the carbon. Each hydrogen atom can be treated as a dipole. (as estimated in Session-01)

Estimate electrostatic potential as function of distance r from the central carbon?

Ans

It is difficult to treat the carbon atom as a multipole since I observed the tetrahedral charge distribution acts as a multipole of order $n = 3$, and I do not possess enough information on how to treat such multipoles.

However, the hydrogen atoms are treated as dipoles. Resulting potential field is plotted as a function of r and θ for a particular ϕ is shown using a 3D plot, with ϕ varying with time, in the script assignment_2_q5_3D.py.

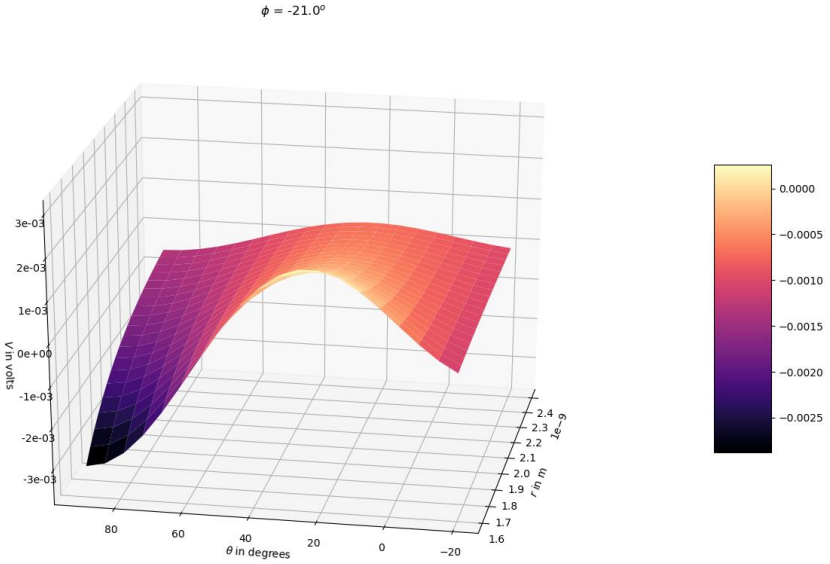


Figure 7: Variation of Potential for CH_4 Charge Distribution

In the script assignment_2_q5_equipot_surf.py, equipotential surface for the described charge distribution is plotted. Please note, the script requires the library Mayavi (Ramachandran and Varoquaux 2011).

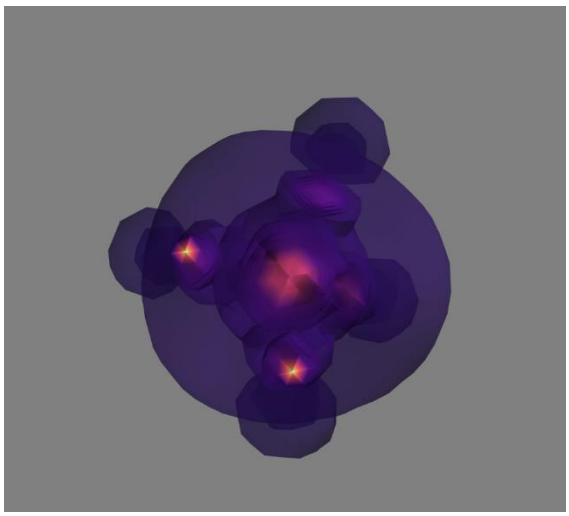


Figure 8: Equipotential surfaces for CH_4 charge distribution

Q6

Can you estimate potential energy of a methane molecule considering its charge distribution: carbon as a multipole and each hydrogen as a dipole?

Ans

Again, treating carbon as a multipole is difficult because of little knowledge on how to treat multipoles of order $n = 3$. Treating hydrogen atoms as dipoles, the potential energy is found by the script assignment_2_q6.py. The output of the script –

```
Total Potential Energy of CH4 :
-5.873169106850645e-17  J
-366.57441639577905  eV
```

Please note, the dipole of hydrogen atoms is assumed to point towards the centre of the carbon atom for all the above calculations involving CH_4 molecule.

References

Ramachandran, P., and G. Varoquaux. 2011. *Mayavi: 3D Visualization of Scientific Data.* IEEE Computing in Science & Engineering, 13 (2), pp. 40-51.
http://docs.enthought.com/mayavi/mayavi/index.html.