Alex Merino

MTH 4311

Dr. Pei Liu

Due: 4/3/2025

Part A.

For the Poisson-Boltzmann equation, the boundary value problem is written out in the work below:

$$\begin{cases} \phi_{xx} = z\sinh(z\phi) \\ \phi(0) = 0 \\ \phi(L) = V \end{cases}$$

First we should check if it is unique $\qquad y'' = z\sinh(zy)$

$z^2 > 0$ and cosh is a strictly positive function so $f_y > 0$

$$f_t = 0 \qquad f_y = z^2\cosh(zy) \qquad f_{y'} = 0$$

All are continuous and $f_{y'} \le M$ is true due to $M > 0$

Finite Difference Method

$$y''(x) = \frac{y(x+h) + y(x-h) - 2y(x)}{h}$$

$$\begin{cases} \dfrac{\phi_{i-1} + \phi_{i+1} - 2\phi_i}{h^2} = z\sinh(z\phi) \\ \phi_0 = 0 \\ \phi_L = V \end{cases}$$

$$\phi_{i-1} + \phi_{i+1} - 2\phi_i = z\sinh(z\phi_i)h^2$$

$$\phi_{i-1} - 2\phi_i - z\sinh(z\phi_i)h^2 + \phi_{i+1} = 0$$

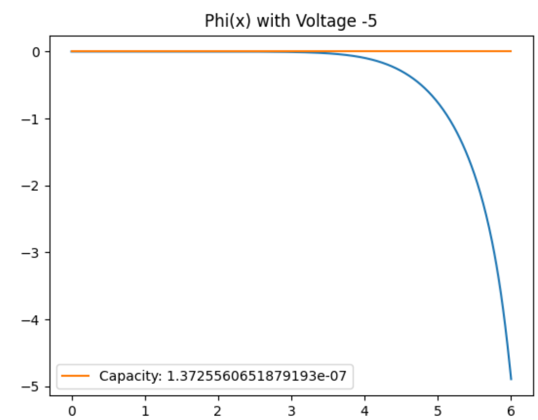
$$\phi_{i-1} - 2\phi_i - zh^2\sinh(z\phi_i) + \phi_{i+1} = 0$$

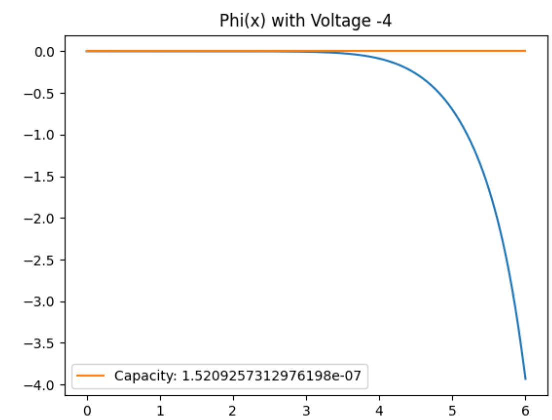
Using DF

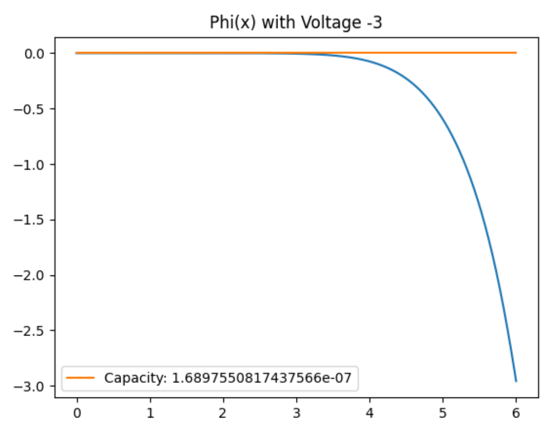
$$\begin{pmatrix} -2 - z^2\cosh(z\phi_i)h^2 & 1 & 0 \\ 1 & \ddots & \ddots \\ 0 & \ddots & \ddots \end{pmatrix}$$

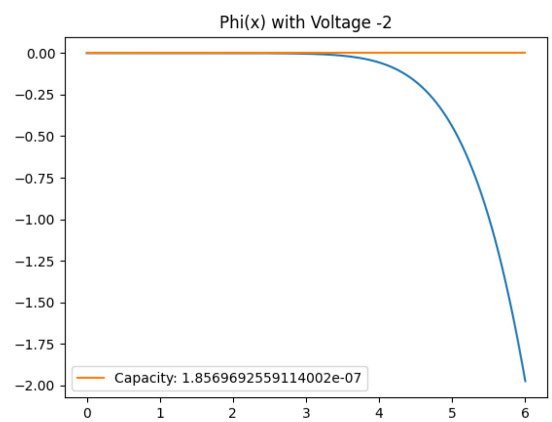
The matrix at the bottom of the work is the jacobian matrix we will be using for Newton's iterative method to calculate the y-values. The program creates the jacobian matrix mentioned above, then the $F(X_K)$ vector which we will use to solve during the iterations. When the Python code is running, the Finite Difference method takes a decent amount of time, due to it being an iterative method.

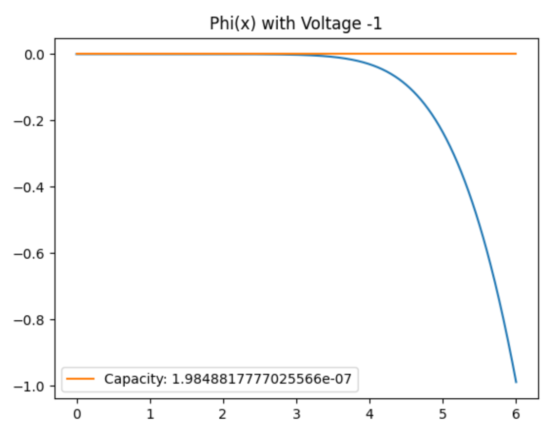
Part B.

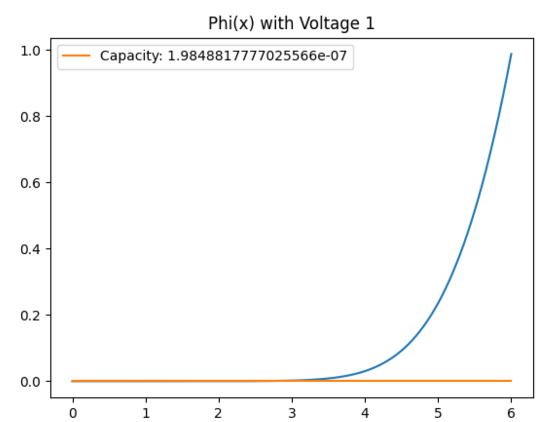


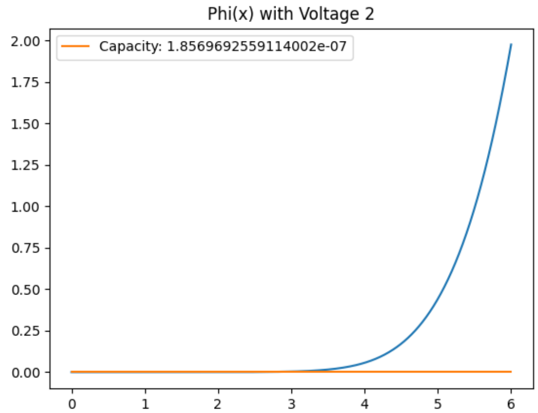


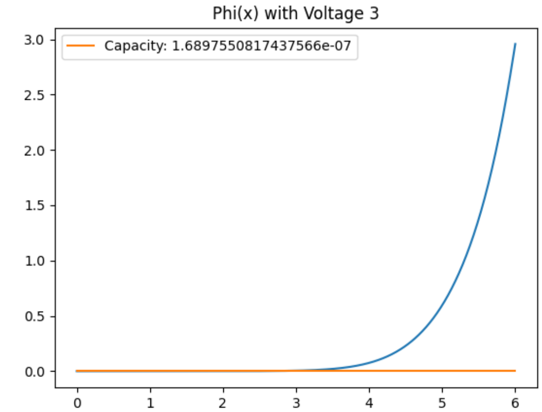


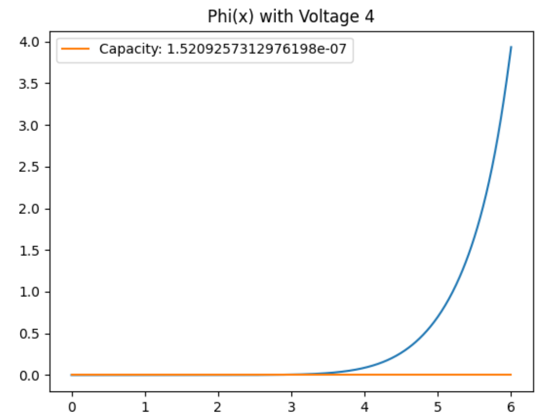


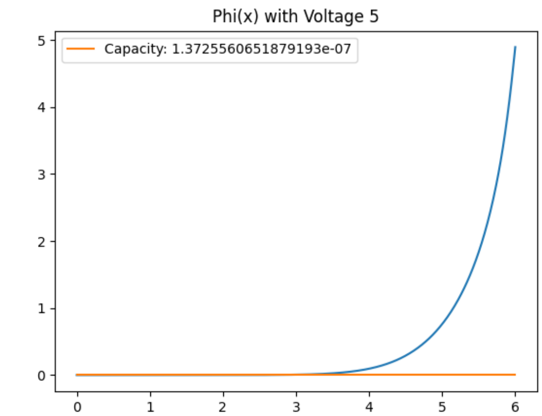




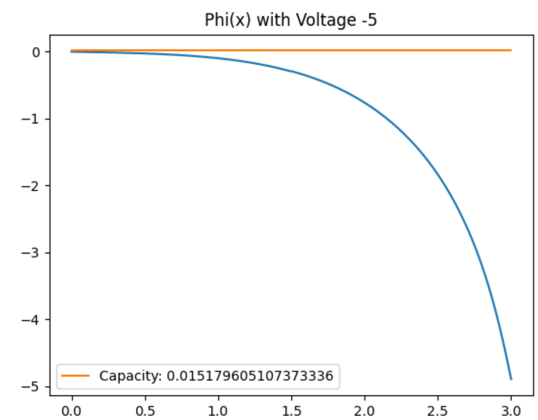

Phi(x) with Voltage 2
Capacity: 1.8569692559114002e-07

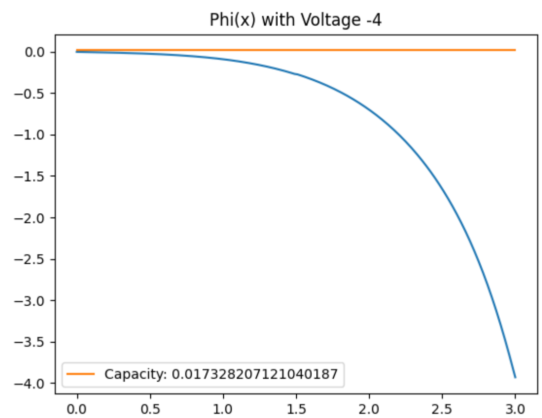

Phi(x) with Voltage 3
Capacity: 1.6897550817437566e-07

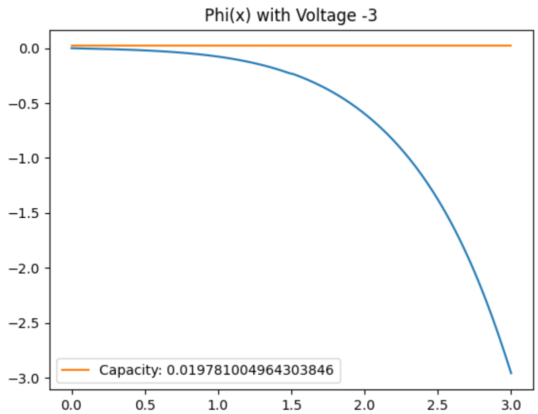

Phi(x) with Voltage 4
Capacity: 1.5209257312976198e-07

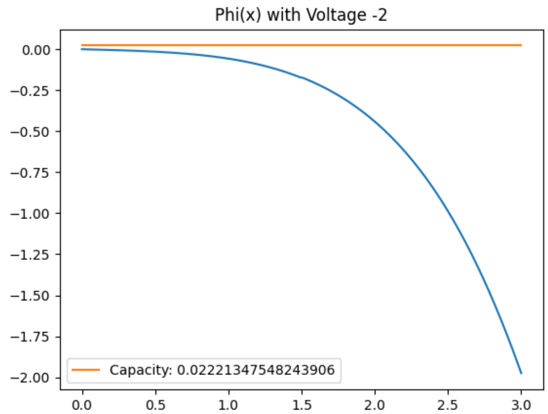

Phi(x) with Voltage 5
Capacity: 1.3725560651879193e-07

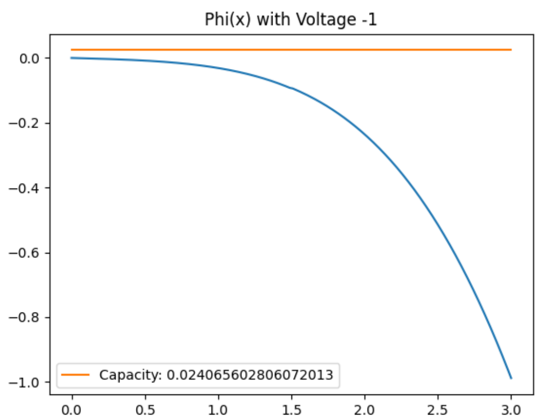
Part C.

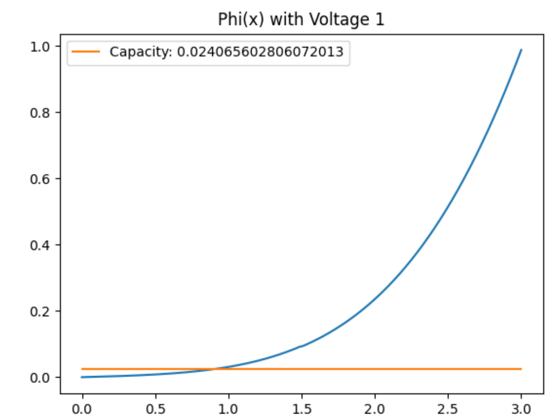

Phi(x) with Voltage -5
Capacity: 0.015179605107373336

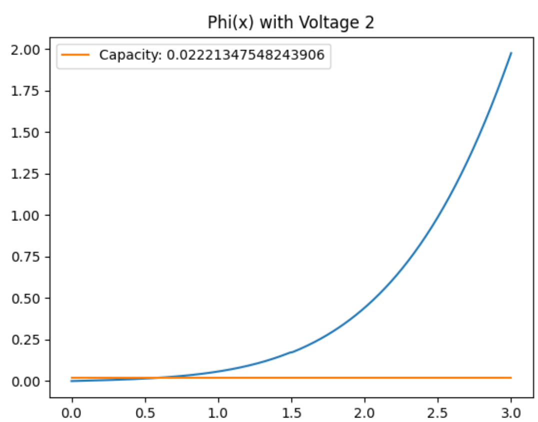

Phi(x) with Voltage -4
Capacity: 0.017328207121040187

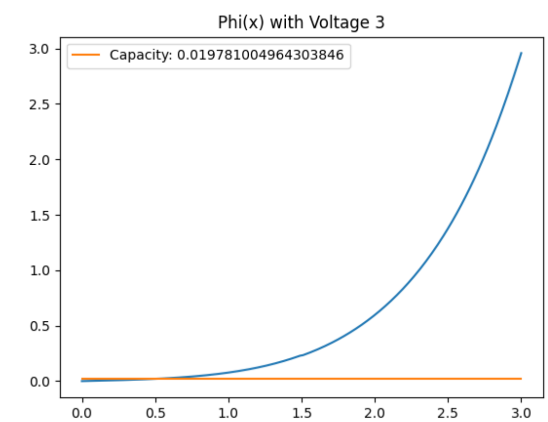

Phi(x) with Voltage -3
Capacity: 0.019781004964303846

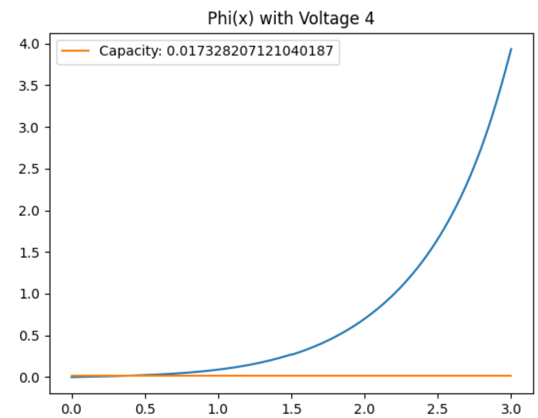

Phi(x) with Voltage -2
Capacity: 0.02221347548243906

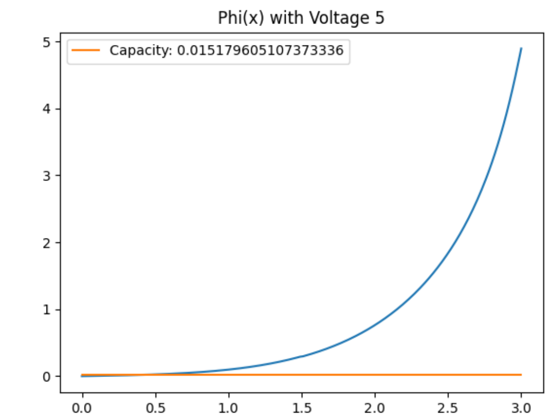

Phi(x) with Voltage -1
Capacity: 0.024065602806072013


Phi(x) with Voltage 1
Capacity: 0.024065602806072013

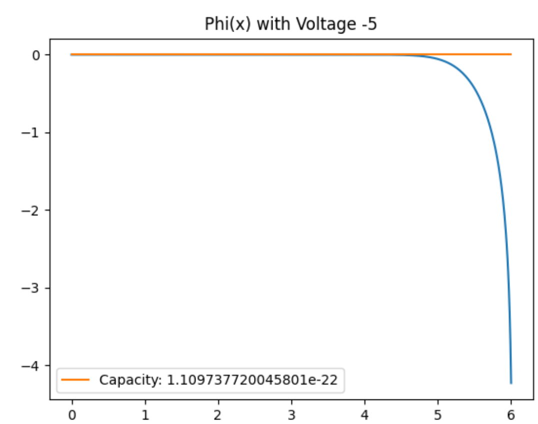

Phi(x) with Voltage 2
Capacity: 0.02221347548243906

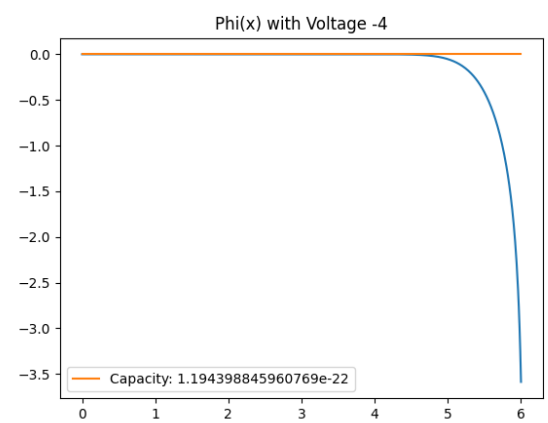

Phi(x) with Voltage 3
Capacity: 0.019781004964303846

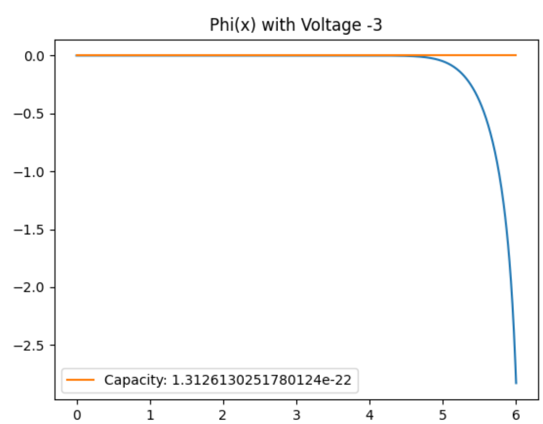

Phi(x) with Voltage 4
Capacity: 0.017328207121040187

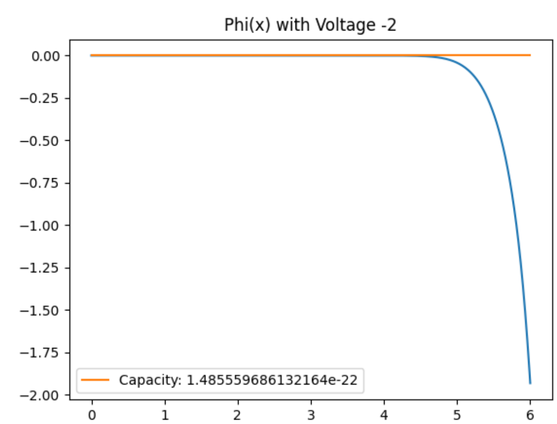

Phi(x) with Voltage 5
Capacity: 0.015179605107373336

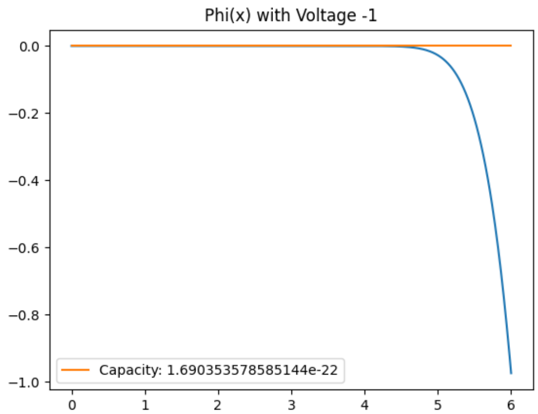
Part D.

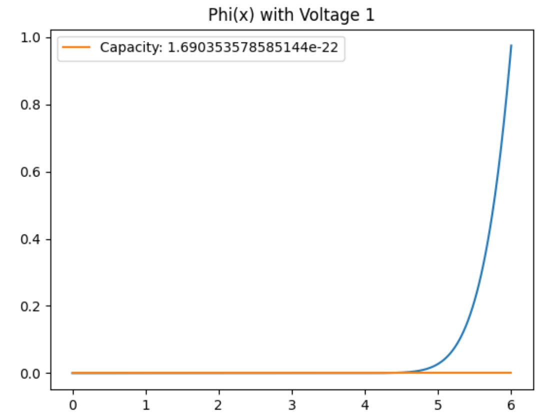

Phi(x) with Voltage -5
Capacity: 1.109737720045801e-22

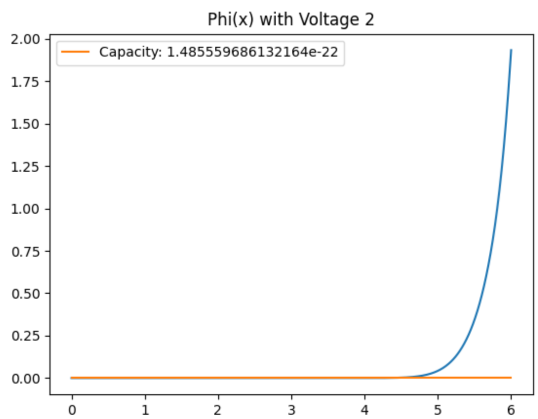

Phi(x) with Voltage -4
Capacity: 1.194398845960769e-22

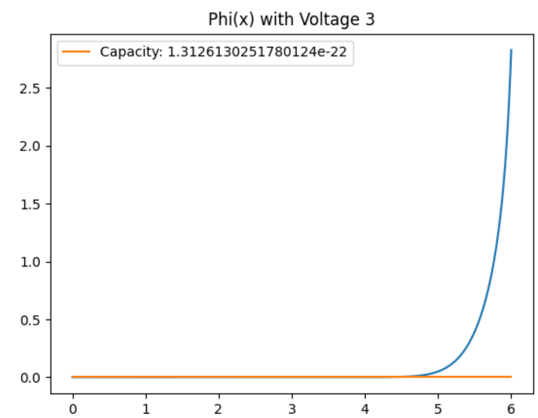

Phi(x) with Voltage -3
Capacity: 1.3126130251780124e-22

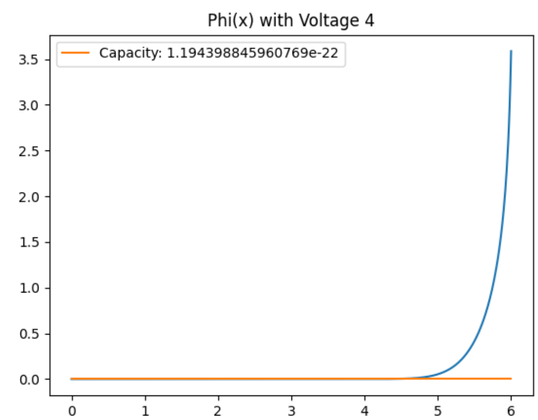

Phi(x) with Voltage -2
Capacity: 1.485559686132164e-22

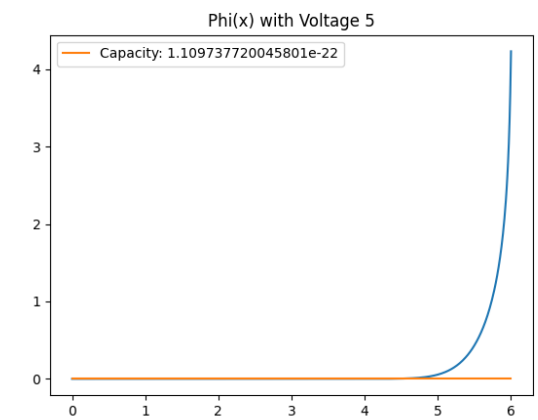












Part E.

For the finite element method, the work is shown below:

$$\begin{cases} \phi_{xx} = z^2 \phi \\ \phi_0 = \emptyset \\ \phi_L = V \end{cases}$$

Weak Form

$$-\int_0^L \phi'(t)\, g'(t)\, dt = \int_0^L (z^2 \phi)\, g(t)\, dt$$

$$-\int_0^L \sum_{i=0}^{N} c_i\, g_i'(t)\, g_j'(t)\, dt = z^2 \int_0^L \sum_{i=0}^{N} c_i\, g_i(t)\, g_j(t)\, dt$$

$$\frac{c_{j-1}}{h} - \frac{2c_j}{h} + \frac{c_{j+1}}{h} = z^2\left(\frac{h c_{j-1}}{6} + \frac{2hc_j}{3} + \frac{h c_{j+1}}{6}\right)$$

$$\frac{c_{j-1}}{h} - z^2\frac{h c_{j-1}}{6} - \frac{2c_j}{h} - \frac{2}{3} z^2 h c_j + \frac{c_{j+1}}{h} - \frac{z^2 h c_{j+1}}{6}$$

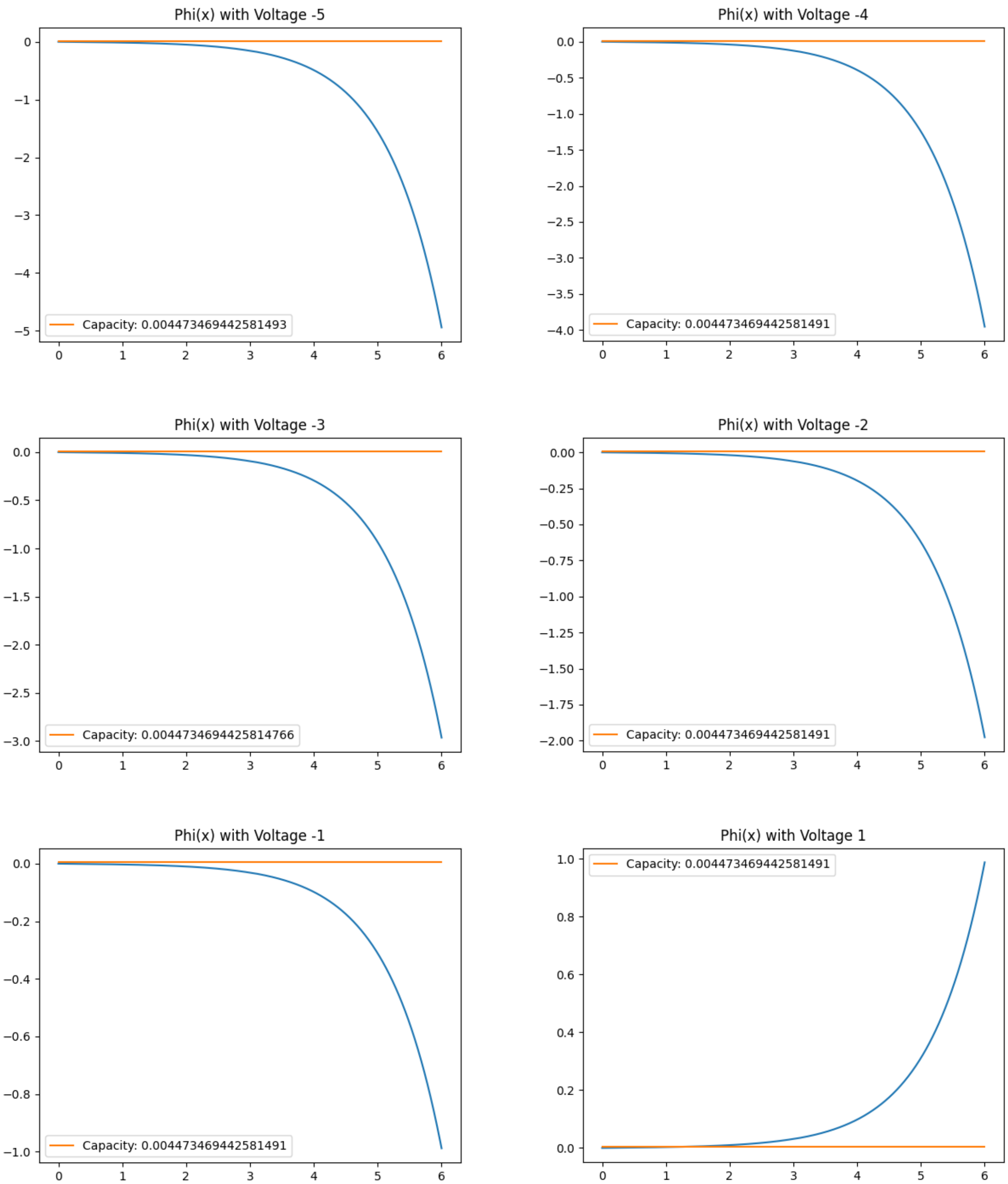
$$c_{j-1}\left(\frac{1}{h} - \frac{z^2 h}{6}\right) - c_j\left(\frac{2}{h} + \frac{2z^2 h}{3}\right) + c_{j+1}\left(\frac{1}{h} - \frac{z^2 h}{6}\right) = \emptyset$$

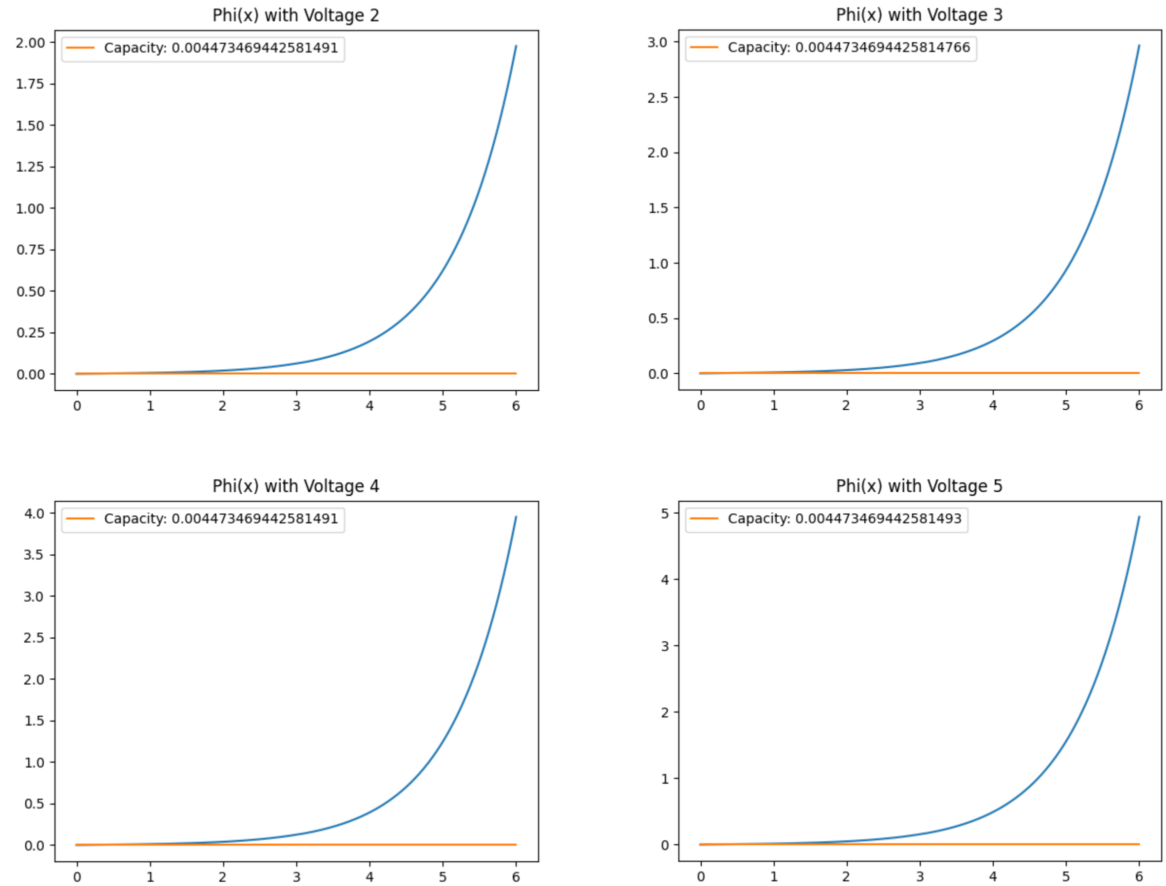
$$\alpha = \frac{2}{h} + \frac{2z^2 h}{3} \qquad \beta = \frac{1}{h} - \frac{z^2 h}{6}$$

$$\begin{pmatrix} -\alpha & \beta & & \emptyset \\ \beta & -\alpha & \beta & \\ & \ddots & \ddots & \ddots \\ \emptyset & & \beta & -\alpha \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} \emptyset \\ \emptyset \\ \vdots \\ \emptyset \\ -\beta V \end{pmatrix}$$

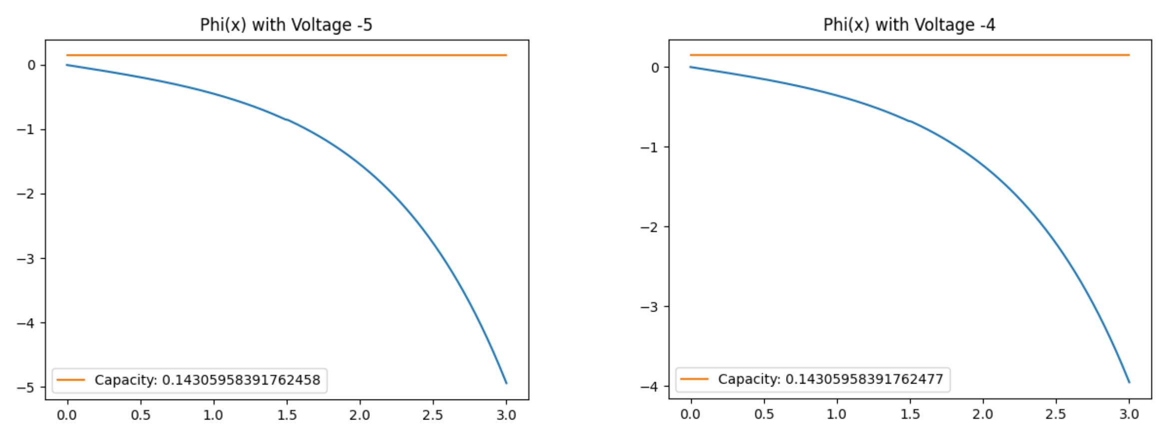
The B-Spline was used to convert the integral into a tri-diagonal matrix of alphas and betas. To compute the finite element method, all that was needed was the solving of one matrix, which ran much faster than the Finite difference method. The results of the graphs show that the curve starts to increase faster in the Finite element method because of the greater values in the matrix (alpha ~ 200, beta ~ 100).

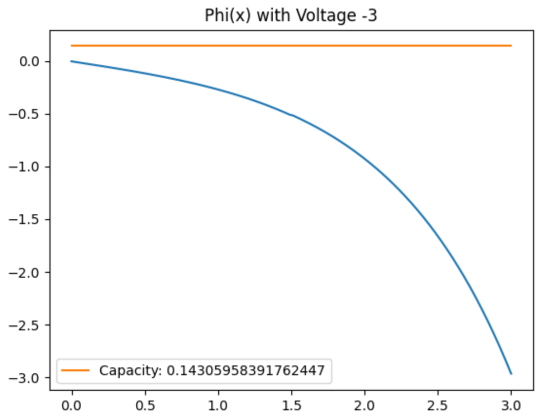
Part F1.

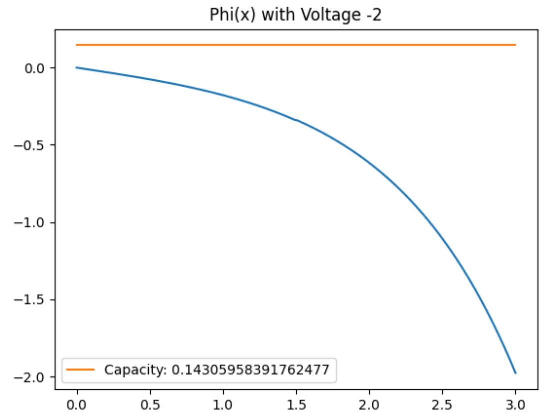

Phi(x) with Voltage -5
Capacity: 0.004473469442581493
Phi(x) with Voltage -4
Capacity: 0.004473469442581491
Phi(x) with Voltage -3
Capacity: 0.0044734694425814766
Phi(x) with Voltage -2
Capacity: 0.004473469442581491
Phi(x) with Voltage -1
Capacity: 0.004473469442581491
Phi(x) with Voltage 1
Capacity: 0.004473469442581491

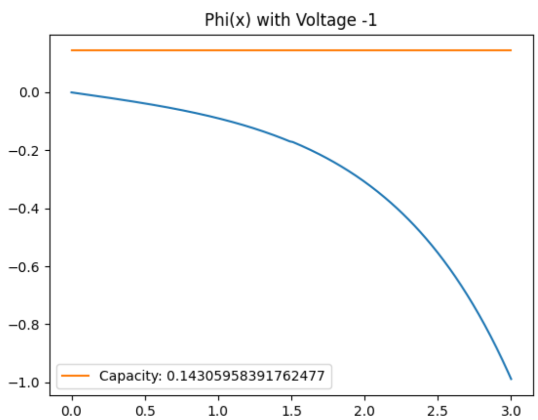

Phi(x) with Voltage 2
Capacity: 0.004473469442581491
Phi(x) with Voltage 3
Capacity: 0.0044734694425814766
Phi(x) with Voltage 4
Capacity: 0.004473469442581491
Phi(x) with Voltage 5
Capacity: 0.004473469442581493

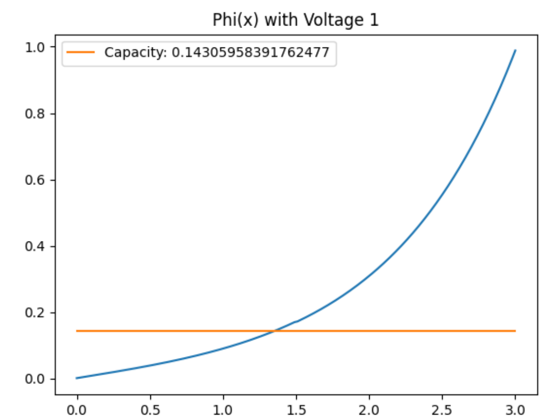
Part F2.

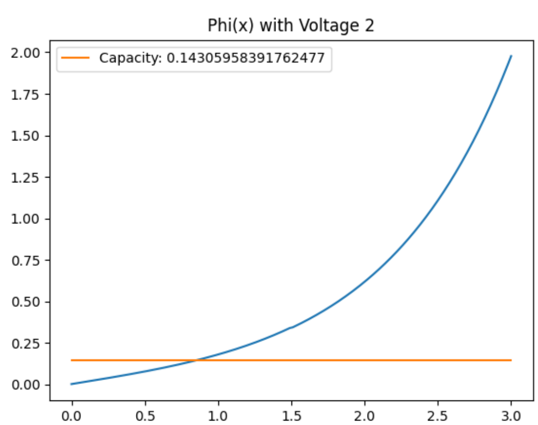

Phi(x) with Voltage -5
Capacity: 0.14305958391762458
Phi(x) with Voltage -4
Capacity: 0.14305958391762477

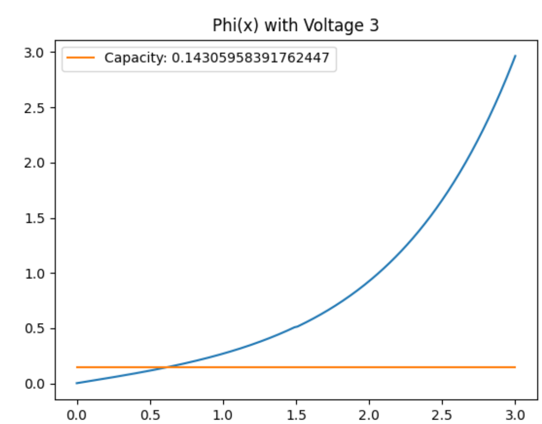

Phi(x) with Voltage -3
Capacity: 0.14305958391762447

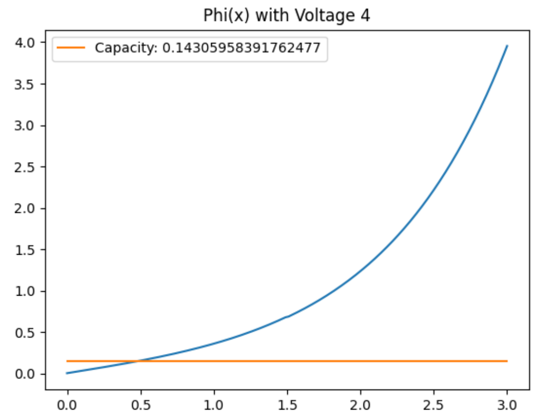

Phi(x) with Voltage -2
Capacity: 0.14305958391762477

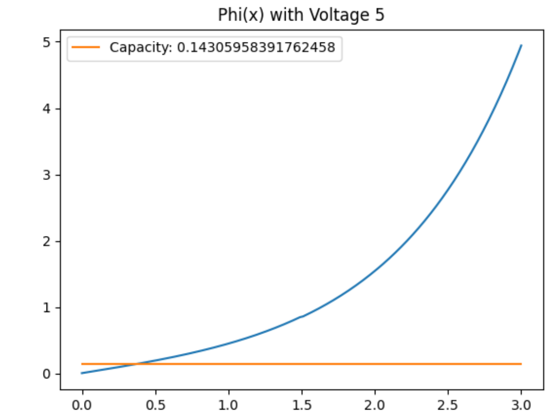

Phi(x) with Voltage -1
Capacity: 0.14305958391762477


Phi(x) with Voltage 1
Capacity: 0.14305958391762477

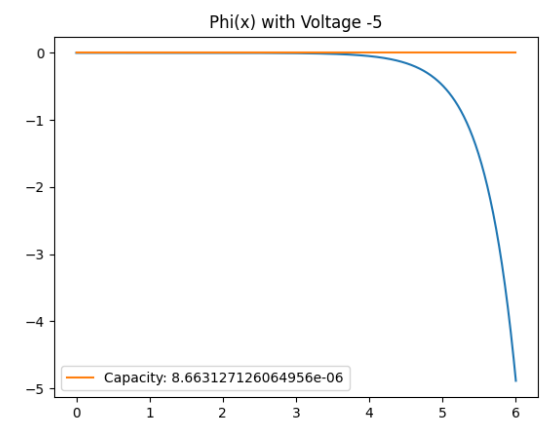

Phi(x) with Voltage 2
Capacity: 0.14305958391762477

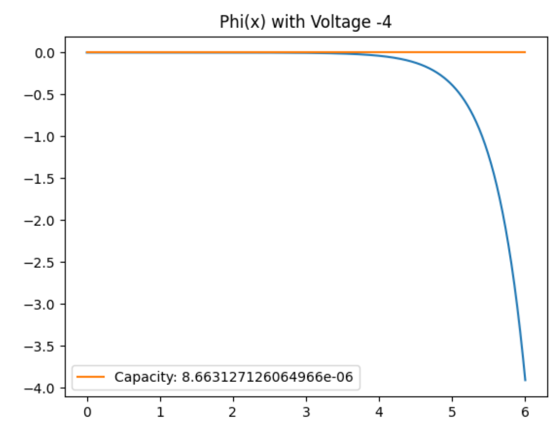

Phi(x) with Voltage 3
Capacity: 0.14305958391762447

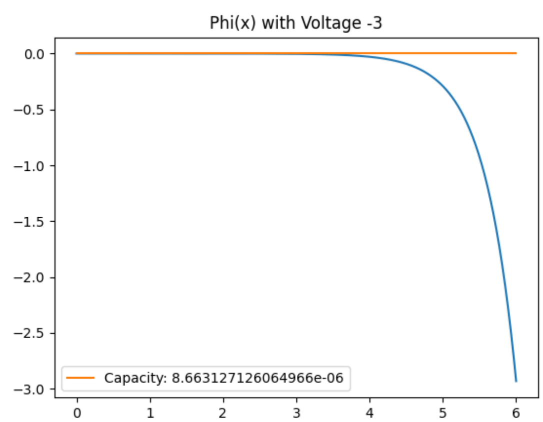

Phi(x) with Voltage 4
Capacity: 0.14305958391762477

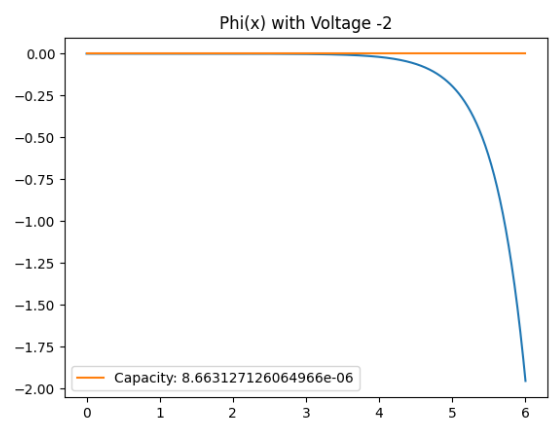

Phi(x) with Voltage 5
Capacity: 0.14305958391762458

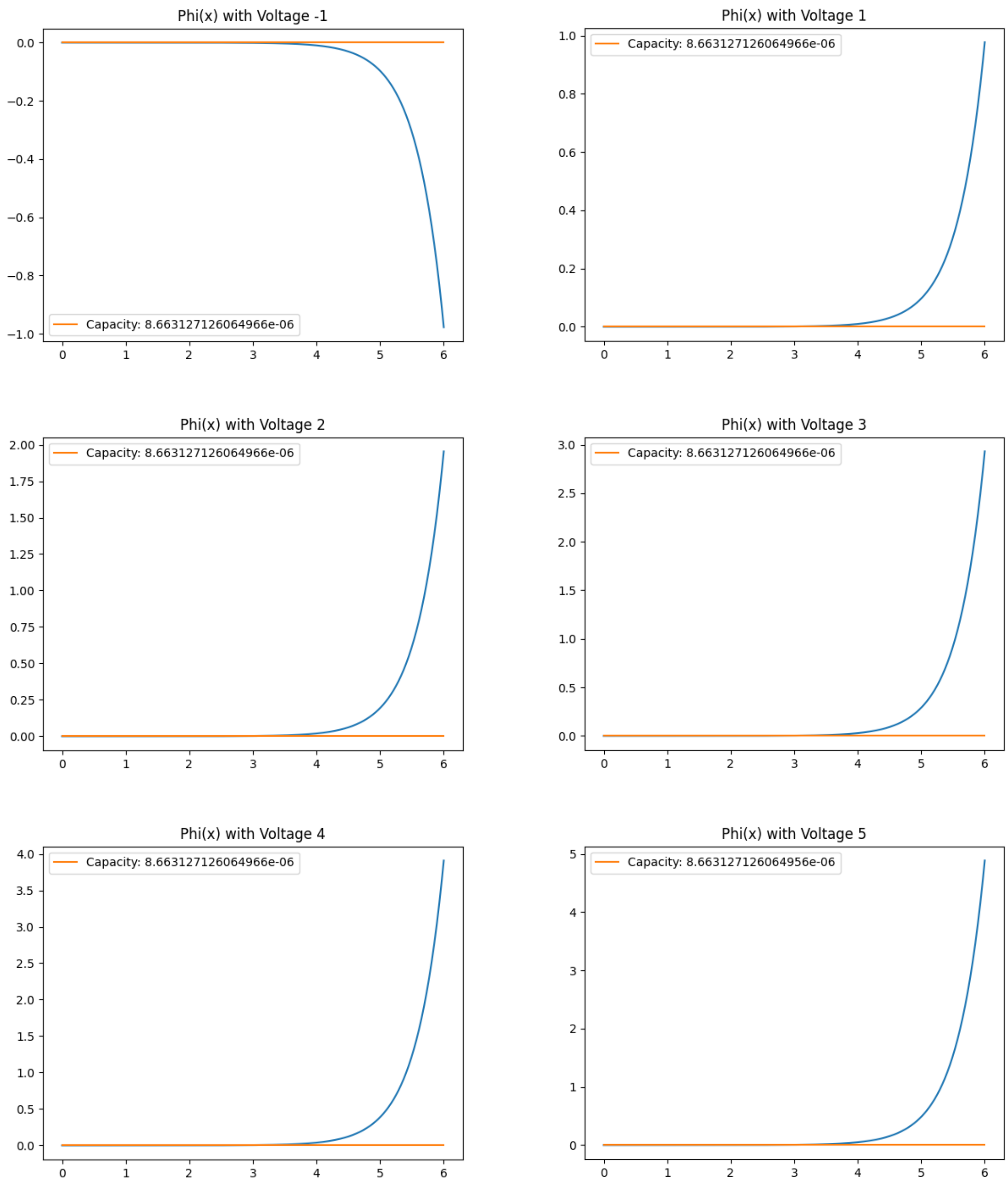
Part F3.


Phi(x) with Voltage -5
Capacity: 8.663127126064956e-06


Phi(x) with Voltage -4
Capacity: 8.663127126064966e-06


Phi(x) with Voltage -3
Capacity: 8.663127126064966e-06


Phi(x) with Voltage -2
Capacity: 8.663127126064966e-06


Phi(x) with Voltage -1
Capacity: 8.663127126064966e-06
Phi(x) with Voltage 1
Capacity: 8.663127126064966e-06
Phi(x) with Voltage 2
Capacity: 8.663127126064966e-06
Phi(x) with Voltage 3
Capacity: 8.663127126064966e-06
Phi(x) with Voltage 4
Capacity: 8.663127126064966e-06
Phi(x) with Voltage 5
Capacity: 8.663127126064956e-06