Propagation Matrix Method.

We know that the time independent Schrodinger equation is given by,

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + V(x)\phi(x) = E\phi(x).$$

It is the 1 dimensional, 2nd order differential equation, which can be rewritten as,

$$\frac{d^2}{dx^2}\phi(x) = -\frac{2m}{\hbar^2}\left[E - V(x)\right]\phi(x)$$

$$\frac{d^2}{dx^2}\phi(x) = -k^2(x)\,\phi(x)$$

where,

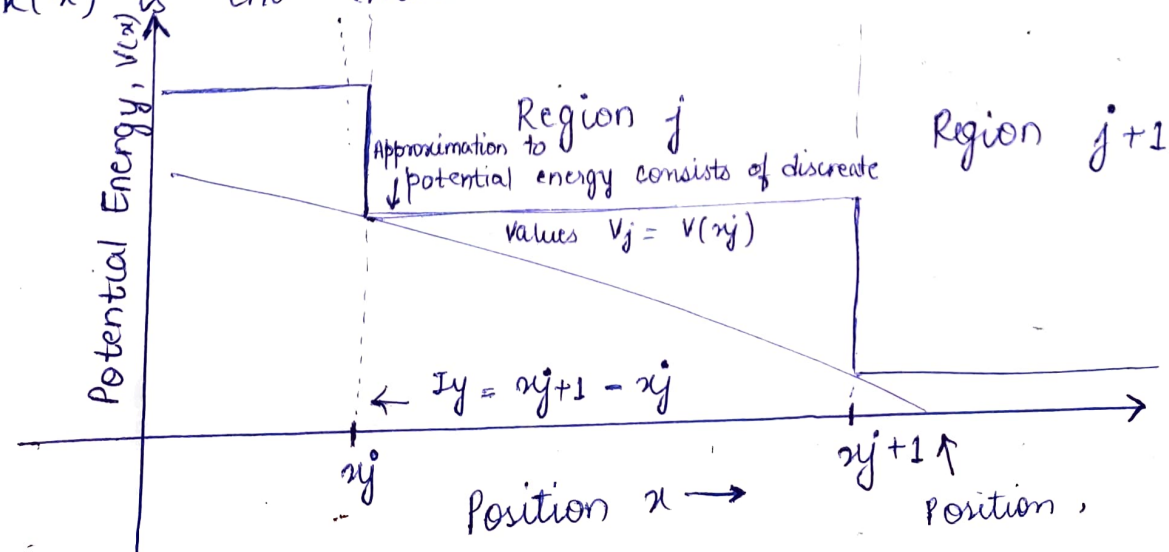
$$k = \sqrt{\frac{2m\left[E - V(x)\right]}{\hbar}}$$

, k is positive and definite

$$\phi(x) = A^r e^{ik(x)x} + A^l e^{-ik(x)x}.$$

where, amplitudes for left and right side are given by A^r and A^l.

$k(x)$ is the momentum.



① We will find Propogation between x_j and x_{j+1}

② What is the propogation across the step x_{j+1}.

Let us first propogator matrix for propagation between the potential step,

(1) Propagation between potential step separated by distanc L_j carries phase information only so that

$$A^r_j e^{ik_j L_j} = A^r_{j+1} \quad \text{and} \quad A^l_j e^{-ik_j L_j} = A^l_{j+1}.$$

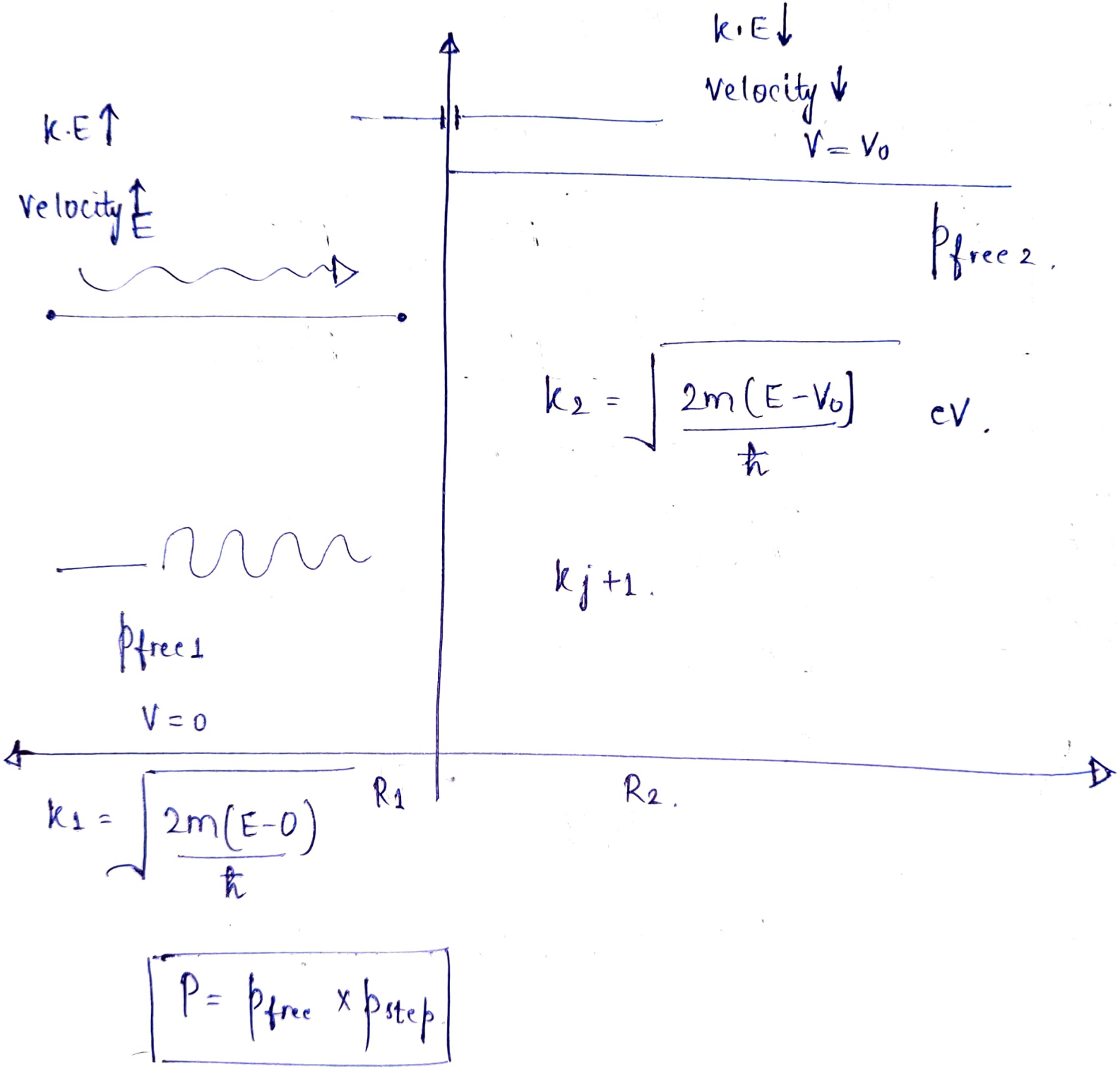
(2) This may be expressed in matrix form as,

$$\begin{bmatrix} e^{ik_j L_j} & 0 \\ 0 & e^{-ik_j L_j} \end{bmatrix} \begin{bmatrix} A^r_j \\ A^l_j \end{bmatrix} = \begin{bmatrix} A^r_{j+1} \\ A^l_{j+1} \end{bmatrix}.$$

(3) Which can be rewritten as:-

$$\begin{bmatrix} A^r_j \\ A^l_j \end{bmatrix} = P_{free} \begin{bmatrix} A^r_{j+1} \\ A^l_{j+1} \end{bmatrix}$$ where, P_{free} is the free propogation matrix, given by.

$$P_{free} = \begin{bmatrix} e^{-ik_j L_j} & 0 \\ 0 & e^{ik_j L_j} \end{bmatrix}$$



$$P = p_{free} \times p_{step}$$

Let us find propagator Matrix for propagation across the potential step →

(1) Propogation between potential step separated by distance l_j carries phase information only so that.

$$\phi_j = A^r_j e^{ik_j x} + A^l_j e^{-ik_j x} \quad \text{and} \quad \phi_{j+1} = A^r_{j+1} e^{ik_{j+1} x} + A^l_{j+1} e^{-ik_{j+1} x} \quad -(7)$$

(2) The boundary conditions $\phi_{j/j+1} = \phi_{j+1/j}$ and $\phi_{j/j+1} = \phi_{j+1/j+1}$ then gives;

$$A^r_j e^{ik_j x} + A^l_j e^{-ik_j x} = A^r_{j+1} e^{ik_{j+1} x} + A^l_{j+1} e^{-ik_{j+1} x}$$

$$A^r_j e^{ik_j x} - A^l_j e^{-ik_j x} = \frac{k_{j+1}}{k_j} A^r_{j+1} e^{ik_{j+1} x} - \frac{k_{j+1}}{k_j} A^l_{j+1} e^{-ik_{j+1} x} \quad -(9)$$

One may write Equations for a potential step at positions $x_{j+1} = 0$ as a matrix equation;

$$\begin{bmatrix} A^l_j \\ A^r_j \end{bmatrix} = P_{step} \begin{bmatrix} A^l_{j+1} \\ A^r_{j+1} \end{bmatrix}$$

$$\downarrow$$

$$P_{step} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_{j+1}}{k_j} & 1 - \frac{k_{j+1}}{k_j} \\ 1 - \frac{k_{j+1}}{k_j} & 1 + \frac{k_{j+1}}{k_j} \end{bmatrix} \quad -(10)$$

$$\begin{pmatrix} 1 \\ A^{l}_{in} \end{pmatrix} = p \begin{pmatrix} A^{r}_{out} \\ 0 \end{pmatrix}$$

Hence,

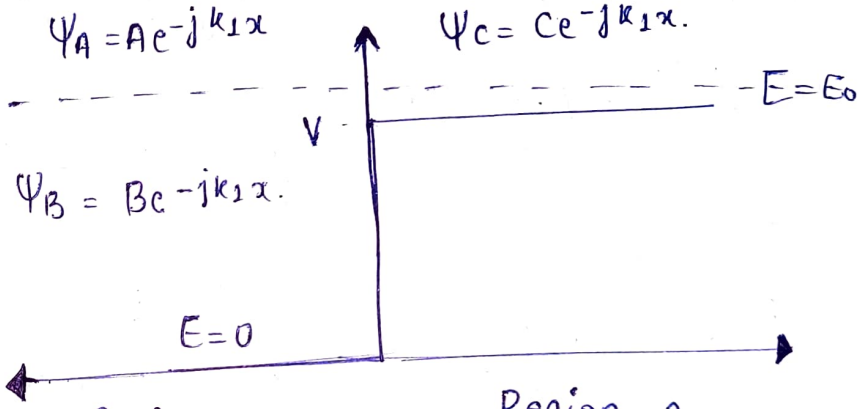
Transmission coefficient is given by A^{r}_{out} and Reflection coefficient is given by A^{l}_{in}.

Transmission Probability = $|A^{r}_{out}|^2$

Reflection Probability = $|A^{l}_{in}|^2$.

Now, Numerical Method for Solving the matrix:-

$E > V_0$



In Region 1 →

$$E_0 \psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

$$k_1^2 = \frac{2mE_0}{\hbar^2}$$

$$k_1 = \sqrt{\frac{2m(E_0 - V)}{\hbar^2}} \quad \text{where } \boxed{V = 0}$$

In Region 2 →

$$(E_0 - V)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \Rightarrow k_2 = \sqrt{\frac{2m(E_0 - V)}{\hbar^2}}.$$

$$\psi_1 = Ae^{-jk_1 x} + Be^{jk_1 x}$$

$$\psi_2 = Ce^{-jk_2 x}$$

ψ is continous

$$\psi_1(0) = \psi_2(0) \Rightarrow A + B = C$$

$\frac{\partial \psi}{\partial x}$ is continous : $\frac{\partial}{\partial x}\psi(0) = \frac{\partial}{\partial x}\psi_2(0) \Rightarrow A - B = \frac{k_2}{k_1} C$

$$\frac{B}{A} = \frac{1 - \frac{k_2}{k_1}}{1 + \frac{k_2}{k_1}} = \frac{k_1 - k_2}{k_1 + k_2}.$$

$$\frac{C}{A} = \frac{2}{1 + k_2/k_1} = \frac{2k_1}{2k_1 + k_2}.$$

$\Leftarrow$

$$\begin{cases} A + B = C \\ A - B = \frac{k_2}{k_1} C. \end{cases}$$

We know, the current density is given by

$$J = -\frac{ic\hbar}{2m}\left(\psi \Delta\psi^* - \psi^* \Delta\psi\right).$$

Electron velocity in the i^{th} region as $v_i = \frac{\hbar k_i}{m}$, transmission probability $|C|^2$ and Reflection probabilities $|B|^2$.

Now,

calculating the Transmission and Reflection Probabilities ;

$$|C|^2 = \frac{4}{\left(1 + \frac{k_2}{k_1}\right)^2} = \frac{4}{\left(1 + \frac{V_2}{V_1}\right)^2}$$

$$|C|^2 = \frac{4}{\left(1 + \frac{m_1 k_2}{m_2 k_1}\right)^2}$$

$$|B|^2 = \frac{\left(1 - k_2/k_1\right)^2}{\left(1 + k_2/k_1\right)^2}$$

Incident current is given by J_I,

The Reflected current,

$$\boxed{J_R = -\frac{e\hbar k_1}{m_1} |B|^2}$$

Transmitted Current is

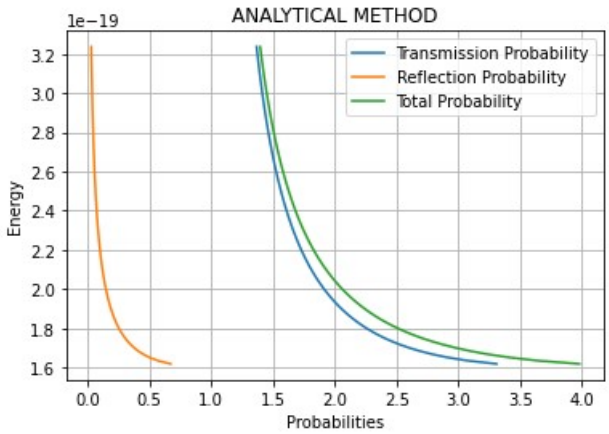
$$\boxed{J_T = \frac{e\hbar k_2}{m_2} |C|^2}$$

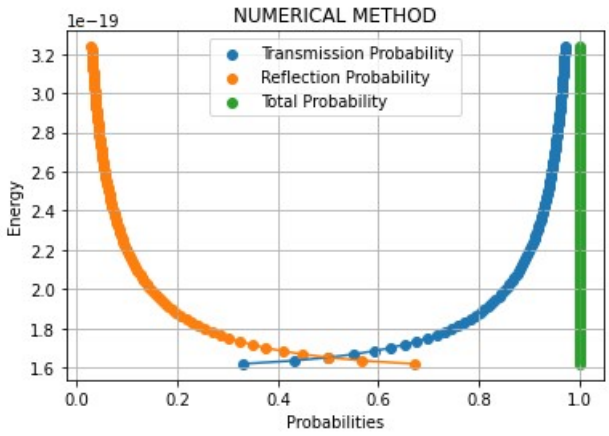
On Simplification,

$$\boxed{J_R = -\frac{e\hbar k_1}{m_1} \frac{\left(1 - \frac{k_2}{k_1}\right)^2}{\left(1 + k_2/k_1\right)^2}}$$

$$\boxed{J_T = +\frac{e\hbar k_2}{m_1} \times \frac{4}{\left(1 + \frac{k_2}{k_1}\right)^2}}$$

```
In [14]: runcell(0, 'C:/Users/hp/Desktop/QUANTUM PHYSICS/SEM
5 CODES/QM Assignment 2.py')
The value of P free : [[-0.6468455+0.76262107j  0.
+0.j         ]
 [ 0.        +0.j         -0.6468455-0.76262107j]]

The value of P step : [[0.54975186 0.45024814]
 [0.45024814 0.54975186]]

The value of P  : [[-0.35560452+0.41925235j
-0.29124098+0.34336872j]
 [-0.29124098-0.34336872j -0.35560452-0.41925235j]]

The value of Tranmission Coefficient :
(-1.1766135753070794-1.387209625188826j)

The value of Reflection Coefficient :
(-0.1336462966880234+0.8080245924721872j)

The value of Tranmission Probability : 3.3087700498134316

The value of Reflection Probability : 0.6707650746582673

The value of Transmission Probability : 0.3292349253417327

The value of Reflection Probability : 0.6707650746582673
```





	Energy	Trans Prob(An)	Refl Prob. (An)	Total Probability	Tran Prob.(Nu)	Ref. Prob. (Nu)	Total Prob.
0	1.618198e-19	3.308770	0.670765	3.979535	0.329235	0.670765	3.308770
1	1.634544e-19	3.073989	0.567430	3.641418	0.432570	0.567430	3.073989
2	1.650889e-19	2.913205	0.499582	3.412787	0.500418	0.499582	2.913205
3	1.667235e-19	2.789208	0.449023	3.238231	0.550977	0.449023	2.789208
4	1.683580e-19	2.687936	0.408951	3.096887	0.591049	0.408951	2.687936
5	1.699926e-19	2.602315	0.375976	2.978291	0.624024	0.375976	2.602315
6	1.716271e-19	2.528213	0.348142	2.876355	0.651858	0.348142	2.528213
7	1.732616e-19	2.462983	0.324204	2.787188	0.675796	0.324204	2.462983
8	1.748962e-19	2.404814	0.303321	2.708135	0.696679	0.303321	2.404814
9	1.765307e-19	2.352406	0.284895	2.637300	0.715105	0.284895	2.352406
10	1.781653e-19	2.304793	0.268484	2.573277	0.731516	0.268484	2.304793
11	1.797998e-19	2.261236	0.253755	2.514991	0.746245	0.253755	2.261236
12	1.814344e-19	2.221155	0.240447	2.461602	0.759553	0.240447	2.221155
13	1.830689e-19	2.184086	0.228355	2.412441	0.771645	0.228355	2.184086
14	1.847035e-19	2.149652	0.217314	2.366966	0.782686	0.217314	2.149652
15	1.863380e-19	2.117543	0.207187				

2.324730 0.792813 0.207187 2.117543
16 1.879725e-19 2.087498 0.197863
2.285361 0.802137 0.197863 2.087498
17 1.896071e-19 2.059301 0.189248
2.248549 0.810752 0.189248 2.059301
18 1.912416e-19 2.032764 0.181263
2.214027 0.818737 0.181263 2.032764
19 1.928762e-19 2.007727 0.173841
2.181568 0.826159 0.173841 2.007727
20 1.945107e-19 1.984052 0.166924
2.150977 0.833076 0.166924 1.984052
21 1.961453e-19 1.961619 0.160463
2.122082 0.839537 0.160463 1.961619
22 1.977798e-19 1.940323 0.154413
2.094736 0.845587 0.154413 1.940323
23 1.994143e-19 1.920069 0.148738
2.068807 0.851262 0.148738 1.920069
24 2.010489e-19 1.900776 0.143403
2.044180 0.856597 0.143403 1.900776
25 2.026834e-19 1.882371 0.138380
2.020751 0.861620 0.138380 1.882371
26 2.043180e-19 1.864787 0.133643
1.998430 0.866357 0.133643 1.864787
27 2.059525e-19 1.847967 0.129168
1.977135 0.870832 0.129168 1.847967
28 2.075871e-19 1.831857 0.124935
1.956792 0.875065 0.124935 1.831857
29 2.092216e-19 1.816410 0.120925
1.937334 0.879075 0.120925 1.816410
30 2.108562e-19 1.801581 0.117121
1.918702 0.882879 0.117121 1.801581
31 2.124907e-19 1.787332 0.113509
1.900842 0.886491 0.113509 1.787332
32 2.141252e-19 1.773627 0.110075
1.883702 0.889925 0.110075 1.773627
33 2.157598e-19 1.760433 0.106807
1.867240 0.893193 0.106807 1.760433
34 2.173943e-19 1.747719 0.103693
1.851412 0.896307 0.103693 1.747719
35 2.190289e-19 1.735459 0.100723
1.836181 0.899277 0.100723 1.735459
36 2.206634e-19 1.723626 0.097887
1.821513 0.902113 0.097887 1.723626
37 2.222980e-19 1.712198 0.095178

```
1.807376        0.904822        0.095178    1.712198
38  2.239325e-19        1.701152        0.092588
1.793739        0.907412        0.092588    1.701152
39  2.255670e-19        1.690468        0.090108
1.780576        0.909892        0.090108    1.690468
40  2.272016e-19        1.680128        0.087733
1.767861        0.912267        0.087733    1.680128
41  2.288361e-19        1.670114        0.085456
1.755571        0.914544        0.085456    1.670114
42  2.304707e-19        1.660411        0.083272
1.743684        0.916728        0.083272    1.660411
43  2.321052e-19        1.651003        0.081176
1.732179        0.918824        0.081176    1.651003
44  2.337398e-19        1.641877        0.079162
1.721039        0.920838        0.079162    1.641877
45  2.353743e-19        1.633018        0.077226
1.710245        0.922774        0.077226    1.633018
46  2.370089e-19        1.624416        0.075364
1.699780        0.924636        0.075364    1.624416
47  2.386434e-19        1.616058        0.073573
1.689630        0.926427        0.073573    1.616058
48  2.402779e-19        1.607933        0.071847
1.679780        0.928153        0.071847    1.607933
49  2.419125e-19        1.600032        0.070185
1.670216        0.929815        0.070185    1.600032
50  2.435470e-19        1.592345        0.068582
1.660926        0.931418        0.068582    1.592345
51  2.451816e-19        1.584862        0.067036
1.651898        0.932964        0.067036    1.584862
52  2.468161e-19        1.577576        0.065544
1.643121        0.934456        0.065544    1.577576
53  2.484507e-19        1.570479        0.064104
1.634583        0.935896        0.064104    1.570479
54  2.500852e-19        1.563563        0.062713
1.626275        0.937287        0.062713    1.563563
55  2.517198e-19        1.556820        0.061368
1.618188        0.938632        0.061368    1.556820
56  2.533543e-19        1.550245        0.060068
1.610313        0.939932        0.060068    1.550245
57  2.549888e-19        1.543830        0.058811
1.602640        0.941189        0.058811    1.543830
58  2.566234e-19        1.537569        0.057594
1.595163        0.942406        0.057594    1.537569
59  2.582579e-19        1.531458        0.056416
```

```
1.587874        0.943584        0.056416    1.531458
60  2.598925e-19        1.525490        0.055275
1.580765        0.944725        0.055275    1.525490
61  2.615270e-19        1.519660        0.054170
1.573830        0.945830        0.054170    1.519660
62  2.631616e-19        1.513964        0.053099
1.567063        0.946901        0.053099    1.513964
63  2.647961e-19        1.508396        0.052060
1.560456        0.947940        0.052060    1.508396
64  2.664306e-19        1.502952        0.051053
1.554005        0.948947        0.051053    1.502952
65  2.680652e-19        1.497628        0.050076
1.547704        0.949924        0.050076    1.497628
66  2.696997e-19        1.492420        0.049127
1.541548        0.950873        0.049127    1.492420
67  2.713343e-19        1.487324        0.048206
1.535531        0.951794        0.048206    1.487324
68  2.729688e-19        1.482337        0.047312
1.529648        0.952688        0.047312    1.482337
69  2.746034e-19        1.477454        0.046443
1.523896        0.953557        0.046443    1.477454
70  2.762379e-19        1.472672        0.045598
1.518270        0.954402        0.045598    1.472672
71  2.778725e-19        1.467989        0.044777
1.512766        0.955223        0.044777    1.467989
72  2.795070e-19        1.463400        0.043979
1.507379        0.956021        0.043979    1.463400
73  2.811415e-19        1.458904        0.043202
1.502106        0.956798        0.043202    1.458904
74  2.827761e-19        1.454497        0.042446
1.496943        0.957554        0.042446    1.454497
75  2.844106e-19        1.450177        0.041711
1.491888        0.958289        0.041711    1.450177
76  2.860452e-19        1.445940        0.040995
1.486935        0.959005        0.040995    1.445940
77  2.876797e-19        1.441785        0.040298
1.482083        0.959702        0.040298    1.441785
78  2.893143e-19        1.437709        0.039619
1.477328        0.960381        0.039619    1.437709
79  2.909488e-19        1.433710        0.038957
1.472668        0.961043        0.038957    1.433710
80  2.925833e-19        1.429786        0.038313
1.468098        0.961687        0.038313    1.429786
81  2.942179e-19        1.425934        0.037684
```

```
1.463618        0.962316         0.037684     1.425934
82  2.958524e-19        1.422152         0.037072
1.459224        0.962928         0.037072     1.422152
83  2.974870e-19        1.418439         0.036474
1.454913        0.963526         0.036474     1.418439
84  2.991215e-19        1.414792         0.035891
1.450684        0.964109         0.035891     1.414792
85  3.007561e-19        1.411210         0.035323
1.446533        0.964677         0.035323     1.411210
86  3.023906e-19        1.407691         0.034768
1.442459        0.965232         0.034768     1.407691
87  3.040252e-19        1.404234         0.034226
1.438460        0.965774         0.034226     1.404234
88  3.056597e-19        1.400836         0.033698
1.434533        0.966302         0.033698     1.400836
89  3.072942e-19        1.397496         0.033181
1.430677        0.966819         0.033181     1.397496
90  3.089288e-19        1.394213         0.032677
1.426890        0.967323         0.032677     1.394213
91  3.105633e-19        1.390984         0.032184
1.423169        0.967816         0.032184     1.390984
92  3.121979e-19        1.387810         0.031703
1.419513        0.968297         0.031703     1.387810
93  3.138324e-19        1.384688         0.031233
1.415921        0.968767         0.031233     1.384688
94  3.154670e-19        1.381617         0.030773
1.412390        0.969227         0.030773     1.381617
95  3.171015e-19        1.378596         0.030323
1.408919        0.969677         0.030323     1.378596
96  3.187360e-19        1.375623         0.029884
1.405507        0.970116         0.029884     1.375623
97  3.203706e-19        1.372698         0.029454
1.402152        0.970546         0.029454     1.372698
98  3.220051e-19        1.369819         0.029034
1.398852        0.970966         0.029034     1.369819
99  3.236397e-19        1.366985         0.028622
1.395607        0.971378         0.028622     1.366985
```

In [**15**]: