

```
In[*]:= ClearAll["Global`*"]
```

```
In[*]:= Table[{R, NIntegrate[8 /  $\pi$  r Exp[-2 r] Exp[-2 r Sqrt[1 + (R / r) ^ 2 - 2 R / r Cos[ $\phi$ ]]],  
  { $\phi$ , 0, 2 Pi}}, {r, 0,  $\infty$ ]], {R, 0, 10, 0.1}]  
S = Interpolation[%]
```

... **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

... **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

... **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

... **General:** Further output of NIntegrate::slwcon will be suppressed during this calculation. [i](#)

```
Out[*]=
```

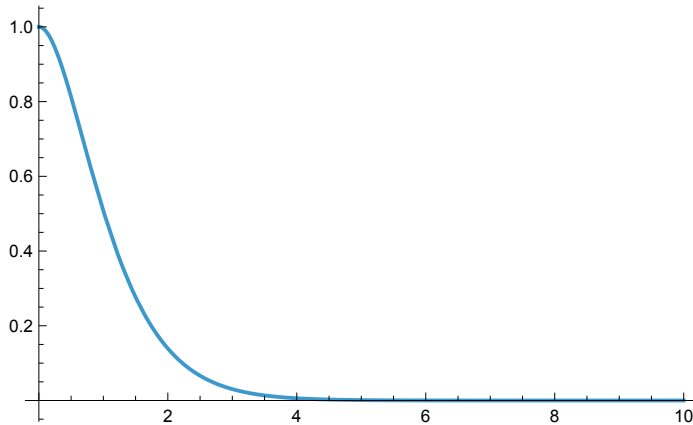
```
{ {0., 1.}, {0.1, 0.990248}, {0.2, 0.962904}, {0.3, 0.921655}, {0.4, 0.870336},  
  {0.5, 0.812419}, {0.6, 0.750837}, {0.7, 0.687952}, {0.8, 0.625596}, {0.9, 0.56513},  
  {1., 0.507519}, {1.1, 0.453404}, {1.2, 0.403166}, {1.3, 0.356985}, {1.4, 0.31489},  
  {1.5, 0.276797}, {1.6, 0.242544}, {1.7, 0.211914}, {1.8, 0.18466}, {1.9, 0.160515},  
  {2., 0.139211}, {2.1, 0.120481}, {2.2, 0.104066}, {2.3, 0.0897231}, {2.4, 0.0772251},  
  {2.5, 0.0663618}, {2.6, 0.0569411}, {2.7, 0.0487887}, {2.8, 0.0417481},  
  {2.9, 0.0356786}, {3., 0.0304554}, {3.1, 0.0259677}, {3.2, 0.0221177},  
  {3.3, 0.0188196}, {3.4, 0.0159978}, {3.5, 0.0135868}, {3.6, 0.0115291},  
  {3.7, 0.00977486}, {3.8, 0.00828101}, {3.9, 0.00701014}, {4., 0.00593002},  
  {4.1, 0.00501284}, {4.2, 0.0042347}, {4.3, 0.00357507}, {4.4, 0.00301633},  
  {4.5, 0.00254343}, {4.6, 0.00214345}, {4.7, 0.00180539}, {4.8, 0.00151985},  
  {4.9, 0.00127882}, {5., 0.00107549}, {5.1, 0.000904066}, {5.2, 0.000759619},  
  {5.3, 0.000637971}, {5.4, 0.000535577}, {5.5, 0.000449432}, {5.6, 0.000376994},  
  {5.7, 0.000316109}, {5.8, 0.000264958}, {5.9, 0.000222004}, {6., 0.000185949},  
  {6.1, 0.000155696}, {6.2, 0.000130322}, {6.3, 0.000109048}, {6.4, 0.0000912189},  
  {6.5, 0.0000762816}, {6.6, 0.0000637715}, {6.7, 0.0000532978}, {6.8, 0.0000445319},  
  {6.9, 0.0000371977}, {7., 0.0000310631}, {7.1, 0.0000259336}, {7.2, 0.0000216457},  
  {7.3, 0.0000180624}, {7.4, 0.0000150687}, {7.5, 0.0000125682}, {7.6, 0.0000104803},  
  {7.7,  $8.73735 \times 10^{-6}$ }, {7.8,  $7.28268 \times 10^{-6}$ }, {7.9,  $6.06891 \times 10^{-6}$ }, {8.,  $5.05639 \times 10^{-6}$ },  
  {8.1,  $4.21195 \times 10^{-6}$ }, {8.2,  $3.50785 \times 10^{-6}$ }, {8.3,  $2.92089 \times 10^{-6}$ }, {8.4,  $2.43169 \times 10^{-6}$ },  
  {8.5,  $2.02405 \times 10^{-6}$ }, {8.6,  $1.68444 \times 10^{-6}$ }, {8.7,  $1.40157 \times 10^{-6}$ }, {8.8,  $1.166 \times 10^{-6}$ },  
  {8.9,  $9.69859 \times 10^{-7}$ }, {9.,  $8.06581 \times 10^{-7}$ }, {9.1,  $6.70682 \times 10^{-7}$ }, {9.2,  $5.57592 \times 10^{-7}$ },  
  {9.3,  $4.635 \times 10^{-7}$ }, {9.4,  $3.85227 \times 10^{-7}$ }, {9.5,  $3.20124 \times 10^{-7}$ }, {9.6,  $2.65985 \times 10^{-7}$ },  
  {9.7,  $2.2097 \times 10^{-7}$ }, {9.8,  $1.83548 \times 10^{-7}$ }, {9.9,  $1.52442 \times 10^{-7}$ }, {10.,  $1.26591 \times 10^{-7}$ }}
```

```
Out[*]=
```

```
InterpolatingFunction[ Domain: {{0., 10.}}  
Output: scalar]
```

```
In[ ]:= Plot[S[R], {R, 0, 10}, PlotRange -> All]
```

```
Out[ ]:=
```



```
In[ ]:=  $\psi g[r\_ , R\_ ] := 1 / \text{Sqrt}[2 (1 + S[R])] \times 4 / \text{Sqrt}[2 \pi]$   

 $\left( \text{Exp}\left[-2 \sqrt{r^2 + R^2 / 4 - r R \cos[\phi]}\right] + \text{Exp}\left[-2 \sqrt{r^2 + R^2 / 4 + r R \cos[\phi]}\right] \right)$ 
```

```
In[ ]:=  $\psi g\text{shift}[r\_ , R\_ ] :=$   

 $1 / \text{Sqrt}[2 (1 + S[R])] \times 4 / \text{Sqrt}[2 \pi] \left( \text{Exp}[-2 r] + \text{Exp}\left[-2 \sqrt{r^2 + R^2 + 2 r R \cos[\phi]}\right] \right)$ 
```

Check normalization

```
In[ ]:= Table[NIntegrate[r  $\psi g[r, R]^2$ , { $\phi$ , 0, 2  $\pi$ }, {r, 0, 10}], {R, 0, 10}]  

Table[NIntegrate[r  $\psi g\text{shift}[r, R]^2$ , { $\phi$ , 0, 2  $\pi$ }, {r, 0, 20}], {R, 0, 10}]
```

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

General: Further output of NIntegrate::slwcon will be suppressed during this calculation. [i](#)

```
Out[ ]:=
```

```
{1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.}
```

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

General: Further output of NIntegrate::slwcon will be suppressed during this calculation. [i](#)

```
Out[ ]:=
```

```
{1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.}
```

```
In[*]:= Vmean = Table[
  {R, 1/R - 2 NIntegrate[  $\psi$ gshift[r, R]^2, { $\phi$ , 0, 2  $\pi$ }, {r, 0, 30}]}, {R, 0.2, 15, 0.1}]
```

... **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

... **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

... **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

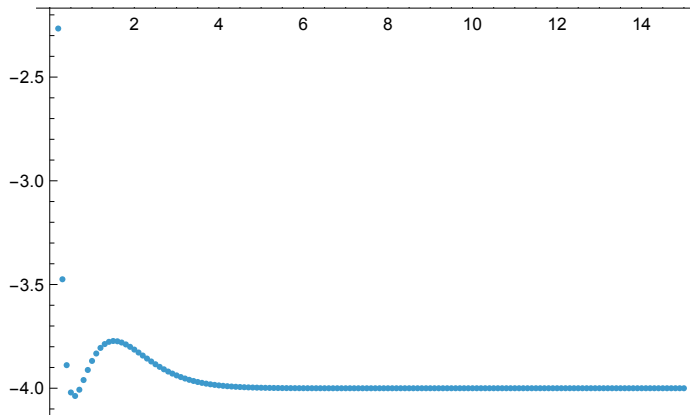
... **General:** Further output of NIntegrate::slwcon will be suppressed during this calculation. [i](#)

```
Out[8]=
```

```
{ {0.2, -2.2659}, {0.3, -3.47477}, {0.4, -3.8888}, {0.5, -4.02051}, {0.6, -4.03737},
  {0.7, -4.00717}, {0.8, -3.96055}, {0.9, -3.91202}, {1., -3.86842}, {1.1, -3.83266},
  {1.2, -3.80564}, {1.3, -3.78714}, {1.4, -3.77637}, {1.5, -3.77228},
  {1.6, -3.77374}, {1.7, -3.77961}, {1.8, -3.78885}, {1.9, -3.8005}, {2., -3.81375},
  {2.1, -3.82793}, {2.2, -3.84247}, {2.3, -3.85694}, {2.4, -3.87102},
  {2.5, -3.88445}, {2.6, -3.89708}, {2.7, -3.90881}, {2.8, -3.91958},
  {2.9, -3.92939}, {3., -3.93825}, {3.1, -3.94619}, {3.2, -3.95327}, {3.3, -3.95955},
  {3.4, -3.96509}, {3.5, -3.96995}, {3.6, -3.97421}, {3.7, -3.97793},
  {3.8, -3.98115}, {3.9, -3.98395}, {4., -3.98636}, {4.1, -3.98845}, {4.2, -3.99024},
  {4.3, -3.99177}, {4.4, -3.99308}, {4.5, -3.99421}, {4.6, -3.99516},
  {4.7, -3.99598}, {4.8, -3.99667}, {4.9, -3.99725}, {5., -3.99775}, {5.1, -3.99817},
  {5.2, -3.99852}, {5.3, -3.99882}, {5.4, -3.99906}, {5.5, -3.99927}, {5.6, -3.99945},
  {5.7, -3.99959}, {5.8, -3.99971}, {5.9, -3.99981}, {6., -3.99989}, {6.1, -3.99996},
  {6.2, -4.00001}, {6.3, -4.00005}, {6.4, -4.00009}, {6.5, -4.00012},
  {6.6, -4.00014}, {6.7, -4.00015}, {6.8, -4.00016}, {6.9, -4.00017}, {7., -4.00018},
  {7.1, -4.00014}, {7.2, -4.00018}, {7.3, -4.00018}, {7.4, -4.00019}, {7.5, -4.00019},
  {7.6, -4.00018}, {7.7, -4.00018}, {7.8, -4.00018}, {7.9, -4.00017}, {8., -4.00017},
  {8.1, -4.00016}, {8.2, -4.00016}, {8.3, -4.00016}, {8.4, -4.00015},
  {8.5, -4.00015}, {8.6, -4.00014}, {8.7, -4.00014}, {8.8, -4.00014},
  {8.9, -4.00013}, {9., -4.00013}, {9.1, -4.00012}, {9.2, -4.00012}, {9.3, -4.00012},
  {9.4, -4.00011}, {9.5, -4.00011}, {9.6, -4.00011}, {9.7, -4.0001}, {9.8, -4.0001},
  {9.9, -4.0001}, {10., -4.00009}, {10.1, -4.00009}, {10.2, -4.00009},
  {10.3, -4.00009}, {10.4, -4.00008}, {10.5, -4.00008}, {10.6, -4.00008},
  {10.7, -4.00008}, {10.8, -4.00008}, {10.9, -4.00008}, {11., -4.00007},
  {11.1, -4.00007}, {11.2, -4.00007}, {11.3, -4.00007}, {11.4, -4.00006},
  {11.5, -4.00006}, {11.6, -4.00006}, {11.7, -4.00006}, {11.8, -4.00006},
  {11.9, -4.00006}, {12., -4.00006}, {12.1, -4.00006}, {12.2, -4.00006},
  {12.3, -4.00006}, {12.4, -4.00006}, {12.5, -4.00006}, {12.6, -4.00006},
  {12.7, -4.00006}, {12.8, -4.00006}, {12.9, -4.00006}, {13., -4.00006},
  {13.1, -4.00006}, {13.2, -4.00006}, {13.3, -4.00006}, {13.4, -4.00006},
  {13.5, -4.00006}, {13.6, -4.00007}, {13.7, -4.00007}, {13.8, -4.00007},
  {13.9, -4.00007}, {14., -4.00007}, {14.1, -4.00007}, {14.2, -4.00007},
  {14.3, -4.00008}, {14.4, -4.00008}, {14.5, -4.00008}, {14.6, -4.00009},
  {14.7, -4.00009}, {14.8, -4.00009}, {14.9, -4.0001}, {15., -4.0001} }
```

```
In[ ]:= ListPlot[Vmean, PlotRange -> All]
```

```
Out[ ]:=
```



```
In[ ]:= KE1 =
```

```
Table[{R, NIntegrate[ψgshift[r, R]^2, {φ, 0, 2 π}, {r, 0, 30}]}, {R, 0.2, 15, 0.1}]
```

```
KE2 =
```

```
Table[{R, NIntegrate[1 / r Cos[φ] R / 2 ψgshift[r, R]^2, {φ, 0, 2 π}, {r, 0.00001, 30}]}, {R, 0.2, 15, 0.1}]
```

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

General: Further output of NIntegrate::slwcon will be suppressed during this calculation. [i](#)

Out[*n*]=

```
{ {0.2, 3.63295}, {0.3, 3.40405}, {0.4, 3.1944}, {0.5, 3.01026}, {0.6, 2.85202},
  {0.7, 2.71787}, {0.8, 2.60528}, {0.9, 2.51157}, {1., 2.43421}, {1.1, 2.37088},
  {1.2, 2.31949}, {1.3, 2.27818}, {1.4, 2.24533}, {1.5, 2.21948}, {1.6, 2.19937},
  {1.7, 2.18392}, {1.8, 2.1722}, {1.9, 2.16341}, {2., 2.15688}, {2.1, 2.15206},
  {2.2, 2.14851}, {2.3, 2.14586}, {2.4, 2.14384}, {2.5, 2.14223}, {2.6, 2.14085},
  {2.7, 2.13959}, {2.8, 2.13836}, {2.9, 2.13711}, {3., 2.13579}, {3.1, 2.13439},
  {3.2, 2.13289}, {3.3, 2.13129}, {3.4, 2.12961}, {3.5, 2.12783}, {3.6, 2.12599},
  {3.7, 2.1241}, {3.8, 2.12215}, {3.9, 2.12018}, {4., 2.11818}, {4.1, 2.11617},
  {4.2, 2.11417}, {4.3, 2.11216}, {4.4, 2.11018}, {4.5, 2.10821}, {4.6, 2.10628},
  {4.7, 2.10437}, {4.8, 2.1025}, {4.9, 2.10067}, {5., 2.09888}, {5.1, 2.09712},
  {5.2, 2.09541}, {5.3, 2.09375}, {5.4, 2.09212}, {5.5, 2.09055}, {5.6, 2.08901},
  {5.7, 2.08751}, {5.8, 2.08606}, {5.9, 2.08465}, {6., 2.08328}, {6.1, 2.08195},
  {6.2, 2.08065}, {6.3, 2.07939}, {6.4, 2.07817}, {6.5, 2.07698}, {6.6, 2.07583},
  {6.7, 2.0747}, {6.8, 2.07361}, {6.9, 2.07255}, {7., 2.07152}, {7.1, 2.07049},
  {7.2, 2.06954}, {7.3, 2.06858}, {7.4, 2.06766}, {7.5, 2.06676}, {7.6, 2.06588},
  {7.7, 2.06503}, {7.8, 2.06419}, {7.9, 2.06338}, {8., 2.06259}, {8.1, 2.06181},
  {8.2, 2.06106}, {8.3, 2.06032}, {8.4, 2.0596}, {8.5, 2.0589}, {8.6, 2.05821},
  {8.7, 2.05754}, {8.8, 2.05689}, {8.9, 2.05625}, {9., 2.05562}, {9.1, 2.05501},
  {9.2, 2.05441}, {9.3, 2.05382}, {9.4, 2.05325}, {9.5, 2.05269}, {9.6, 2.05214},
  {9.7, 2.0516}, {9.8, 2.05107}, {9.9, 2.05056}, {10., 2.05005}, {10.1, 2.04955},
  {10.2, 2.04906}, {10.3, 2.04859}, {10.4, 2.04812}, {10.5, 2.04766}, {10.6, 2.04721},
  {10.7, 2.04677}, {10.8, 2.04634}, {10.9, 2.04591}, {11., 2.04549}, {11.1, 2.04508},
  {11.2, 2.04468}, {11.3, 2.04428}, {11.4, 2.04389}, {11.5, 2.04351}, {11.6, 2.04314},
  {11.7, 2.04277}, {11.8, 2.0424}, {11.9, 2.04205}, {12., 2.0417}, {12.1, 2.04135},
  {12.2, 2.04101}, {12.3, 2.04068}, {12.4, 2.04035}, {12.5, 2.04003},
  {12.6, 2.03971}, {12.7, 2.0394}, {12.8, 2.03909}, {12.9, 2.03879}, {13., 2.03849},
  {13.1, 2.0382}, {13.2, 2.03791}, {13.3, 2.03762}, {13.4, 2.03734}, {13.5, 2.03707},
  {13.6, 2.0368}, {13.7, 2.03653}, {13.8, 2.03626}, {13.9, 2.03601}, {14., 2.03575},
  {14.1, 2.0355}, {14.2, 2.03525}, {14.3, 2.035}, {14.4, 2.03476}, {14.5, 2.03452},
  {14.6, 2.03429}, {14.7, 2.03406}, {14.8, 2.03383}, {14.9, 2.03361}, {15., 2.03338}}
```

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

General: Further output of NIntegrate::slwcon will be suppressed during this calculation. [i](#)

Out[8]=

```
{ {0.2, -0.24823}, {0.3, -0.365647}, {0.4, -0.451311}, {0.5, -0.508232},
  {0.6, -0.541688}, {0.7, -0.556832}, {0.8, -0.558054}, {0.9, -0.548908},
  {1., -0.532215}, {1.1, -0.510198}, {1.2, -0.48461}, {1.3, -0.456828},
  {1.4, -0.427938}, {1.5, -0.398783}, {1.6, -0.370017}, {1.7, -0.342132},
  {1.8, -0.315487}, {1.9, -0.290332}, {2., -0.266822}, {2.1, -0.245041},
  {2.2, -0.225011}, {2.3, -0.206711}, {2.4, -0.190082}, {2.5, -0.17504},
  {2.6, -0.161487}, {2.7, -0.149314}, {2.8, -0.138407}, {2.9, -0.128653},
  {3., -0.11994}, {3.1, -0.112162}, {3.2, -0.105222}, {3.3, -0.0990259},
  {3.4, -0.0934906}, {3.5, -0.0885395}, {3.6, -0.0841039}, {3.7, -0.0801223},
  {3.8, -0.07654}, {3.9, -0.0733087}, {4., -0.0703857}, {4.1, -0.0677335},
  {4.2, -0.0653192}, {4.3, -0.063114}, {4.4, -0.061093}, {4.5, -0.0592342},
  {4.6, -0.0575187}, {4.7, -0.0559298}, {4.8, -0.0544531}, {4.9, -0.0530762},
  {5., -0.0517882}, {5.1, -0.0505796}, {5.2, -0.0494421}, {5.3, -0.0483685},
  {5.4, -0.0473527}, {5.5, -0.0463891}, {5.6, -0.0454729}, {5.7, -0.0445999},
  {5.8, -0.0437664}, {5.9, -0.0429692}, {6., -0.0422053}, {6.1, -0.0414723},
  {6.2, -0.0407679}, {6.3, -0.04009}, {6.4, -0.0394368}, {6.5, -0.0388068},
  {6.6, -0.0381984}, {6.7, -0.0376104}, {6.8, -0.0370416}, {6.9, -0.0364909},
  {7., -0.0359572}, {7.1, -0.0354398}, {7.2, -0.0349378}, {7.3, -0.0344504},
  {7.4, -0.0339769}, {7.5, -0.0335167}, {7.6, -0.0330692}, {7.7, -0.0326338},
  {7.8, -0.0322099}, {7.9, -0.0317972}, {8., -0.0313951}, {8.1, -0.0310033},
  {8.2, -0.0306212}, {8.3, -0.0302486}, {8.4, -0.029885}, {8.5, -0.0295302},
  {8.6, -0.0291838}, {8.7, -0.0288455}, {8.8, -0.0285151}, {8.9, -0.0281921},
  {9., -0.0278765}, {9.1, -0.0275679}, {9.2, -0.0272661}, {9.3, -0.0269708},
  {9.4, -0.0266819}, {9.5, -0.0263992}, {9.6, -0.0261224}, {9.7, -0.0258514},
  {9.8, -0.025586}, {9.9, -0.025326}, {10., -0.0250713}, {10.1, -0.0248216},
  {10.2, -0.0245769}, {10.3, -0.024337}, {10.4, -0.0241017}, {10.5, -0.023871},
  {10.6, -0.0236446}, {10.7, -0.0234225}, {10.8, -0.0232046},
  {10.9, -0.0229906}, {11., -0.0227806}, {11.1, -0.0225745}, {11.2, -0.022372},
  {11.3, -0.0221731}, {11.4, -0.0219777}, {11.5, -0.0217859},
  {11.6, -0.0215972}, {11.7, -0.0214118}, {11.8, -0.0212296},
  {11.9, -0.0210505}, {12., -0.0208744}, {12.1, -0.0207012}, {12.2, -0.0205309},
  {12.3, -0.0203633}, {12.4, -0.0201985}, {12.5, -0.0200363}, {12.6, -0.0198767},
  {12.7, -0.0197197}, {12.8, -0.0195651}, {12.9, -0.0194129}, {13., -0.0192631},
  {13.1, -0.0191155}, {13.2, -0.0189703}, {13.3, -0.0188272}, {13.4, -0.0186862},
  {13.5, -0.0185474}, {13.6, -0.0184106}, {13.7, -0.0182758}, {13.8, -0.018143},
  {13.9, -0.0180121}, {14., -0.0178831}, {14.1, -0.0177559}, {14.2, -0.0176305},
  {14.3, -0.0175069}, {14.4, -0.017385}, {14.5, -0.0172648}, {14.6, -0.0171462},
  {14.7, -0.0170293}, {14.8, -0.016914}, {14.9, -0.0168002}, {15., -0.0166879}}
```

```

In[*]:= Dimensions[KE1]
Dimensions[KE2]
Dimensions[Vmean]

Out[*]=
{149, 2}

Out[*]=
{149, 2}

Out[*]=
{149, 2}

In[*]:= KE = Table[{KE1[[i, 1]], KE1[[i, 2]] + KE2[[i, 2]]}, {i, 1, 119}]

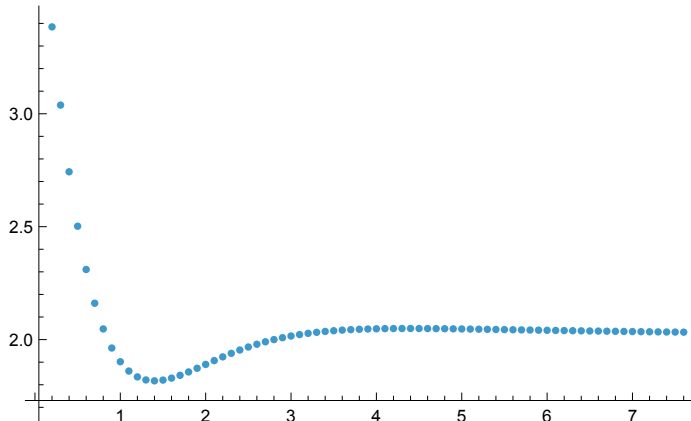
Out[*]=
{{0.2, 3.38472}, {0.3, 3.03841}, {0.4, 2.74309}, {0.5, 2.50202}, {0.6, 2.31033},
{0.7, 2.16104}, {0.8, 2.04722}, {0.9, 1.96266}, {1., 1.90199}, {1.1, 1.86068},
{1.2, 1.83488}, {1.3, 1.82136}, {1.4, 1.81739}, {1.5, 1.82069}, {1.6, 1.82935},
{1.7, 1.84179}, {1.8, 1.85671}, {1.9, 1.87307}, {2., 1.89005}, {2.1, 1.90702},
{2.2, 1.9235}, {2.3, 1.93915}, {2.4, 1.95376}, {2.5, 1.96719}, {2.6, 1.97936},
{2.7, 1.99028}, {2.8, 1.99996}, {2.9, 2.00846}, {3., 2.01585}, {3.1, 2.02222},
{3.2, 2.02766}, {3.3, 2.03226}, {3.4, 2.03612}, {3.5, 2.03929}, {3.6, 2.04189},
{3.7, 2.04398}, {3.8, 2.04561}, {3.9, 2.04687}, {4., 2.04779}, {4.1, 2.04844},
{4.2, 2.04885}, {4.3, 2.04905}, {4.4, 2.04909}, {4.5, 2.04898}, {4.6, 2.04876},
{4.7, 2.04844}, {4.8, 2.04805}, {4.9, 2.04759}, {5., 2.04709}, {5.1, 2.04654},
{5.2, 2.04597}, {5.3, 2.04538}, {5.4, 2.04477}, {5.5, 2.04416}, {5.6, 2.04354},
{5.7, 2.04291}, {5.8, 2.0423}, {5.9, 2.04168}, {6., 2.04107}, {6.1, 2.04047},
{6.2, 2.03988}, {6.3, 2.0393}, {6.4, 2.03873}, {6.5, 2.03817}, {6.6, 2.03763},
{6.7, 2.03709}, {6.8, 2.03657}, {6.9, 2.03606}, {7., 2.03556}, {7.1, 2.03505},
{7.2, 2.0346}, {7.3, 2.03413}, {7.4, 2.03368}, {7.5, 2.03324}, {7.6, 2.03281},
{7.7, 2.03239}, {7.8, 2.03198}, {7.9, 2.03158}, {8., 2.03119}, {8.1, 2.03081},
{8.2, 2.03043}, {8.3, 2.03007}, {8.4, 2.02971}, {8.5, 2.02937}, {8.6, 2.02903},
{8.7, 2.0287}, {8.8, 2.02837}, {8.9, 2.02805}, {9., 2.02774}, {9.1, 2.02744},
{9.2, 2.02714}, {9.3, 2.02685}, {9.4, 2.02657}, {9.5, 2.02629}, {9.6, 2.02601},
{9.7, 2.02575}, {9.8, 2.02549}, {9.9, 2.02523}, {10., 2.02498}, {10.1, 2.02473},
{10.2, 2.02449}, {10.3, 2.02425}, {10.4, 2.02402}, {10.5, 2.02379},
{10.6, 2.02356}, {10.7, 2.02335}, {10.8, 2.02313}, {10.9, 2.02292}, {11., 2.02271},
{11.1, 2.0225}, {11.2, 2.02231}, {11.3, 2.02211}, {11.4, 2.02191}, {11.5, 2.02172},
{11.6, 2.02154}, {11.7, 2.02135}, {11.8, 2.02117}, {11.9, 2.021}, {12., 2.02082}}

```



```
In[*]:= ListPlot[KE, PlotRange -> All]
```

```
Out[*]:=
```



```
In[*]:= Vg = Table[{KE1[[i, 1]], Vmean[[i, 2]] + KE[[i, 2]]}, {i, 1, 119}]
```

```
Out[*]:=
```

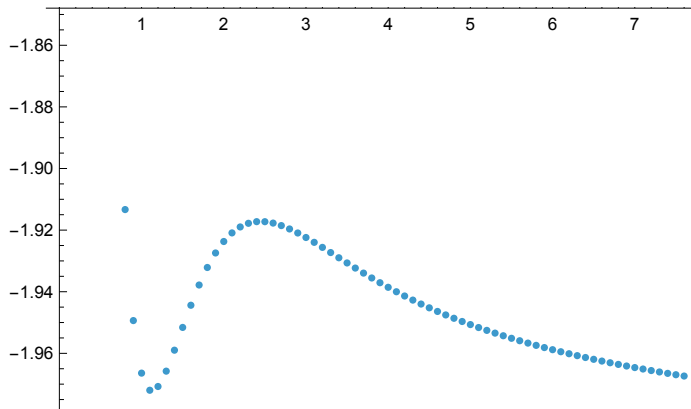
```
{ {0.2, 1.11882}, {0.3, -0.436367}, {0.4, -1.14571}, {0.5, -1.51849}, {0.6, -1.72704},
  {0.7, -1.84613}, {0.8, -1.91333}, {0.9, -1.94936}, {1., -1.96642}, {1.1, -1.97198},
  {1.2, -1.97076}, {1.3, -1.96578}, {1.4, -1.95898}, {1.5, -1.95159}, {1.6, -1.94439},
  {1.7, -1.93782}, {1.8, -1.93213}, {1.9, -1.92742}, {2., -1.9237}, {2.1, -1.92091},
  {2.2, -1.91897}, {2.3, -1.91779}, {2.4, -1.91726}, {2.5, -1.91727},
  {2.6, -1.91772}, {2.7, -1.91853}, {2.8, -1.91963}, {2.9, -1.92093}, {3., -1.9224},
  {3.1, -1.92397}, {3.2, -1.92561}, {3.3, -1.92729}, {3.4, -1.92898},
  {3.5, -1.93066}, {3.6, -1.93232}, {3.7, -1.93395}, {3.8, -1.93554},
  {3.9, -1.93708}, {4., -1.93856}, {4.1, -1.94}, {4.2, -1.94139}, {4.3, -1.94272},
  {4.4, -1.944}, {4.5, -1.94523}, {4.6, -1.9464}, {4.7, -1.94754}, {4.8, -1.94862},
  {4.9, -1.94966}, {5., -1.95066}, {5.1, -1.95162}, {5.2, -1.95255}, {5.3, -1.95344},
  {5.4, -1.95429}, {5.5, -1.95512}, {5.6, -1.95591}, {5.7, -1.95668},
  {5.8, -1.95741}, {5.9, -1.95813}, {6., -1.95882}, {6.1, -1.95948}, {6.2, -1.96013},
  {6.3, -1.96075}, {6.4, -1.96136}, {6.5, -1.96194}, {6.6, -1.96251},
  {6.7, -1.96306}, {6.8, -1.96359}, {6.9, -1.96411}, {7., -1.96462}, {7.1, -1.96509},
  {7.2, -1.96559}, {7.3, -1.96605}, {7.4, -1.9665}, {7.5, -1.96694}, {7.6, -1.96737},
  {7.7, -1.96779}, {7.8, -1.9682}, {7.9, -1.96859}, {8., -1.96898}, {8.1, -1.96936},
  {8.2, -1.96973}, {8.3, -1.97009}, {8.4, -1.97044}, {8.5, -1.97078}, {8.6, -1.97112},
  {8.7, -1.97144}, {8.8, -1.97176}, {8.9, -1.97208}, {9., -1.97238}, {9.1, -1.97268},
  {9.2, -1.97298}, {9.3, -1.97327}, {9.4, -1.97355}, {9.5, -1.97382}, {9.6, -1.97409},
  {9.7, -1.97436}, {9.8, -1.97462}, {9.9, -1.97487}, {10., -1.97512},
  {10.1, -1.97536}, {10.2, -1.9756}, {10.3, -1.97584}, {10.4, -1.97607},
  {10.5, -1.97629}, {10.6, -1.97651}, {10.7, -1.97673}, {10.8, -1.97695},
  {10.9, -1.97716}, {11., -1.97736}, {11.1, -1.97756}, {11.2, -1.97776},
  {11.3, -1.97796}, {11.4, -1.97815}, {11.5, -1.97834}, {11.6, -1.97853},
  {11.7, -1.97871}, {11.8, -1.97889}, {11.9, -1.97906}, {12., -1.97924}}
```

```
\\
```

2

```
In[ ]:= g1 = ListPlot[Vg]
```

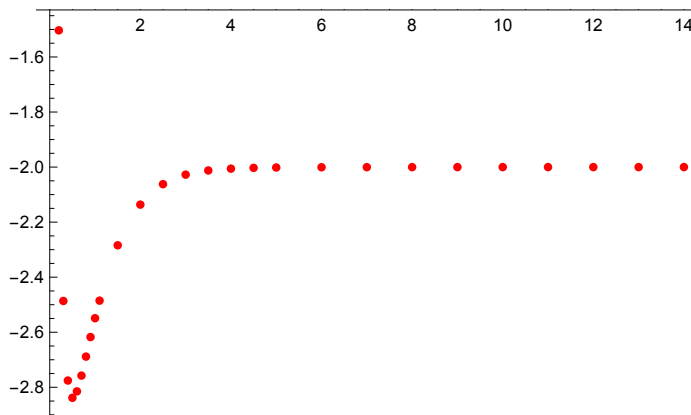
```
Out[ ]:=
```



```
In[ ]:= geradeAccurate = {{0.2`, -1.5032842174691563`},
  {0.30000000000000004`, -2.486387012340349`}, {0.4`, -2.775482794272996`},
  {0.5`, -2.8382004175318905`}, {0.6000000000000001`, -2.8148087552980185`},
  {0.7`, -2.7575873912342637`}, {0.8`, -2.6885226394307153`},
  {0.9000000000000001`, -2.6174940314358572`}, {1.`, -2.549044361047986`},
  {1.1`, -2.485203068355592`}, {1.5`, -2.284163517706141`},
  {2.`, -2.1363792605416463`}, {2.5`, -2.0620994675224718`},
  {3.`, -2.027525786359168`}, {3.5`, -2.012261705447291`},
  {4.`, -2.0056825752101832`}, {4.5`, -2.002835251510367`},
  {5.`, -2.001563627276939`}, {6, -2.000650380284965`},
  {7, -2.0003628296082634`}, {8, -2.000233447243552`}, {9, -2.00016118749333`},
  {10, -2.000115980937658`}, {11, -2.000085087656995`}, {12, -2.000061031526381`},
  {13, -2.0000376138544573`}, {14, -2.0000079088805016`}};
```

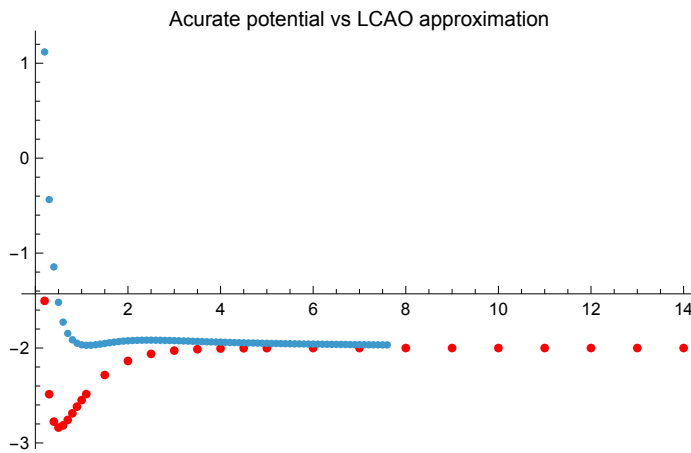
```
In[ ]:= g2 = ListPlot[geradeAccurate, PlotStyle -> Red]
```

```
Out[ ]:=
```

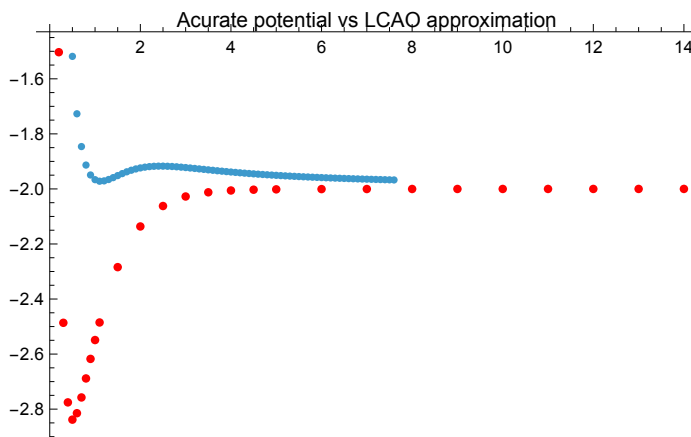


```
In[ ]:= Show[g2, g1, PlotRange -> All, PlotLabel -> "Acurate potential vs LCAO approximation"]
Show[g2, g1, PlotLabel -> "Acurate potential vs LCAO approximation"]
```

Out[]=

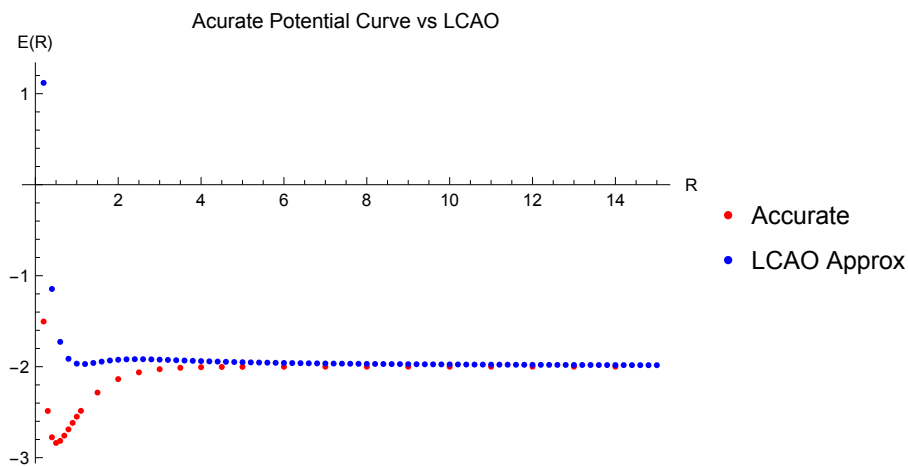


Out[]=



```
ListPlot[{Zgerade, Vg}, PlotRange → All,
  PlotLabel → "Acurate Potential Curve vs LCAO", PlotStyle → {Red, Blue},
  PlotLegends → {"Accurate", "LCAO Approx"}, AxesLabel → {"R", "E(R)"}]
```

Out[8] =



Above graph shows accurate gerade potentials (red icons), versus the ones obtained with the simplistic LCAO method described in my Notes.

Note that for $R > 10$ there is fair agreement; not so good for $R < 10$. This is a reasonable result as the LCAO including only the ground state orbital is a poor description in the molecular region.