

```
In[1]:= ClearAll["Global`*"]

In[1]:= 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, 30, 0.1}};

S = Interpolation[%];
```

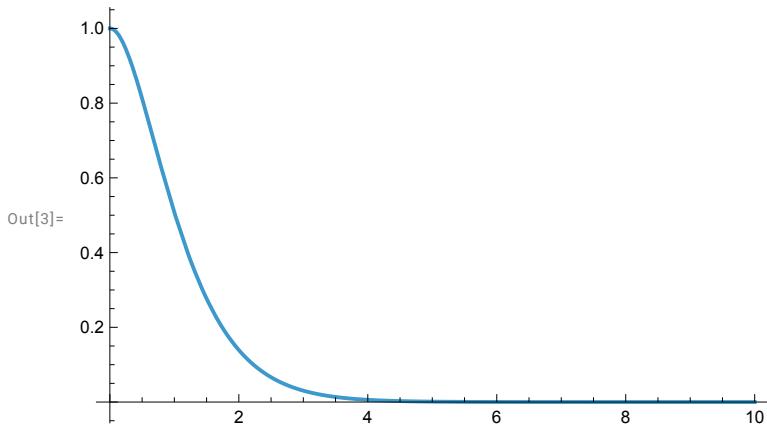
••• **NIntegrate:** Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand or WorkingPrecision too small. [i](#)

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```
In[3]:= Plot[S[R], {R, 0, 10}, PlotRange -> All]
```



```
In[4]:= \psi u[r_, R_] := 1/Sqrt[2(1-S[R])] \times 4/Sqrt[2\pi]
          \left(Exp[-2\sqrt{r^2+R^2/4-rR Cos[\phi]}] - Exp[-2\sqrt{r^2+R^2/4+rR Cos[\phi]}]\right)
```

```
In[5]:= \psi ushift[r_, R_] :=
  1/Sqrt[2(1-S[R])] \times 4/Sqrt[2\pi] \left(Exp[-2r] - Exp[-2\sqrt{r^2+R^2+2rR Cos[\phi]}]\right)
```

Check normalization

```
In[6]:= Table[NIntegrate[r \!~\! u[r, R]^2, {\phi, 0, 2 \pi}, {r, 0, 10}], {R, 0.2, 10}]
Table[NIntegrate[r \!~\! ushift[r, R]^2, {\phi, 0, 2 \pi}, {r, 0, 20}], {R, 0.2, 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
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Out[6]= {0.999999, 1., 1., 1., 1., 1., 1., 1., 1.}

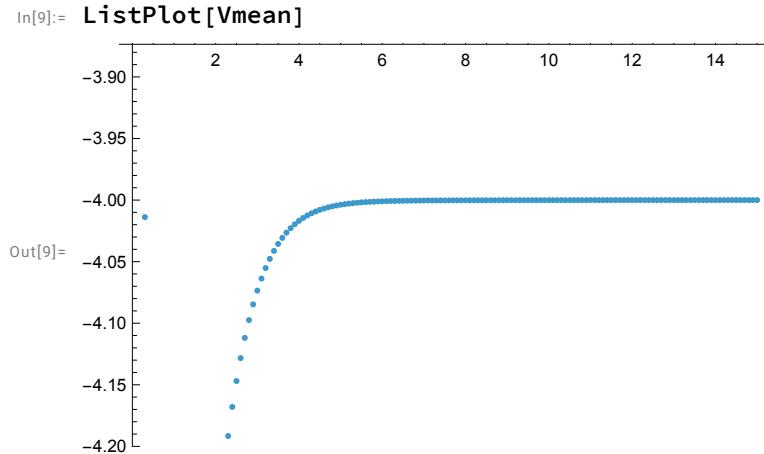
... NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the
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Out[7]= {1.00001, 1., 1., 1., 1., 1., 1., 1., 1.}

In[8]:= Vmean = Table[
  {R, 1/R - 2 NIntegrate[\!~\! ushift[r, R]^2, {\phi, 0, 2 \pi}, {r, 0, 30}]}, {R, 0.2, 15, 0.1}]

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... General: Further output of NIntegrate::slwcon will be suppressed during this calculation. i
```

```
Out[8]= {{0.2, -2.61285}, {0.3, -4.01384}, {0.4, -4.58292}, {0.5, -4.83}, {0.6, -4.92603}, {0.7, -4.94401}, {0.8, -4.91988}, {0.9, -4.87302}, {1., -4.81449}, {1.1, -4.75088}, {1.2, -4.68615}, {1.3, -4.62272}, {1.4, -4.56204}, {1.5, -4.50495}, {1.6, -4.45188}, {1.7, -4.40299}, {1.8, -4.35828}, {1.9, -4.31764}, {2., -4.28088}, {2.1, -4.24779}, {2.2, -4.21811}, {2.3, -4.19158}, {2.4, -4.16794}, {2.5, -4.14695}, {2.6, -4.12835}, {2.7, -4.11192}, {2.8, -4.09744}, {2.9, -4.08471}, {3., -4.07354}, {3.1, -4.06376}, {3.2, -4.05521}, {3.3, -4.04775}, {3.4, -4.04127}, {3.5, -4.03562}, {3.6, -4.03072}, {3.7, -4.02648}, {3.8, -4.02281}, {3.9, -4.01964}, {4., -4.01689}, {4.1, -4.01454}, {4.2, -4.01251}, {4.3, -4.01076}, {4.4, -4.00926}, {4.5, -4.00797}, {4.6, -4.00686}, {4.7, -4.00591}, {4.8, -4.00509}, {4.9, -4.0044}, {5., -4.0038}, {5.1, -4.00329}, {5.2, -4.00285}, {5.3, -4.00248}, {5.4, -4.00216}, {5.5, -4.00188}, {5.6, -4.00165}, {5.7, -4.00145}, {5.8, -4.00127}, {5.9, -4.00113}, {6., -4.001}, {6.1, -4.00089}, {6.2, -4.00079}, {6.3, -4.00071}, {6.4, -4.00064}, {6.5, -4.00058}, {6.6, -4.00053}, {6.7, -4.00048}, {6.8, -4.00044}, {6.9, -4.00041}, {7., -4.00037}, {7.1, -4.00031}, {7.2, -4.00032}, {7.3, -4.0003}, {7.4, -4.00028}, {7.5, -4.00027}, {7.6, -4.00025}, {7.7, -4.00024}, {7.8, -4.00022}, {7.9, -4.00022}, {8., -4.0002}, {8.1, -4.00019}, {8.2, -4.00018}, {8.3, -4.00017}, {8.4, -4.00017}, {8.5, -4.00016}, {8.6, -4.00016}, {8.7, -4.00015}, {8.8, -4.00014}, {8.9, -4.00014}, {9., -4.00013}, {9.1, -4.00013}, {9.2, -4.00012}, {9.3, -4.00012}, {9.4, -4.00012}, {9.5, -4.00011}, {9.6, -4.00011}, {9.7, -4.00011}, {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., -4.00005}, {12.1, -4.00005}, {12.2, -4.00005}, {12.3, -4.00005}, {12.4, -4.00005}, {12.5, -4.00005}, {12.6, -4.00005}, {12.7, -4.00005}, {12.8, -4.00005}, {12.9, -4.00005}, {13., -4.00004}, {13.1, -4.00004}, {13.2, -4.00004}, {13.3, -4.00004}, {13.4, -4.00004}, {13.5, -4.00004}, {13.6, -4.00004}, {13.7, -4.00004}, {13.8, -4.00004}, {13.9, -4.00004}, {14., -4.00003}, {14.1, -4.00003}, {14.2, -4.00003}, {14.3, -4.00003}, {14.4, -4.00003}, {14.5, -4.00003}, {14.6, -4.00003}, {14.7, -4.00003}, {14.8, -4.00003}, {14.9, -4.00003}, {15., -4.00003}}
```



```
In[10]:= KE1 =
Table[{R, NIntegrate[\psiushift[r, R]^2, {\phi, 0, 2 \pi}, {r, 0, 30}]}, {R, 0.2, 15, 0.1}]
KE2 =
Table[{R, NIntegrate[1/r Cos[\phi] R/2 \psiushift[r, R]^2, {\phi, 0, 2 \pi}, {r, 0.00001, 30}]},
{R, 0.2, 15, 0.1}]
```

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Out[10]=

```
{ {0.2, 3.80643}, {0.3, 3.67358}, {0.4, 3.54146}, {0.5, 3.415}, {0.6, 3.29635},
{0.7, 3.18629}, {0.8, 3.08494}, {0.9, 2.99206}, {1., 2.90725}, {1.1, 2.82998},
{1.2, 2.75974}, {1.3, 2.69597}, {1.4, 2.63816}, {1.5, 2.58581}, {1.6, 2.53844},
{1.7, 2.49561}, {1.8, 2.45692}, {1.9, 2.42198}, {2., 2.39044}, {2.1, 2.36199},
{2.2, 2.33633}, {2.3, 2.31318}, {2.4, 2.2923}, {2.5, 2.27347}, {2.6, 2.25648},
{2.7, 2.24115}, {2.8, 2.22729}, {2.9, 2.21477}, {3., 2.20344}, {3.1, 2.19317},
{3.2, 2.18385}, {3.3, 2.17539}, {3.4, 2.16769}, {3.5, 2.16067}, {3.6, 2.15425},
{3.7, 2.14838}, {3.8, 2.14298}, {3.9, 2.13802}, {4., 2.13345}, {4.1, 2.12922},
{4.2, 2.1253}, {4.3, 2.12166}, {4.4, 2.11826}, {4.5, 2.11509}, {4.6, 2.11213},
{4.7, 2.10934}, {4.8, 2.10671}, {4.9, 2.10424}, {5., 2.1019}, {5.1, 2.09968},
{5.2, 2.09758}, {5.3, 2.09558}, {5.4, 2.09367}, {5.5, 2.09185}, {5.6, 2.09011},
{5.7, 2.08844}, {5.8, 2.08684}, {5.9, 2.08531}, {6., 2.08383}, {6.1, 2.08241},
{6.2, 2.08104}, {6.3, 2.07972}, {6.4, 2.07845}, {6.5, 2.07721}, {6.6, 2.07602},
{6.7, 2.07487}, {6.8, 2.07375}, {6.9, 2.07267}, {7., 2.07162}, {7.1, 2.07058},
{7.2, 2.0696}, {7.3, 2.06864}, {7.4, 2.06771}, {7.5, 2.0668}, {7.6, 2.06591},
{7.7, 2.06505}, {7.8, 2.06421}, {7.9, 2.0634}, {8., 2.0626}, {8.1, 2.06182},
{8.2, 2.06107}, {8.3, 2.06033}, {8.4, 2.05961}, {8.5, 2.0589}, {8.6, 2.05822},
{8.7, 2.05755}, {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, 2.04313},
{11.7, 2.04276}, {11.8, 2.0424}, {11.9, 2.04204}, {12., 2.04169}, {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, 2.03939}, {12.8, 2.03909}, {12.9, 2.03878}, {13., 2.03848},
{13.1, 2.03819}, {13.2, 2.0379}, {13.3, 2.03761}, {13.4, 2.03733}, {13.5, 2.03706},
{13.6, 2.03679}, {13.7, 2.03652}, {13.8, 2.03625}, {13.9, 2.03599}, {14., 2.03573},
{14.1, 2.03548}, {14.2, 2.03523}, {14.3, 2.03498}, {14.4, 2.03474}, {14.5, 2.0345},
{14.6, 2.03426}, {14.7, 2.03403}, {14.8, 2.0338}, {14.9, 2.03357}, {15., 2.03335} }
```

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```
Out[11]=
{{0.2, 0.818861}, {0.3, 0.874433}, {0.4, 0.854539}, {0.5, 0.797815}, {0.6, 0.724406},
{0.7, 0.645304}, {0.8, 0.566599}, {0.9, 0.491609}, {1., 0.422041},
{1.1, 0.358644}, {1.2, 0.301602}, {1.3, 0.250766}, {1.4, 0.205802},
{1.5, 0.166281}, {1.6, 0.131729}, {1.7, 0.101668}, {1.8, 0.075631},
{1.9, 0.0531784}, {2., 0.0339008}, {2.1, 0.0174232}, {2.2, 0.00340515},
{2.3, -0.00845998}, {2.4, -0.0184469}, {2.5, -0.0268004}, {2.6, -0.0337378},
{2.7, -0.0394511}, {2.8, -0.0441098}, {2.9, -0.0478626}, {3., -0.0508399},
{3.1, -0.0531555}, {3.2, -0.0549086}, {3.3, -0.0561855}, {3.4, -0.0570609},
{3.5, -0.0575993}, {3.6, -0.0578565}, {3.7, -0.0578801}, {3.8, -0.0577113},
{3.9, -0.0573851}, {4., -0.0569312}, {4.1, -0.0563752}, {4.2, -0.0557383},
{4.3, -0.0550388}, {4.4, -0.0542919}, {4.5, -0.0535102}, {4.6, -0.0527043},
{4.7, -0.0518832}, {4.8, -0.0510539}, {4.9, -0.0502225}, {5., -0.0493938},
{5.1, -0.0485716}, {5.2, -0.047759}, {5.3, -0.0469585}, {5.4, -0.046172},
{5.5, -0.0454008}, {5.6, -0.0446461}, {5.7, -0.0439085}, {5.8, -0.0431884},
{5.9, -0.0424862}, {6., -0.0418019}, {6.1, -0.0411354}, {6.2, -0.0404867},
{6.3, -0.0398553}, {6.4, -0.0392411}, {6.5, -0.0386435}, {6.6, -0.0380623},
{6.7, -0.037497}, {6.8, -0.0369471}, {6.9, -0.0364121}, {7., -0.0358917},
{7.1, -0.0353853}, {7.2, -0.0348924}, {7.3, -0.0344126}, {7.4, -0.0339455},
{7.5, -0.0334906}, {7.6, -0.0330474}, {7.7, -0.0326157}, {7.8, -0.0321949},
{7.9, -0.0317847}, {8., -0.0313848}, {8.1, -0.0309947}, {8.2, -0.0306141},
{8.3, -0.0302427}, {8.4, -0.0298801}, {8.5, -0.0295261}, {8.6, -0.0291804},
{8.7, -0.0288427}, {8.8, -0.0285127}, {8.9, -0.0281902}, {9., -0.0278749},
{9.1, -0.0275665}, {9.2, -0.0272649}, {9.3, -0.0269699}, {9.4, -0.0266812},
{9.5, -0.0263986}, {9.6, -0.0261219}, {9.7, -0.025851}, {9.8, -0.0255857},
{9.9, -0.0253257}, {10., -0.025071}, {10.1, -0.0248214}, {10.2, -0.0245767},
{10.3, -0.0243368}, {10.4, -0.0241016}, {10.5, -0.0238709}, {10.6, -0.0236445},
{10.7, -0.0234225}, {10.8, -0.0232045}, {10.9, -0.0229906}, {11., -0.0227806},
{11.1, -0.0225744}, {11.2, -0.0223719}, {11.3, -0.0221731}, {11.4, -0.0219777},
{11.5, -0.0217858}, {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, -0.0205308},
{12.3, -0.0203633}, {12.4, -0.0201985}, {12.5, -0.0200363}, {12.6, -0.0198767},
{12.7, -0.0197196}, {12.8, -0.019565}, {12.9, -0.0194128}, {13., -0.019263},
{13.1, -0.0191155}, {13.2, -0.0189702}, {13.3, -0.0188271}, {13.4, -0.0186861},
{13.5, -0.0185473}, {13.6, -0.0184105}, {13.7, -0.0182757}, {13.8, -0.0181429},
{13.9, -0.018012}, {14., -0.0178829}, {14.1, -0.0177557}, {14.2, -0.0176303},
{14.3, -0.0175067}, {14.4, -0.0173848}, {14.5, -0.0172646}, {14.6, -0.017146},
{14.7, -0.0170291}, {14.8, -0.0169137}, {14.9, -0.0167999}, {15., -0.0166876}}
```

```

In[12]:= Dimensions[KE1]
Dimensions[KE2]
Out[12]= {149, 2}

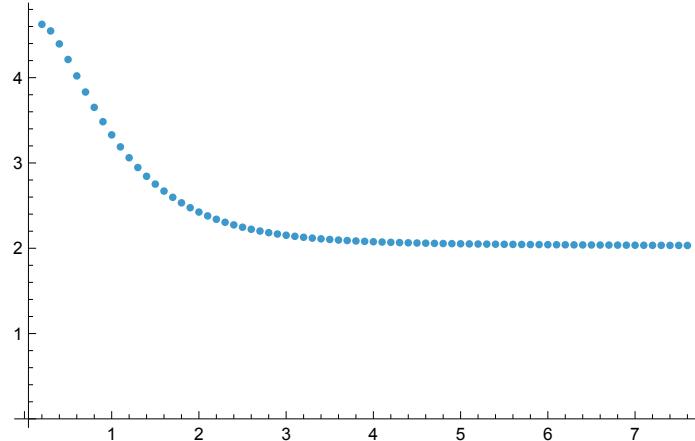
Out[13]= {149, 2}

In[26]:= KE = Table[{KE1[[i, 1]], KE1[[i, 2]] + KE2[[i, 2]]}, {i, 1, 119}]
Out[26]= {{0.2, 4.62529}, {0.3, 4.54802}, {0.4, 4.396}, {0.5, 4.21282}, {0.6, 4.02075},
{0.7, 3.83159}, {0.8, 3.65154}, {0.9, 3.48367}, {1., 3.32929}, {1.1, 3.18863},
{1.2, 3.06134}, {1.3, 2.94674}, {1.4, 2.84397}, {1.5, 2.75209}, {1.6, 2.67017},
{1.7, 2.59728}, {1.8, 2.53255}, {1.9, 2.47515}, {2., 2.42434}, {2.1, 2.37941},
{2.2, 2.33973}, {2.3, 2.30472}, {2.4, 2.27386}, {2.5, 2.24667}, {2.6, 2.22275},
{2.7, 2.2017}, {2.8, 2.18318}, {2.9, 2.16691}, {3., 2.1526}, {3.1, 2.14001},
{3.2, 2.12895}, {3.3, 2.11921}, {3.4, 2.11063}, {3.5, 2.10307}, {3.6, 2.09639},
{3.7, 2.0905}, {3.8, 2.08527}, {3.9, 2.08064}, {4., 2.07651}, {4.1, 2.07285},
{4.2, 2.06956}, {4.3, 2.06662}, {4.4, 2.06397}, {4.5, 2.06158}, {4.6, 2.05942},
{4.7, 2.05745}, {4.8, 2.05566}, {4.9, 2.05402}, {5., 2.05251}, {5.1, 2.05111},
{5.2, 2.04982}, {5.3, 2.04862}, {5.4, 2.0475}, {5.5, 2.04645}, {5.6, 2.04546},
{5.7, 2.04453}, {5.8, 2.04366}, {5.9, 2.04282}, {6., 2.04203}, {6.1, 2.04128},
{6.2, 2.04056}, {6.3, 2.03987}, {6.4, 2.0392}, {6.5, 2.03857}, {6.6, 2.03796},
{6.7, 2.03737}, {6.8, 2.0368}, {6.9, 2.03625}, {7., 2.03572}, {7.1, 2.03519},
{7.2, 2.03471}, {7.3, 2.03423}, {7.4, 2.03376}, {7.5, 2.03331}, {7.6, 2.03287},
{7.7, 2.03244}, {7.8, 2.03202}, {7.9, 2.03161}, {8., 2.03122}, {8.1, 2.03083},
{8.2, 2.03045}, {8.3, 2.03009}, {8.4, 2.02973}, {8.5, 2.02938}, {8.6, 2.02904},
{8.7, 2.0287}, {8.8, 2.02838}, {8.9, 2.02806}, {9., 2.02775}, {9.1, 2.02744},
{9.2, 2.02714}, {9.3, 2.02685}, {9.4, 2.02657}, {9.5, 2.02629}, {9.6, 2.02602},
{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, 2.02334}, {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, 2.02099}, {12., 2.02082}}

```

```
In[15]:= ListPlot[KE, PlotRange -> All]
```

```
Out[15]=
```



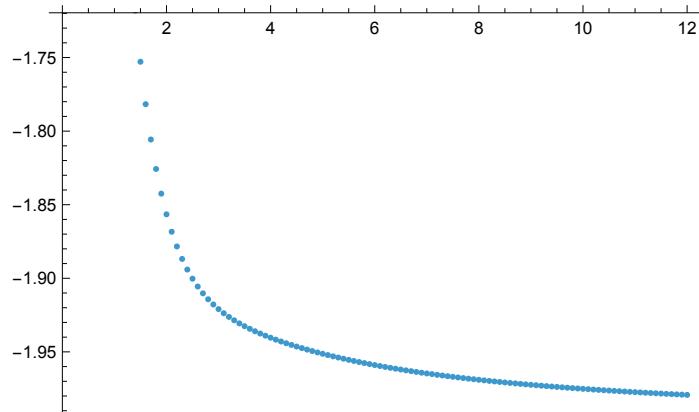
```
In[27]:= Vu = Table[{KE1[[i, 1]], Vmean[[i, 2]] + KE[[i, 2]]}, {i, 1, 119}]
```

```
Out[27]=
```

```
{ {0.2, 2.01244}, {0.3, 0.534181}, {0.4, -0.186921}, {0.5, -0.617186},
{0.6, -0.905274}, {0.7, -1.11241}, {0.8, -1.26834}, {0.9, -1.38934},
{1., -1.48521}, {1.1, -1.56225}, {1.2, -1.6248}, {1.3, -1.67598}, {1.4, -1.71808},
{1.5, -1.75286}, {1.6, -1.78171}, {1.7, -1.80571}, {1.8, -1.82573}, {1.9, -1.84248},
{2., -1.85654}, {2.1, -1.86838}, {2.2, -1.87838}, {2.3, -1.88686}, {2.4, -1.89408},
{2.5, -1.90027}, {2.6, -1.90561}, {2.7, -1.91023}, {2.8, -1.91426},
{2.9, -1.9178}, {3., -1.92094}, {3.1, -1.92374}, {3.2, -1.92626}, {3.3, -1.92855},
{3.4, -1.93064}, {3.5, -1.93255}, {3.6, -1.93433}, {3.7, -1.93599},
{3.8, -1.93754}, {3.9, -1.939}, {4., -1.94038}, {4.1, -1.94169}, {4.2, -1.94294},
{4.3, -1.94414}, {4.4, -1.94528}, {4.5, -1.94638}, {4.6, -1.94744},
{4.7, -1.94845}, {4.8, -1.94943}, {4.9, -1.95038}, {5., -1.95129}, {5.1, -1.95218},
{5.2, -1.95303}, {5.3, -1.95386}, {5.4, -1.95466}, {5.5, -1.95543},
{5.6, -1.95618}, {5.7, -1.95691}, {5.8, -1.95762}, {5.9, -1.9583}, {6., -1.95897},
{6.1, -1.95961}, {6.2, -1.96024}, {6.3, -1.96085}, {6.4, -1.96144},
{6.5, -1.96201}, {6.6, -1.96257}, {6.7, -1.96311}, {6.8, -1.96364},
{6.9, -1.96415}, {7., -1.96465}, {7.1, -1.96512}, {7.2, -1.96561}, {7.3, -1.96607},
{7.4, -1.96652}, {7.5, -1.96696}, {7.6, -1.96738}, {7.7, -1.9678}, {7.8, -1.9682},
{7.9, -1.9686}, {8., -1.96899}, {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, -1.97145},
{8.8, -1.97177}, {8.9, -1.97208}, {9., -1.97239}, {9.1, -1.97269}, {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., -1.97923} }
```

```
In[28]:= g1 = ListPlot[Vu]
```

```
Out[28]=
```



```
In[22]:= ungeradeAccurate =
```

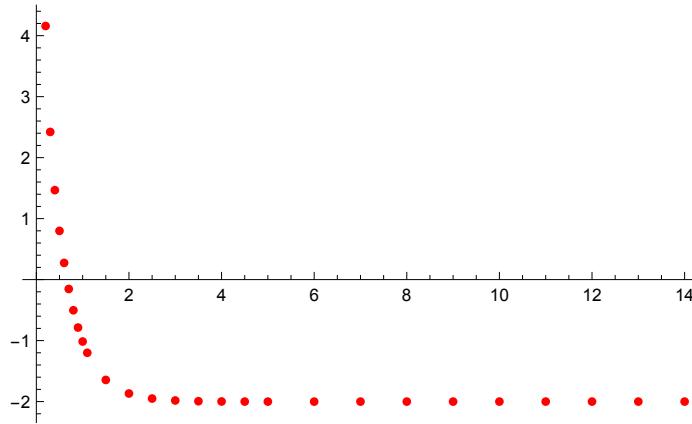
```
{ {0.2` , 4.158676158754618`}, {0.3` , 2.4214819602700515`},
{0.4` , 1.4667568527594321`}, {0.5` , 0.798837037484202`},
{0.6` , 0.27398329203366`}, {0.7` , -0.15355838170615854`},
{0.8` , -0.502668845061603`}, {0.9` , -0.7861427341683027`},
{1.` , -1.0152146767380725`}, {1.1` , -1.1999001015268562`},
{1.5` , -1.6449404033311605`}, {2.` , -1.8674405785498043`},
{2.5` , -1.9502894862529478`}, {3.` , -1.98193057045757`},
{3.5` , -1.9939879161467178`}, {4.` , -1.9984548827903468`},
{4.5` , -2.000004357615667`}, {5.` , -2.000463004394309`}, {6, -2.000486680182881`},
{7, -2.000338857366044`}, {8, -2.000229992718693`}, {9, -2.0001607943205273`},
{10, -2.0001163734073755`}, {11, -2.000086707793727`}, {12, -2.0000658320684908`},
{13, -2.0000498631142434`}, {14, -2.0000356666547345`}}
```

```
Out[22]=
```

```
{ {0.2, 4.15868}, {0.3, 2.42148}, {0.4, 1.46676}, {0.5, 0.798837},
{0.6, 0.273983}, {0.7, -0.153558}, {0.8, -0.502669}, {0.9, -0.786143},
{1., -1.01521}, {1.1, -1.1999}, {1.5, -1.64494}, {2., -1.86744},
{2.5, -1.95029}, {3., -1.98193}, {3.5, -1.99399}, {4., -1.99845}, {4.5, -2.},
{5., -2.00046}, {6, -2.00049}, {7, -2.00034}, {8, -2.00023}, {9, -2.00016},
{10, -2.00012}, {11, -2.00009}, {12, -2.00007}, {13, -2.00005}, {14, -2.00004} }
```

```
In[29]:= g2 = ListPlot[ungeradeAccurate, PlotStyle -> Red]
```

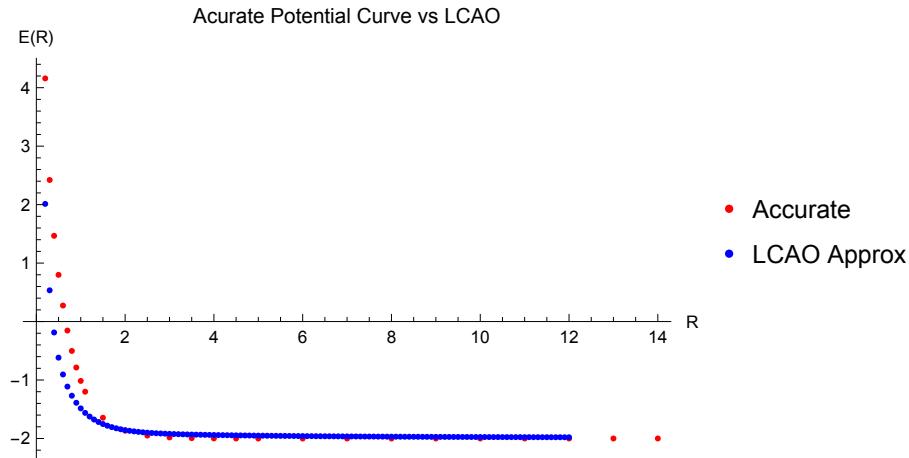
```
Out[29]=
```



```
Show[g2, g1, PlotRange -> All, PlotLabel -> "Accurate potential vs LCAO approximation"]
Show[g2, g1, PlotLabel -> "Accurate potential vs LCAO approximation"]
```

```
In[30]:= ListPlot[{ungeradeAccurate, Vu}, PlotRange -> All,
PlotLabel -> "Accurate Potential Curve vs LCAO", PlotStyle -> {Red, Blue},
PlotLegends -> {"Accurate", "LCAO Approx"}, AxesLabel -> {"R", "E(R)"}]
```

```
Out[30]=
```



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

Note that for  $R > 2$  the there is fair agreement.