

Appendix

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#Joe Angelo
#Quantum Paper Work
#Finite Nuclear Size Perturbation Theory
# Computes energy shifts due to finite nuclear size.
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```
restart;
with(orthopoly);
```

[G, H, L, P, T, U] (1)

```
L(5, x);      ### These are the Laguerres polynomials
```

$$1 - 5x + 5x^2 - \frac{5}{3}x^3 + \frac{5}{24}x^4 - \frac{1}{120}x^5 \quad (2)$$

```
g(5, 0, x) := L(5, x);  ### begins process for computing Associated Laguerres polynomials
```

$$1 - 5x + 5x^2 - \frac{5}{3}x^3 + \frac{5}{24}x^4 - \frac{1}{120}x^5 \quad (3)$$

```
for i from 1 to 7 do
```

```
g(5, i, x) := diff(g(5, i - 1, x), x) : print(5, i - 1, g(5, i - 1, x)) :od:
```

$$5, 0, 1 - 5x + 5x^2 - \frac{5}{3}x^3 + \frac{5}{24}x^4 - \frac{1}{120}x^5$$

$$5, 1, -5 + 10x - 5x^2 + \frac{5}{6}x^3 - \frac{1}{24}x^4$$

$$5, 2, 10 - 10x + \frac{5}{2}x^2 - \frac{1}{6}x^3$$

$$5, 3, -10 + 5x - \frac{1}{2}x^2$$

$$5, 4, 5 - x$$

$$5, 5, -1$$

$$5, 6, 0$$

(4)

```
for j from 0 to 12 do g(j, 0, x) := L(j, x); for i from 1 to j + 2 do
```

```
g(j, i, x) := diff(g(j, i - 1, x), x) :od:od:## Lots of assoc lag.
```

```
for n from 1 to 5 do for l from 0 to n - 1 do
```

$$R(n, l, x) := g(n + l, 2 \cdot l + 1, x) \cdot \exp\left(-\frac{x}{2}\right) \cdot (x)^l; \quad RR(n, l, r) := \text{subs}\left(x = \frac{2 \cdot r}{n}, g(n + l, 2 \cdot l + 1, x) \cdot \exp\left(-\frac{x}{2}\right) \cdot (x)^l\right);$$

```
N(n, l) := int(r^2 \cdot RR(n, l, r)^2, r = 0 .. \infty);
```

$$RX(n, l, r) := \frac{RR(n, l, r)}{\text{sqrt}(N(n, l))}; \quad \text{### constructs normalized hydrogenic radial wavefunctions}$$

```
print(n, l, RX(n, l, r))
```

```
:od:od;
```

$$1, 0, -2e^{-r}$$

$$\begin{aligned}
& 2, 0, \frac{1}{4} (-2 + r) e^{-\frac{1}{2} r} \sqrt{2} \\
& 2, 1, -\frac{1}{12} e^{-\frac{1}{2} r} r \sqrt{6} \\
& 3, 0, \frac{2}{27} \left(-3 + 2r - \frac{2}{9} r^2 \right) e^{-\frac{1}{3} r} \sqrt{3} \\
& 3, 1, \frac{1}{81} \left(-4 + \frac{2}{3} r \right) e^{-\frac{1}{3} r} r \sqrt{6} \\
& 3, 2, -\frac{2}{1215} e^{-\frac{1}{3} r} r^2 \sqrt{30} \\
& 4, 0, \frac{1}{16} \left(-4 + 3r - \frac{1}{2} r^2 + \frac{1}{48} r^3 \right) e^{-\frac{1}{4} r} \\
& 4, 1, \frac{1}{480} \left(-10 + \frac{5}{2} r - \frac{1}{8} r^2 \right) e^{-\frac{1}{4} r} r \sqrt{15} \\
& 4, 2, \frac{1}{1920} \left(-6 + \frac{1}{2} r \right) e^{-\frac{1}{4} r} r^2 \sqrt{5} \\
& 4, 3, -\frac{1}{26880} e^{-\frac{1}{4} r} r^3 \sqrt{35} \\
& 5, 0, \frac{2}{125} \left(-5 + 4r - \frac{4}{5} r^2 + \frac{4}{75} r^3 - \frac{2}{1875} r^4 \right) e^{-\frac{1}{5} r} \sqrt{5} \\
& 5, 1, \frac{1}{1875} \left(-20 + 6r - \frac{12}{25} r^2 + \frac{4}{375} r^3 \right) e^{-\frac{1}{5} r} r \sqrt{30} \\
& 5, 2, \frac{2}{65625} \left(-21 + \frac{14}{5} r - \frac{2}{25} r^2 \right) e^{-\frac{1}{5} r} r^2 \sqrt{70} \\
& 5, 3, \frac{1}{328125} \left(-8 + \frac{2}{5} r \right) e^{-\frac{1}{5} r} r^3 \sqrt{70} \\
& 5, 4, -\frac{2}{4921875} e^{-\frac{1}{5} r} r^4 \sqrt{70}
\end{aligned} \tag{5}$$

$int(RX(1, 0, r)^2 \cdot r^2, r=0.. \infty)$; ### Normalized??

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(6)

for n from 1 to 5 do for l from 1 to n - 1 do

$over(n, l) := int(RX(n, l, r) \cdot RX(n, l - 1, r) \cdot r \cdot r^2, r=0.. \infty) : print(n, l, over(n, l));$

: od:od

$$\begin{aligned}
& 2, 1, -3\sqrt{3} \\
& 3, 1, -9\sqrt{2} \\
& 3, 2, -\frac{9}{2}\sqrt{5} \\
& 4, 1, -6\sqrt{15} \\
& 4, 2, -12\sqrt{3} \\
& 4, 3, -6\sqrt{7} \\
& 5, 1, -15\sqrt{6} \\
& 5, 2, -\frac{15}{2}\sqrt{7}\sqrt{3} \\
& 5, 3, -30 \\
& 5, 4, -\frac{45}{2}
\end{aligned} \tag{7}$$

for n from 1 to 5 do for l from 0 to $n - 1$ do

$over(n, l) := int(RX(n, l, r) \cdot RX(n, l, r) \cdot r^2 \cdot r^2, r=0.. \infty) : print(n, l, over(n, l));$
:od:od:

$$\begin{aligned}
& 1, 0, 3 \\
& 2, 0, 42 \\
& 2, 1, 30 \\
& 3, 0, 207 \\
& 3, 1, 180 \\
& 3, 2, 126 \\
& 4, 0, 648 \\
& 4, 1, 600 \\
& 4, 2, 504 \\
& 4, 3, 360 \\
& 5, 0, 1575 \\
& 5, 1, 1500 \\
& 5, 2, 1350 \\
& 5, 3, 1125 \\
& 5, 4, 825
\end{aligned} \tag{8}$$

for n from 1 to 5 do for l from 2 to $n - 1$ do

$over(n, l) := int(RX(n, l, r) \cdot RX(n, l - 2, r) \cdot r^2 \cdot r^2, r=0.. \infty); print(n, l, over(n, l));$
:od:od:

$$\begin{aligned}
& 3, 2, 45\sqrt{10} \\
& 4, 2, 240\sqrt{5}
\end{aligned}$$

$$\begin{aligned}
& 4, 3, 80 \sqrt{7} \sqrt{3} \\
& 5, 2, 375 \sqrt{14} \\
& 5, 3, 250 \sqrt{7} \sqrt{3} \\
& 5, 4, 750
\end{aligned} \tag{9}$$

$$pert1 := -\frac{3}{2 \cdot K} + \frac{r^2}{2 \cdot K^3} + \frac{1}{r};$$

$$-\frac{3}{2 K} + \frac{1}{2} \frac{r^2}{K^3} + \frac{1}{r} \tag{10}$$

$$pert2 := -\frac{1}{K} + \frac{1}{r};$$

$$-\frac{1}{K} + \frac{1}{r} \tag{11}$$

$int(RX(1, 0, r)^2 \cdot r^2 \cdot pert1, r=0..K); taylor(%, K=0, 10);$

$$\frac{1}{2} \frac{2 K^3 + 3 - 3 K^2 - 3 e^{-2K} - 3 e^{-2K} K^2 - 6 e^{-2K} K}{K^3}$$

$$\frac{2}{5} K^2 - \frac{1}{3} K^3 + \frac{6}{35} K^4 - \frac{1}{15} K^5 + \frac{4}{189} K^6 + O(K^7) \tag{12}$$

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(13)

$int(RX(1, 0, r)^2 \cdot r^2 \cdot pert2, r=0..K); taylor(%, K=0, 10);$

$$\frac{K - 1 + e^{-2K} K + e^{-2K}}{K}$$

$$\frac{2}{3} K^2 - \frac{2}{3} K^3 + \frac{2}{5} K^4 - \frac{8}{45} K^5 + \frac{4}{63} K^6 - \frac{2}{105} K^7 + \frac{2}{405} K^8 + O(K^9) \tag{14}$$

for n from 1 to 5 do for l from 0 to n - 1 do

$z := int(RX(n, l, r)^2 \cdot r^2 \cdot pert1, r=0..K); corr1(n, l) := taylor(z, K=0, 8 + 2^l) : print(n, l, corr1(n, l))$

:od:od:

$$1, 0, \frac{2}{5} K^2 - \frac{1}{3} K^3 + \frac{6}{35} K^4 - \frac{1}{15} K^5 + O(K^6)$$

$$2, 0, \frac{1}{20} K^2 - \frac{1}{24} K^3 + \frac{3}{160} K^4 - \frac{11}{1920} K^5 + O(K^6)$$

$$2, 1, \frac{1}{1120} K^4 - \frac{1}{1920} K^5 + \frac{1}{6048} K^6 + O(K^7)$$

$$3, 0, \frac{2}{135} K^2 - \frac{1}{81} K^3 + \frac{46}{8505} K^4 - \frac{17}{10935} K^5 + O(K^6)$$

$$3, 1, \frac{8}{25515} K^4 - \frac{2}{10935} K^5 + \frac{68}{1240029} K^6 + O(K^7)$$

$$3, 2, \frac{4}{6200145} K^6 - \frac{1}{3444525} K^7 + \frac{2}{29229255} K^8 + O(K^9)$$

$$\begin{aligned}
& 4, 0, \frac{1}{160} K^2 - \frac{1}{192} K^3 + \frac{81}{35840} K^4 - \frac{13}{20480} K^5 + O(K^6) \\
& \quad 4, 1, \frac{1}{7168} K^4 - \frac{1}{12288} K^5 + \frac{37}{1548288} K^6 + O(K^7) \\
& \quad 4, 2, \frac{1}{2580480} K^6 - \frac{1}{5734400} K^7 + \frac{31}{778567680} K^8 + O(K^9) \\
4, 3, & \frac{1}{5449973760} K^8 - \frac{1}{14863564800} K^9 + \frac{1}{78721843200} K^{10} - \frac{1}{610397061120} K^{11} \\
& + \frac{1}{6183242956800} K^{12} + O(K^{13}) \\
& \quad 5, 0, \frac{2}{625} K^2 - \frac{1}{375} K^3 + \frac{18}{15625} K^4 - \frac{1}{3125} K^5 + O(K^6) \\
& \quad 5, 1, \frac{8}{109375} K^4 - \frac{2}{46875} K^5 + \frac{916}{73828125} K^6 + O(K^7) \\
& \quad 5, 2, \frac{4}{17578125} K^6 - \frac{1}{9765625} K^7 + \frac{334}{14501953125} K^8 + O(K^9) \\
5, 3, & \frac{16}{101513671875} K^8 - \frac{8}{138427734375} K^9 + \frac{28}{2618408203125} K^{10} \\
& - \frac{118}{88824462890625} K^{11} + \frac{4}{32135009765625} K^{12} + O(K^{13}) \\
5, 4, & \frac{4}{164959716796875} K^{10} - \frac{2}{266473388671875} K^{11} + \frac{4}{3374176025390625} K^{12} \\
& - \frac{1}{7873077392578125} K^{13} + \frac{8}{772167205810546875} K^{14} - \frac{1}{1459980010986328125} K^{15} \\
& + \frac{2}{52397060394287109375} K^{16} - \frac{8}{4343440532684326171875} K^{17} \\
& + \frac{8}{101943104267120361328125} K^{18} - \frac{4}{1334969222545623779296875} K^{19} \\
& + \frac{8}{77128006517887115478515625} K^{20} + O(K^{21})
\end{aligned} \tag{15}$$

for n from 1 to 5 do for l from 0 to n - 1 do

$z := \text{int}(RX(n, l, r)^2 \cdot r^2 \cdot \text{pert2}, r=0..K)$; $\text{corr}l(n, l) := \text{taylor}(z, K=0, (6 + 2 \cdot l))$; $\text{print}(n, l, \text{corr}l(n, l))$ **:od:od:**

$$\begin{aligned}
& 1, 0, \frac{2}{3} K^2 - \frac{2}{3} K^3 + \frac{2}{5} K^4 + O(K^5) \\
& 2, 0, \frac{1}{12} K^2 - \frac{1}{12} K^3 + \frac{7}{160} K^4 + O(K^5) \\
& 2, 1, \frac{1}{480} K^4 - \frac{1}{720} K^5 + \frac{1}{2016} K^6 + O(K^7) \\
& 3, 0, \frac{2}{81} K^2 - \frac{2}{81} K^3 + \frac{46}{3645} K^4 + O(K^5)
\end{aligned}$$

$$\begin{aligned}
& 3, 1, \frac{8}{10935} K^4 - \frac{16}{32805} K^5 + \frac{68}{413343} K^6 + O(K^7) \\
& 3, 2, \frac{4}{2066715} K^6 - \frac{2}{2066715} K^7 + \frac{2}{7971615} K^8 + O(K^9) \\
& \quad 4, 0, \frac{1}{96} K^2 - \frac{1}{96} K^3 + \frac{27}{5120} K^4 + O(K^5) \\
& \quad 4, 1, \frac{1}{3072} K^4 - \frac{1}{4608} K^5 + \frac{37}{516096} K^6 + O(K^7) \\
& \quad 4, 2, \frac{1}{860160} K^6 - \frac{1}{1720320} K^7 + \frac{31}{212336640} K^8 + O(K^9) \\
& 4, 3, \frac{1}{1486356480} K^8 - \frac{1}{3715891200} K^9 + \frac{1}{18166579200} K^{10} + O(K^{11}) \\
& \quad 5, 0, \frac{2}{375} K^2 - \frac{2}{375} K^3 + \frac{42}{15625} K^4 + O(K^5) \\
& \quad 5, 1, \frac{8}{46875} K^4 - \frac{16}{140625} K^5 + \frac{916}{24609375} K^6 + O(K^7) \\
& \quad 5, 2, \frac{4}{5859375} K^6 - \frac{2}{5859375} K^7 + \frac{334}{3955078125} K^8 + O(K^9) \\
& \quad 5, 3, \frac{16}{27685546875} K^8 - \frac{32}{138427734375} K^9 + \frac{28}{604248046875} K^{10} + O(K^{11}) \\
& 5, 4, \frac{4}{38067626953125} K^{10} - \frac{4}{114202880859375} K^{11} + \frac{4}{674835205078125} K^{12} + O(K^{13}) \quad (16)
\end{aligned}$$

#graph for analytic potential

with(plots) :

R := 1.4 :

Vanalytic := proc(r)

- 1
r

end proc:

Vr := proc(r)

if $r \geq R$ **then**

- 1
r

elif $r < R$ **then**

- 3 1 + 1 1 . (r)²
2 R R R

end if

end proc:

```

liney := PLOT(CURVES([ [0,-1.8], [0, .1]], )) :
linex := PLOT(CURVES([ [-.2, 0], [4.5, 0]], )) :
Text := textplot([ 1.5,-.3, "Rn", font = [TIMES, ROMAN, 13]], align = right) :
t2 := textplot([ 3,-.42, "V(r)/e", font = [TIMES, ROMAN, 13]], align = right) :
t3 := textplot([ -.03,-.8, "E/e", font = [TIMES, ROMAN, 13]], align = left) :
t4 := textplot([ 2, .03, "r", font = [TIMES, ROMAN, 13]], align = above) :
line := PLOT(CURVES([ [R, -1.5], [R, 0]], linestyle = dots)) :
Vees := plot([ Vanalytic, Vr], .6..5, labels = [r,  $\frac{V(r)}{e}$ ], linestyle = [solid, dash], title = "Potential

```

Curves for a point particle and a finite size nucleus

```

", font = [TIMES, ROMAN, 13], legend = [V(analytic), V(real)] ) :
display(Vees, line, Text, t2, t3, t4, liney, linex)

```

Potential Curves for a point particle and a finite size nucleus

