

## Hydrogen Radial Wave Functions

Define operators

```
(%i1) assume(h[bar]>0, m>0, a>0, b>0);
(%o1) [ hbar>0 , m>0 , a>0 , b>0 ]

(%i2) /* Norm of function */
N(f) := (integrate(conjugate(f)*f*r^2, r, 0, inf));
(%o2) N(f) :=  $\int_0^{\infty} \text{conjugate}(f) f r^2 dr$ 

(%i3) /* Expectation value of function */
Ex(f,op) := (integrate(conjugate(f)*op*f*r^2, r, 0, inf));
(%o3) Ex(f, op) :=  $\int_0^{\infty} \text{conjugate}(f) op f r^2 dr$ 

(%i4) /* Nabla operator */
Nabla(f) := diff(f,r);
(%o4) Nabla(f) := diff(f, r)

(%i5) /* Hamilton operator
H(f) := -h[bar]^2/(2*m)*(1/r^2)*diff(r^2*diff(f,r),r)
+ l*(l+1)*h[bar]^2/(2*m*r^2)*f - (e^2/(4*pi*epsilon[0]*r))*f)/nil;
(%o5) nil

(%i6) /* Hamilton operator */
H(f) := -h[bar]^2/(2*m)*(1/r^2)*diff(r^2*diff(f,r),r)
+ l*(l+1)*h[bar]^2/(2*m*r^2)*f - (h[bar]^2/(a*m*r))*f;
(%o6) H(f) :=  $\frac{-h_{\text{bar}}^2}{2m} \frac{1}{r^2} \text{diff}(r^2 \text{diff}(f, r), r) + \frac{l(l+1)h_{\text{bar}}^2}{2mr^2} f - \frac{h_{\text{bar}}^2}{amr} f$ 
```

Define energy levels of harmonic oscillator

```
(%i7) for n: 1 thru 3 do (
/*E[n]: -m*b^2/(2*h[bar]^2*n^2),*/
E[n]: -h[bar]^2/(2*m*a^2*n^2),
print (n, ":", E[n])
);
1 :  $-\frac{h_{\text{bar}}^2}{2a^2m}$ 
2 :  $-\frac{h_{\text{bar}}^2}{8a^2m}$ 
3 :  $-\frac{h_{\text{bar}}^2}{18a^2m}$ 
(%o7) done
```

Define Eigenfunctions

(%i8)  $\text{rhon}: 2r/(n\alpha);$   
 (%o8)  $\frac{2 r}{\alpha n}$

(%i9)  $\text{rho}: \text{ev}(\text{rhon}, [n=1]);$   
 (%o9)  $\frac{2 r}{\alpha}$

(%i10)  $\text{psi}[0]: 2*(1/\alpha)^{(3/2)}*\exp(-\text{rho}/2);$   
 (%o10)  $\frac{2 \%e^{-\frac{r}{\alpha}}}{\alpha^{3/2}}$

(%i11)  $\text{rho}: \text{ev}(\text{rhon}, [n=2]);$   
 (%o11)  $\frac{r}{\alpha}$

(%i12)  $\text{psi}[1]: 1/(2*\sqrt(2))*(1/\alpha)^{(3/2)}*(2-\text{rho})*\exp(-\text{rho}/2);$   
 (%o12) 
$$\frac{\left(2 - \frac{r}{\alpha}\right) \%e^{-\frac{r}{2 \alpha}}}{2^{3/2} \alpha^{3/2}}$$

(%i13)  $\text{psi}[2]: 1/(2*\sqrt(6))*(1/\alpha)^{(3/2)}*(\text{rho})*\exp(-\text{rho}/2);$   
 (%o13) 
$$\frac{r \%e^{-\frac{r}{2 \alpha}}}{2 \sqrt{6} \alpha^{5/2}}$$

(%i14)  $\text{rho}: \text{ev}(\text{rhon}, [n=3]);$   
 (%o14)  $\frac{2 r}{3 \alpha}$

(%i15)  $\text{psi}[3]: 1/(\sqrt(243))*(1/\alpha)^{(3/2)}*(6-6*\text{rho}+\text{rho}^2)*\exp(-\text{rho}/2);$   
 (%o15) 
$$\frac{\left(\frac{4 r^2}{9 \alpha^2} - \frac{4 r}{\alpha} + 6\right) \%e^{-\frac{r}{3 \alpha}}}{3^{5/2} \alpha^{3/2}}$$

(%i16)  $\text{psi}[4]: 1/(\sqrt(486))*(1/\alpha)^{(3/2)}*(4-\text{rho})*\text{rho}*\exp(-\text{rho}/2);$   
 (%o16) 
$$\frac{2 r \left(4 - \frac{2 r}{3 \alpha}\right) \%e^{-\frac{r}{3 \alpha}}}{27 \sqrt{6} \alpha^{5/2}}$$

```

(%i17) psi[5]: 1/(sqrt(2430))*(1/a)^(3/2)*(rho^2)*exp(-rho/2);
(%o17) 
$$\frac{4 r^2 e^{-\frac{r}{3 a}}}{81 \sqrt{30} a^{7/2}}$$


```

## Derivatives of Eigenfunctions

```

(%i18) for i: 0 thru 5 do (
  dpsi[i]: ratsimp(diff(psi[i],r)),
  print (i, ":", dpsi[i])
);

0 : 
$$-\frac{2 e^{-\frac{r}{a}}}{a^{5/2}}$$

1 : 
$$\frac{(\sqrt{2} r - 2^{5/2} a) e^{-\frac{r}{2 a}}}{8 a^{7/2}}$$

2 : 
$$-\frac{(\sqrt{6} r - 2 \sqrt{6} a) e^{-\frac{r}{2 a}}}{24 a^{7/2}}$$

3 : 
$$-\frac{(4 \sqrt{3} r^2 - 20 3^{3/2} a r + 2 3^{9/2} a^2) e^{-\frac{r}{3 a}}}{729 a^{9/2}}$$

4 : 
$$\frac{(4 r^2 - 48 a r + 72 a^2) e^{-\frac{r}{3 a}}}{243 \sqrt{6} a^{9/2}}$$

5 : 
$$-\frac{(2 \sqrt{30} r^2 - 12 \sqrt{30} a r) e^{-\frac{r}{3 a}}}{3645 a^{9/2}}$$

(%o18) done

```

## Normalization check

```

(%i19) for i: 0 thru 5 do (
    print (i, "N(psi): ", N(psi[i]), "      N(dpsi): ", N(dpsi[i]))
);

0 N(psi): 1      N(dpsi):  $\frac{1}{a^2}$ 
1 N(psi): 1      N(dpsi):  $\frac{1}{4 a^2}$ 
2 N(psi): 1      N(dpsi):  $\frac{1}{12 a^2}$ 
3 N(psi): 1      N(dpsi):  $\frac{1}{9 a^2}$ 
4 N(psi): 1      N(dpsi):  $\frac{5}{81 a^2}$ 
5 N(psi): 1      N(dpsi):  $\frac{1}{45 a^2}$ 

(%o19) done

```

Force eigenvalues F, first method (with Hamiltonian)

```

(%i20) for i: 0 thru 5 do (
    if i=0 then (Ei: E[1], l: 0)
    else if i=1 then (Ei: E[2], l: 1)
    else if i=2 then (Ei: E[2], l: 1)
    else (Ei: E[3], l: 2),
    Fpsi: H(dpsi[i])-Ei*dpsi[i],
    Fpsi: ratsimp(Fpsi),
    F1[i]: Fpsi/psi[i],
    F1[i]: (ratsimp(F1[i])),
    /*print (i, " H(dpsi): ", H(dpsi[i])),
    print (i, " Ei*dpsi: ", Ei*dpsi[i]),
    print (i, " F*psi: ", Fpsi),
    print (i, " E: ", Ei, " , F1: ", F1[i]),*/
    print (i, " E: ", Ei, " , F1: ", (F1[i]))
);

0 E:  $-\frac{h_{\text{bar}}^2}{2 a^2 m}$ , F1: 0
1 E:  $-\frac{h_{\text{bar}}^2}{8 a^2 m}$ , F1:  $-\frac{h_{\text{bar}}^2}{a m r^2}$ 
2 E:  $-\frac{h_{\text{bar}}^2}{8 a^2 m}$ , F1:  $-\frac{h_{\text{bar}}^2 r - 2 a h_{\text{bar}}^2}{2 a m r^3}$ 
3 E:  $-\frac{h_{\text{bar}}^2}{18 a^2 m}$ , F1:  $-\frac{10 h_{\text{bar}}^2 r^2 - 114 a h_{\text{bar}}^2 r + 243 a^2 h_{\text{bar}}^2}{6 a m r^4 - 54 a^2 m r^3 + 81 a^3 m r^2}$ 
4 E:  $-\frac{h_{\text{bar}}^2}{18 a^2 m}$ , F1:  $-\frac{4 h_{\text{bar}}^2 r^2 - 36 a h_{\text{bar}}^2 r + 54 a^2 h_{\text{bar}}^2}{3 a m r^4 - 18 a^2 m r^3}$ 
5 E:  $-\frac{h_{\text{bar}}^2}{18 a^2 m}$ , F1:  $-\frac{2 h_{\text{bar}}^2 r - 12 a h_{\text{bar}}^2}{3 a m r^3}$ 

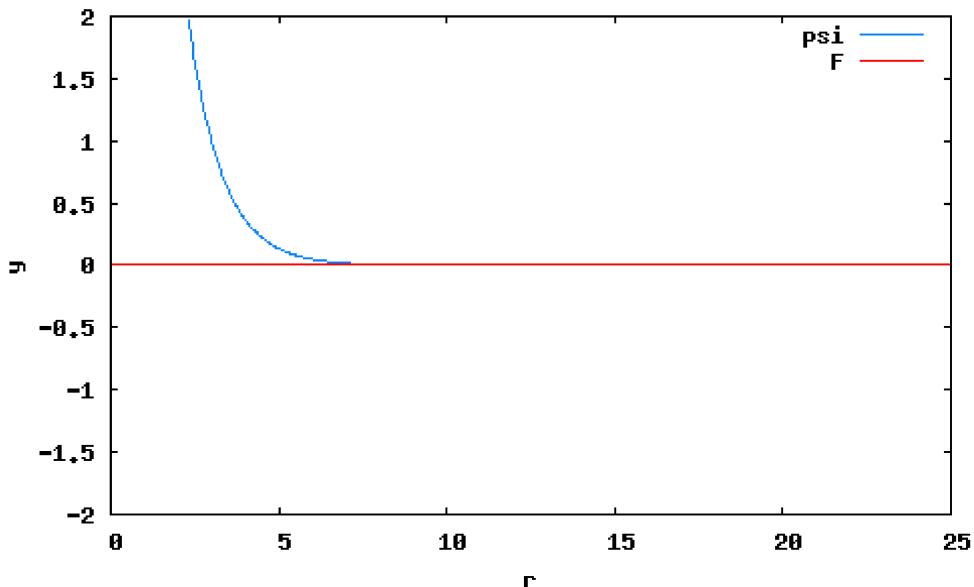
(%o20) done

```

## Plot F

```
(%i21) a: 1;
      b: 1;
      m: 1;
      h[bar]:1;
(%o21) 1
(%o22) 1
(%o23) 1
(%o24) 1
```

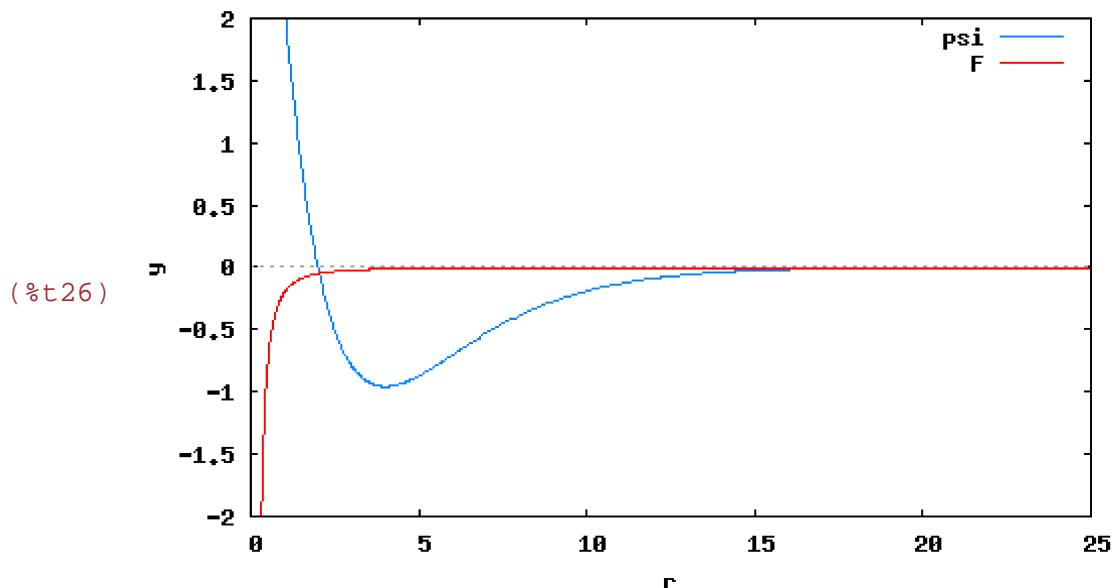
```
(%i25) for i: 0 thru 2 do (
    F1[i]: ev(F1[i]),
    psi[i]: ev(psi[i]),
    wxplot2d([10*psi[i],1/5*F1[i]],[r,0,25], [y,-2,2], [legend, "psi", "F"]);
)
plot2d: some values were clipped.
```



plot2d: some values were clipped.

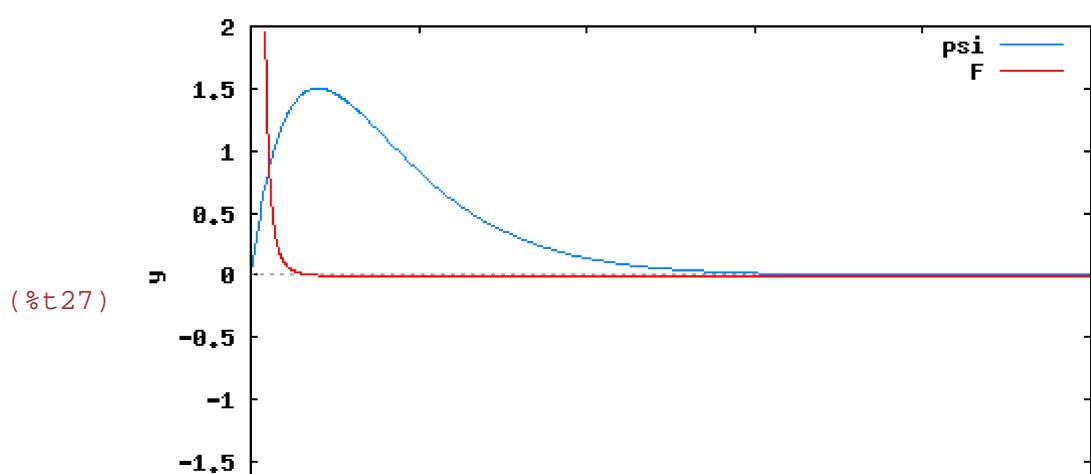
plot2d: expression evaluates to non-numeric value somewhere in plotting range

plot2d: some values were clipped.



plot2d: expression evaluates to non-numeric value somewhere in plotting range

plot2d: some values were clipped.

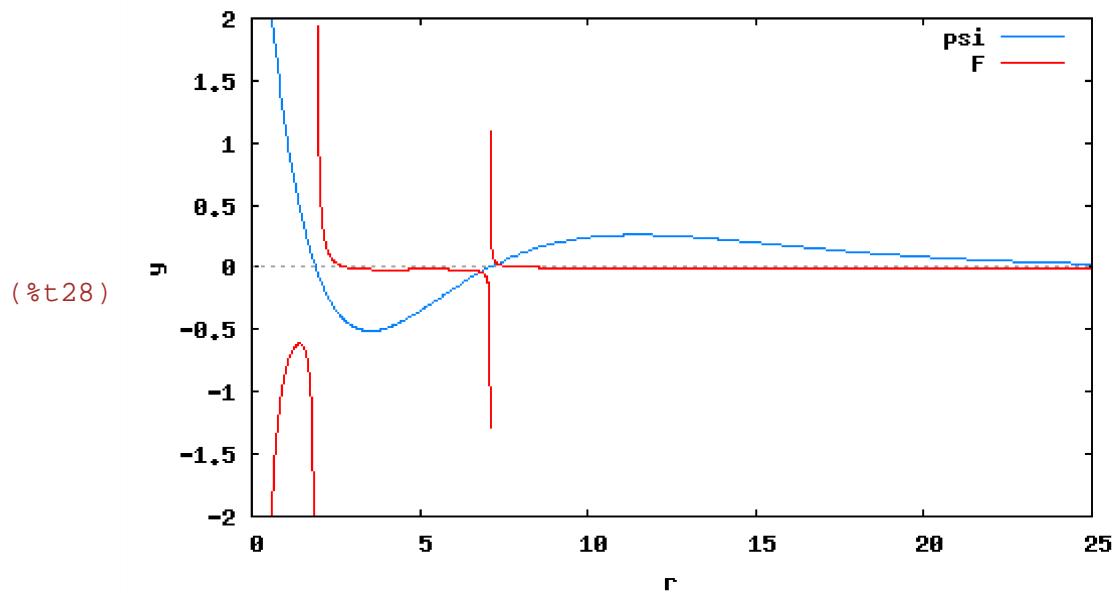


```
(%i28) for i: 3 thru 5 do (
    F1[i]: ev(F1[i]),
    psi[i]: ev(psi[i]),
    wxplot2d([10*psi[i],1/5*F1[i]],[r,0,25], [y,-2,2], [legend, "psi", "F"]);
)
```

plot2d: some values were clipped.

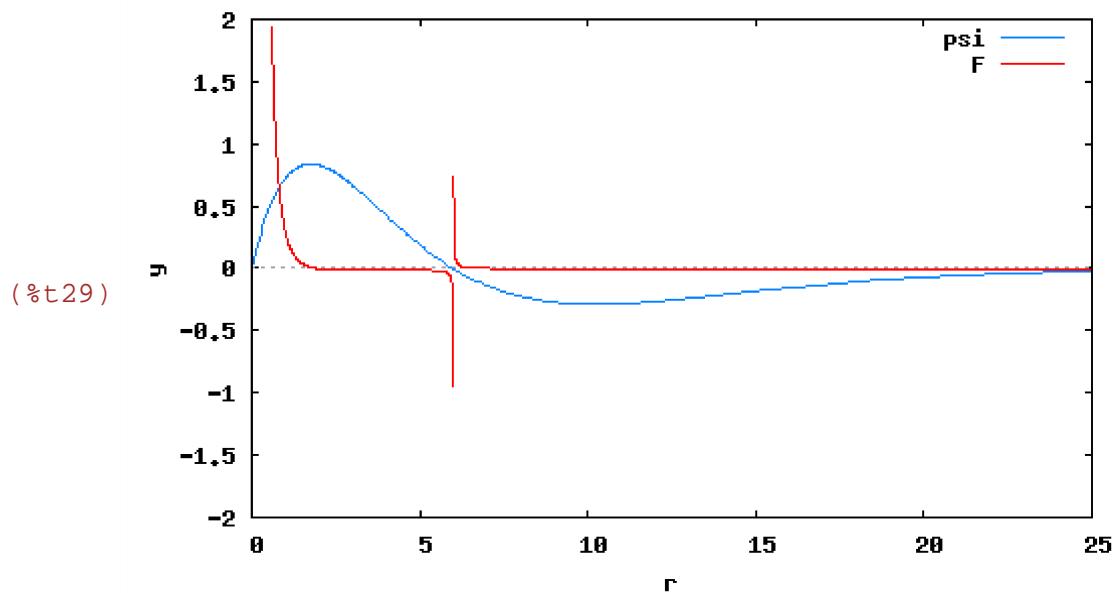
plot2d: expression evaluates to non-numeric value somewhere in plotting range

plot2d: some values were clipped.



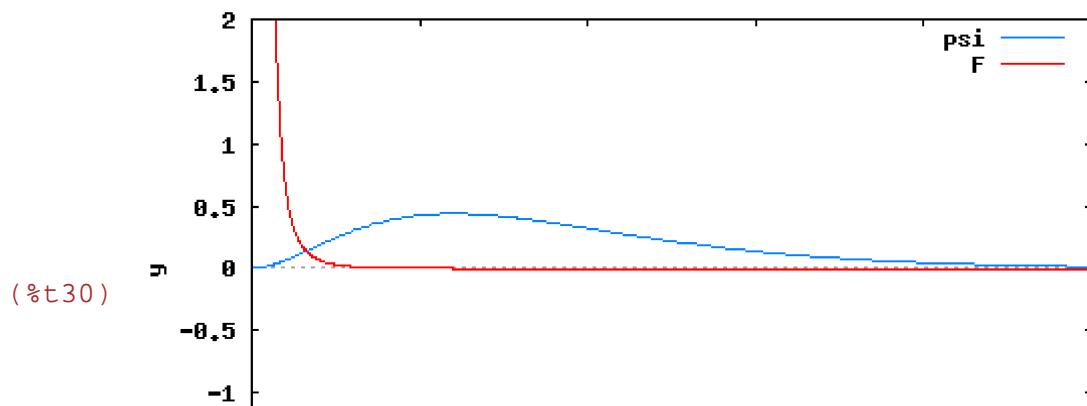
plot2d: expression evaluates to non-numeric value somewhere in plotting range

plot2d: some values were clipped.



plot2d: expression evaluates to non-numeric value somewhere in plotting range

plot2d: some values were clipped.



Expectation values of F

```
▽ (%i31) for i: 0 thru 5 do (
    ExF: Ex(psi[i],F1[i]),
    print(i, ExF)
);
```

0 0

1 - $\frac{1}{4}$

2 0

3 - $\frac{2}{9}$

4 0

5 0

(%o31) done