

## □ Spherical Harmonic Functions, F(phi)

└ Define operators

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

```
(%i2) /* Norm of function */
N(f) := integrate(integrate(conjugate(f)*f*sin(theta), theta, 0, %pi)
(%o2) N(f) := ∫02 π ∫0π conjugate(f)f sin(θ)dθ dφ
```

```
(%i3) /* Hamilton operator */
H(f) := (-h[bar]^2/(2*m*r^2)*(1/sin(theta)*diff(sin(theta)*diff(f, theta), theta)
+ 1/sin(theta)^2*diff(f, phi, 2))
));
(%o3) H(f) := 
$$\frac{-h_{\text{bar}}^2}{2mr^2} \left( \frac{1}{\sin(\theta)} \text{diff}(\sin(\theta)\text{diff}(f, \theta), \theta) + \frac{1}{\sin(\theta)^2} \text{diff}(f, \phi, 2) \right)$$

```

└ Define energy levels of harmonic oscillator

```
(%i4) for l: 0 thru 2 do (
E[l]: h[bar]^2/(2*m*r^2)*l*(l+1),
print (n, ":", E[l])
);
n : 0
n :  $\frac{h_{\text{bar}}^2}{mr^2}$ 
n :  $\frac{3h_{\text{bar}}^2}{mr^2}$ 
(%o4) done
```

└ Define Eigenfunctions

└ Y(0,0)

```
(%i5) psi[0]: 1/(2*sqrt(%pi));
(%o5)  $\frac{1}{2\sqrt{\pi}}$ 
```

└ Y(1,0)

```
(%i6) psi[1]: 1/2*sqrt(3/%pi)*cos(theta);
(%o6)  $\frac{\sqrt{3}\cos(\theta)}{2\sqrt{\pi}}$ 
```

Y(1,1)

(%i7)  $\psi[2]: -1/2\sqrt{3/(2\pi)} \sin(\theta) e^{i\phi} \exp(i\phi);$   
 (%o7) 
$$-\frac{\sqrt{3} e^{i\phi} \sin(\theta)}{2^{3/2} \sqrt{\pi}}$$

Y(2,0)

(%i8)  $\psi[3]: 1/4\sqrt{5/\pi} (3\cos^2(\theta) - 1);$   
 (%o8) 
$$\frac{\sqrt{5} (3 \cos^2(\theta) - 1)}{4 \sqrt{\pi}}$$

Y(2,1)

(%i9)  $\psi[4]: -1/2\sqrt{15/(2\pi)} \sin(\theta) \cos(\theta) e^{i\phi} \exp(i\phi);$   
 (%o9) 
$$-\frac{\sqrt{15} e^{i\phi} \cos(\theta) \sin(\theta)}{2^{3/2} \sqrt{\pi}}$$

Y(2,2)

(%i10)  $\psi[5]: 1/4\sqrt{15/(2\pi)} \sin(\theta)^2 e^{2i\phi} \exp(2i\phi);$   
 (%o10) 
$$\frac{\sqrt{15} e^{2i\phi} \sin(\theta)^2}{2^{5/2} \sqrt{\pi}}$$

phi-Derivatives of Eigenfunctions

(%i11) for i: 0 thru 5 do (  
 dps[i]: ratsimp(1/(r\*sin(theta))\*diff(psi[i],phi)),  
 print (i, ":", dps[i])  
);  
0 : 0  
1 : 0  
2 : 
$$-\frac{\sqrt{3} i e^{i\phi}}{2^{3/2} \sqrt{\pi} r}$$
  
3 : 0  
4 : 
$$-\frac{\sqrt{15} i e^{i\phi} \cos(\theta)}{2^{3/2} \sqrt{\pi} r}$$
  
5 : 
$$\frac{\sqrt{15} i e^{2i\phi} \sin(\theta)}{2^{3/2} \sqrt{\pi} r}$$
  
(%o11) done

Normalization check

```

(%i12) for i: 0 thru 5 do (
    print (i, "N(psi): ", N(psi[i]), "      N(dpsi): ", N(dpsi[i]))
);
0 N(psi): 1      N(dpsi): 0
1 N(psi): 1      N(dpsi): 0
2 N(psi): 1      N(dpsi):  $\frac{3}{2 r^2}$ 
3 N(psi): 1      N(dpsi): 0
4 N(psi): 1      N(dpsi):  $\frac{5}{2 r^2}$ 
5 N(psi): 1      N(dpsi):  $\frac{5}{r^2}$ 
(%o12) done

```

```

(%i13) E[1];
(%o13)  $\frac{h_{bar}^2}{m r^2}$ 

```

Force eigenvalues F, phi component

```

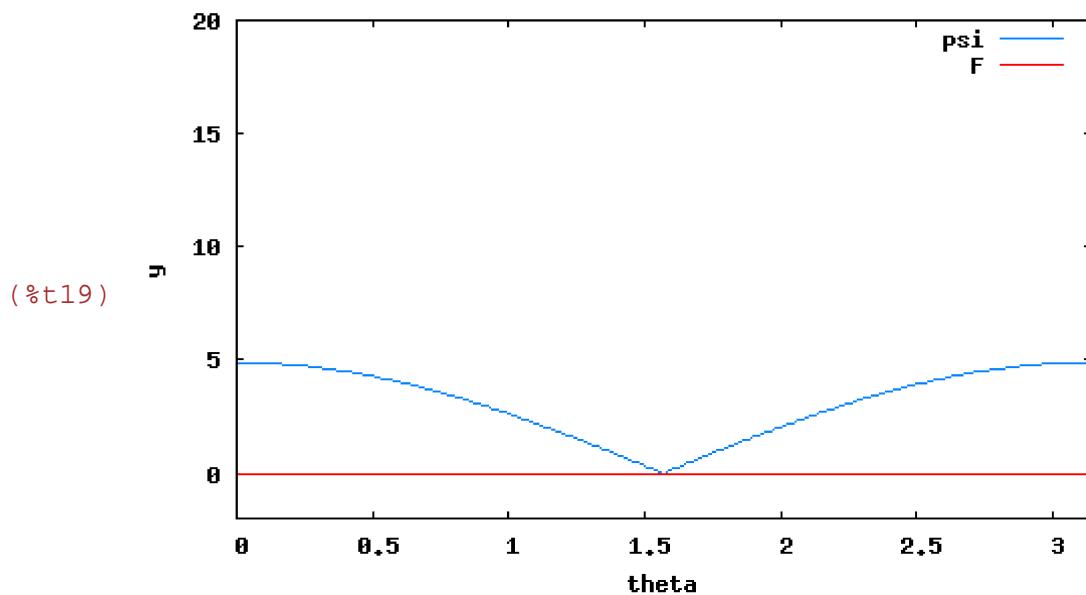
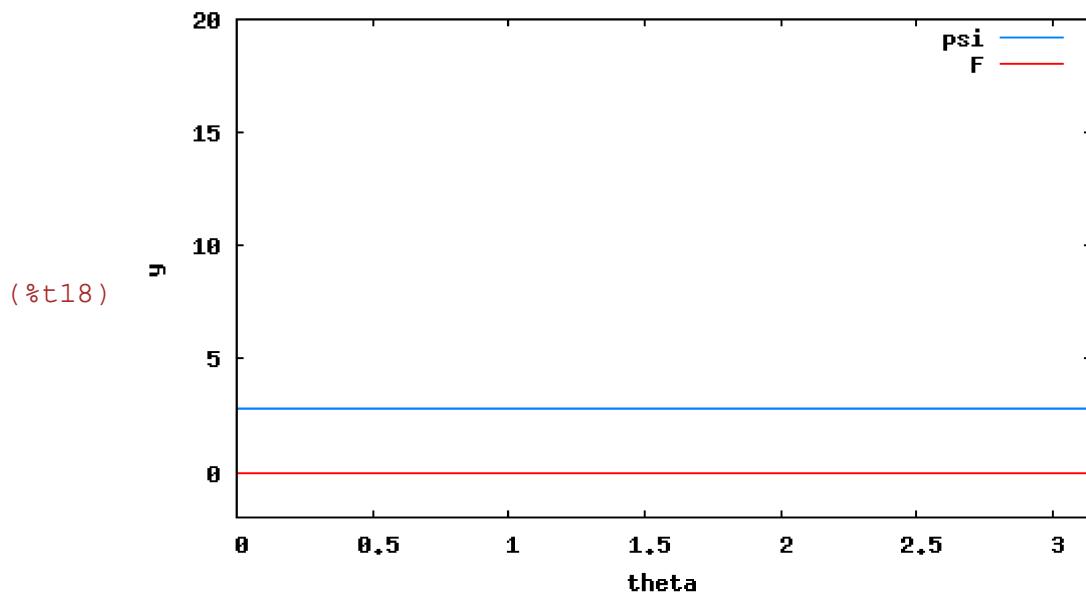
(%i14) for i: 0 thru 5 do (
    if i=0 then (Ei: E[0], l: 0)
    else if i=1 then (Ei: E[1], l: 1)
    else if i=2 then (Ei: E[1], l: 1)
    else (Ei: E[2], l: 2),
    Fpsi: H(dpsi[i])-Ei*dpsi[i],
    Fpsi: ratsimp(Fpsi),
    F1[i]: Fpsi/psi[i],
    F1[i]: factor(trigsimp((F1[i]))),
    /*print (i, " 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: 0 , F1: 0
1 E:  $\frac{h_{bar}^2}{m r^2}$  , F1: 0
2 E:  $\frac{h_{bar}^2}{m r^2}$  , F1:  $\frac{\%i h_{bar}^2 (2 \cos(\theta)^2 - 1)}{2 m r^3 \sin(\theta)^3}$ 
3 E:  $\frac{3 h_{bar}^2}{m r^2}$  , F1: 0
4 E:  $\frac{3 h_{bar}^2}{m r^2}$  , F1:  $\frac{\%i h_{bar}^2 (4 \cos(\theta)^2 - 3)}{2 m r^3 \sin(\theta)^3}$ 
5 E:  $\frac{3 h_{bar}^2}{m r^2}$  , F1:  $-\frac{\%i h_{bar}^2 (4 \sin(\theta)^2 - 3)}{m r^3 \sin(\theta)^3}$ 
(%o14) done

```

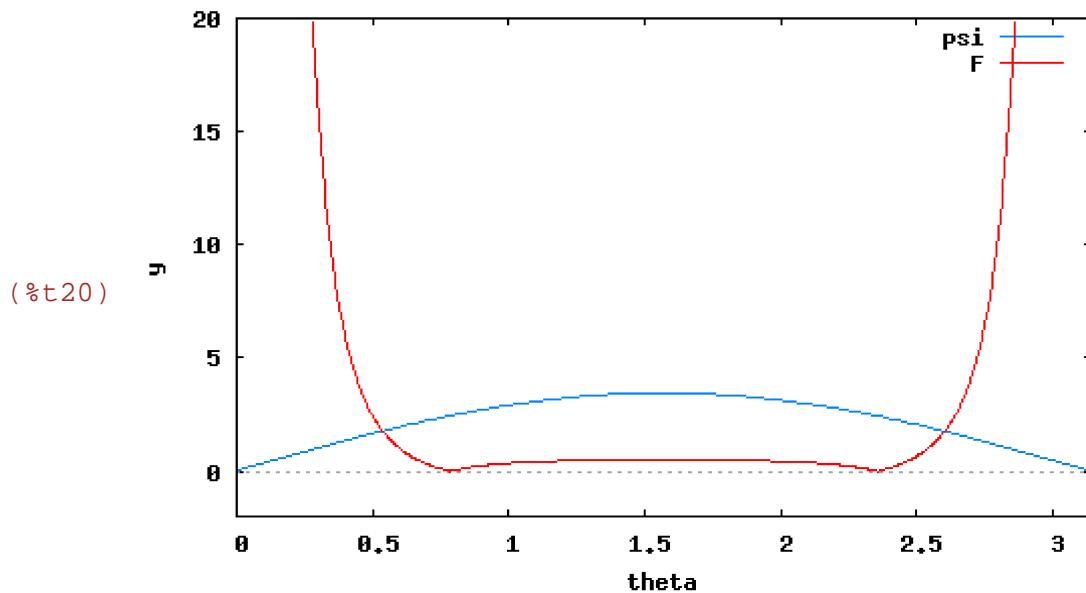
Plot F

```
(%i15) r: 1;
          m: 1;
          h[bar]:1;
(%o15) 1
(%o16) 1
(%o17) 1
```

```
(%i18) for i: 0 thru 2 do (
    F1[i]: abs(ev(F1[i])),
    wxplot2d([10*abs(psi[i]),F1[i]], [theta,0,%pi], [y,-2,20], [legend, "psi
    );
```

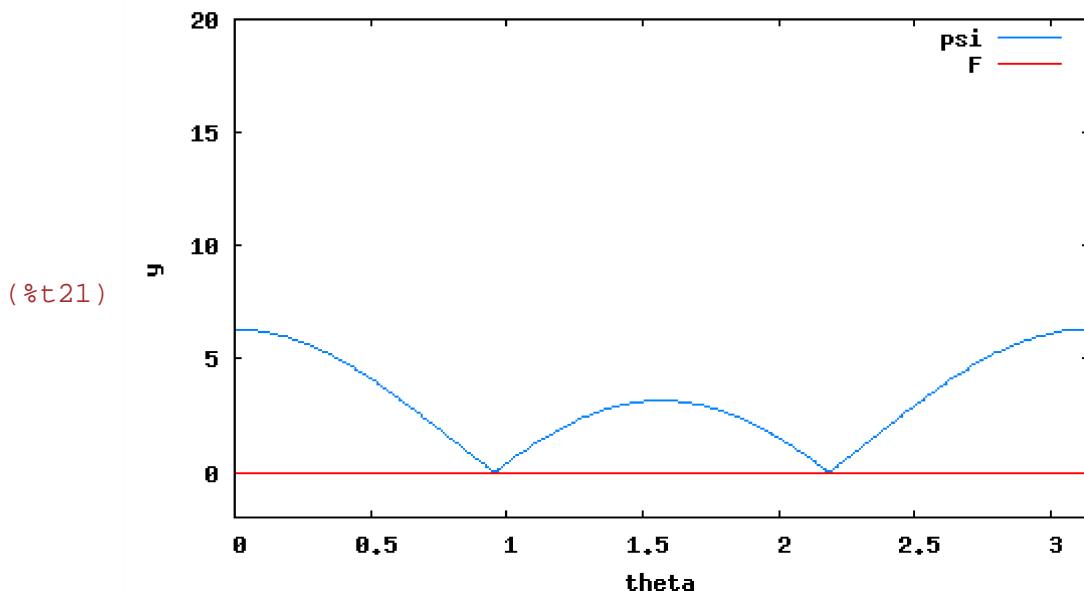


plot2d: expression evaluates to non-numeric value somewhere in plotting range  
 plot2d: some values were clipped.

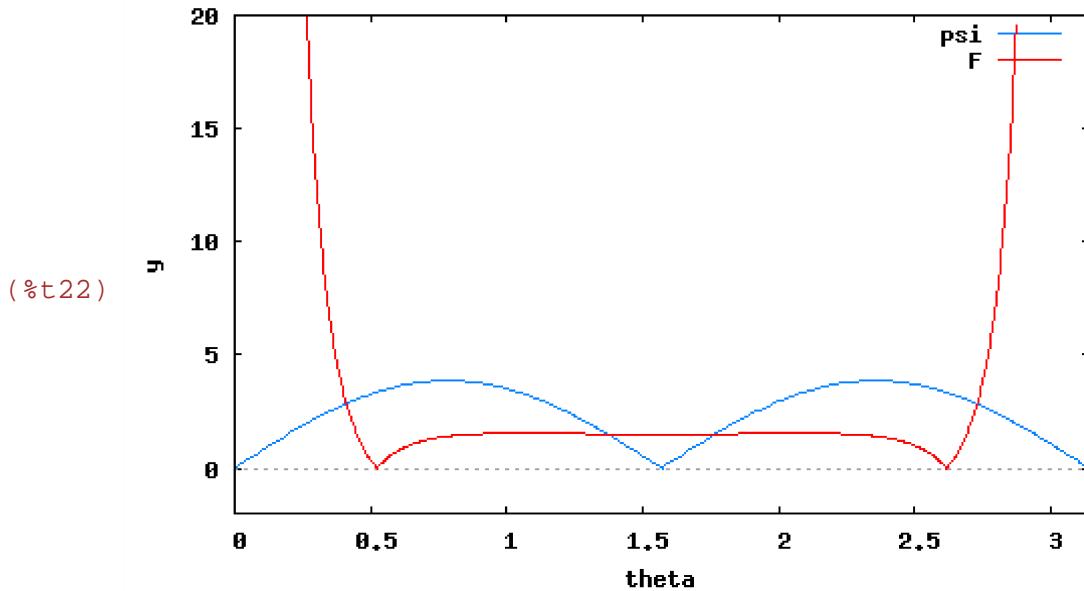


(%o20) done

```
(%i21) for i: 3 thru 5 do (
    F1[i]: abs(ev(F1[i])),
    wxplot2d([10*abs(psi[i]),F1[i]],[theta,0,%pi], [y,-2,20], [legend, "psi
    );
```



plot2d: expression evaluates to non-numeric value somewhere in plotting range  
plot2d: some values were clipped.



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