

```
(%i1) kill(all);  
(%o0) done
```

1 Virial theorem

```
(%i1) T: -1/2*U;
```

```
(T) -\frac{U}{2}
```

```
(%i2) T+U;
```

```
(%o2) \frac{U}{2}
```

```
(%i3) E: T+U;
```

```
(E) \frac{U}{2}
```

2 H energy levels

(%i4) load("D:/Work/Maxima/Ry-Hydrogen.wxm")\$

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for |\$r|

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for |\$dR|

$$0: -\frac{2 Z^{5/2} e^{-\frac{Zr}{a_0}}}{a_0^{5/2}}$$

$$1: \frac{\sqrt{Z}(\sqrt{2} Z^3 r - 2^{5/2} a_0 Z^2) e^{-\frac{Zr}{2 a_0}}}{8 a_0^{7/2}}$$

$$2: -\frac{\sqrt{Z}(\sqrt{6} Z^3 r - 2\sqrt{6} a_0 Z^2) e^{-\frac{Zr}{2 a_0}}}{24 a_0^{7/2}}$$

$$3: -\frac{\sqrt{Z}(4\sqrt{3} Z^4 r^2 - 20 \cdot 3^{3/2} a_0 Z^3 r + 2 \cdot 3^{9/2} a_0^2 Z^2) e^{-\frac{Zr}{3 a_0}}}{729 a_0^{9/2}}$$

$$4: \frac{\sqrt{Z}(4 Z^4 r^2 - 48 a_0 Z^3 r + 72 a_0^2 Z^2) e^{-\frac{Zr}{3 a_0}}}{243 \sqrt{6} a_0^{9/2}}$$

$$5: -\frac{\sqrt{Z}(2\sqrt{30} Z^4 r^2 - 12\sqrt{30} a_0 Z^3 r) e^{-\frac{Zr}{3 a_0}}}{3645 a_0^{9/2}}$$

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for |\$d2R|

$$0: \frac{2 Z^{7/2} e^{-\frac{Zr}{a_0}}}{a_0^{7/2}}$$

$$1: -\frac{\sqrt{Z}(Z^4 r - 6 a_0 Z^3) e^{-\frac{Zr}{2 a_0}}}{2^{7/2} a_0^{9/2}}$$

$$2: \frac{\sqrt{Z}(Z^4 r - 4 a_0 Z^3) e^{-\frac{Zr}{2 a_0}}}{8 \sqrt{6} a_0^{9/2}}$$

$$3: \frac{\sqrt{Z}(4\sqrt{3} Z^5 r^2 - 28 \cdot 3^{3/2} a_0 Z^4 r + 38 \cdot 3^{5/2} a_0^2 Z^3) e^{-\frac{Zr}{3 a_0}}}{2187 a_0^{11/2}}$$

$$4: -\frac{\sqrt{Z}(2\sqrt{6} Z^5 r^2 - 6^{5/2} a_0 Z^4 r + 3 \cdot 6^{5/2} a_0^2 Z^3) e^{-\frac{Zr}{3 a_0}}}{2187 a_0^{11/2}}$$

$$5: \frac{\sqrt{Z}(2\sqrt{30} Z^5 r^2 - 24\sqrt{30} a_0 Z^4 r + 36\sqrt{30} a_0^2 Z^3) e^{-\frac{Zr}{3 a_0}}}{10935 a_0^{11/2}}$$

$$0 \quad N(R): 1 \quad N(dR): \frac{Z^2}{a_0^2} \quad N(d2R): \frac{Z^4}{a_0^4}$$

$$1 \quad N(R): 1 \quad N(dR): \frac{Z^2}{4 a_0^2} \quad N(d2R): \frac{3 Z^4}{16 a_0^4}$$

$$2 \quad N(R): 1 \quad N(dR): \frac{Z^2}{12 a_0^2} \quad N(d2R): \frac{Z^4}{48 a_0^4}$$

$$3 \quad N(R): 1 \quad N(dR): \frac{Z^2}{9 a_0^2} \quad N(d2R): \frac{49 Z^4}{729 a_0^4}$$

$$4 \quad N(R): 1 \quad N(dR): \frac{5 Z^2}{81 a_0^2} \quad N(d2R): \frac{Z^4}{81 a_0^4}$$

$$5 \quad N(R): 1 \quad N(dR): \frac{Z^2}{45 a_0^2} \quad N(d2R): \frac{Z^4}{729 a_0^4}$$

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for |\$y|

ARRSTORE: use_fast_arrays=false; allocate a new property hash table for |\$dYt|

0: 0

$$1: -\frac{\sqrt{3} \sin(\theta)}{2 \sqrt{\pi}}$$

$$2: -\frac{\sqrt{3} e^{i \varphi} \cos(\theta)}{2^{3/2} \sqrt{\pi}}$$

$$3: -\frac{3 \sqrt{5} \cos(\theta) \sin(\theta)}{2 \sqrt{\pi}}$$

$$4: \frac{\sqrt{2} \sqrt{15} e^{i \varphi} \sin(\theta)^2 - \sqrt{2} \sqrt{15} e^{i \varphi} \cos(\theta)^2}{2 \sqrt{\pi}}$$

3 H energy levels

3.1 With radial functions only

```
(%i7) Ek: -1/2*(Ex32(psi[0], 1., d2psi[0]) + Ex32(psi[0],2/r,dpsi[0]));
      Ep: -Ex32(psi[0], 1/r, psi[0]);
      E: Ek+Ep;
```

$$(Ek) \quad \frac{Z^2}{2 a_0^2}$$

$$(Ep) \quad -\frac{Z}{a_0}$$

$$(E) \quad \frac{Z^2}{2 a_0^2} - \frac{Z}{a_0}$$

```
(%i8) ev(E, [Z=1, a[0]=1]);
```

$$(%o8) \quad -\frac{1}{2}$$

3.2 With 3D wave functions

```
(%i9) nabla2_psi(ps) := 1/r^2*diff(r^2*diff(ps,r),r)
      +1/(r^2*sin(theta))*diff(sin(theta)*diff(ps,theta),theta)
      +1/(r^2*sin(theta)^2)*diff(ps,phi,2);
```

$$(%o9) \quad \text{nabla}_2 \text{psi}(ps) := \frac{1}{r^2} \left(\frac{d}{dr} \left(r^2 \left(\frac{d}{dr} ps \right) \right) \right) + \frac{1}{r^2 \sin(\theta)} \left(\frac{d}{d\theta} \left(\sin(\theta) \left(\frac{d}{d\theta} ps \right) \right) \right) + \frac{1}{r^2 \sin(\theta)^2} \left(\frac{d^2}{d\phi^2} ps \right)$$

```
(%i10) nabla2_psi: ratsimp(ev(nabla2_psi(psi[0]),diff));
```

$$(\text{nabla}_2 \text{psi}) \quad \frac{\sqrt{Z} (Z^3 r - 2 a_0 Z^2) \%e^{-\frac{Zr}{a_0}}}{\sqrt{\pi} a_0^{7/2} r}$$

```
(%i14) Ek: -1/2*Ex32(psi[0], 1., nabla2_psi(psi[0]));
      Ep: -Ex32(psi[0], 1/r, psi[0]);
      E: Ek+Ep;
      ex: ev(E, [Z=1, a[0]=1]);
```

$$(Ek) \quad \frac{Z^2}{2 a_0^2}$$

$$(Ep) \quad -\frac{Z}{a_0}$$

$$(E) \quad \frac{Z^2}{2 a_0^2} - \frac{Z}{a_0}$$

$$(%o14) \quad -\frac{1}{2}$$

4 H energy levels with m(r) function

```
(%i25) m(r) := x;
```

```
(%o25) m(r) := x
```

```
(%i34) Ek: -1/2*(Ex32(psi[0], 1, nabla2_psi(1/m(r)*psi[0]));
      Ep: -Ex32(psi[0], m(r)^(1/2)/r, psi[0]);
      E: Ek+Ep;
      Ex: ev(E, [Z=1, a[0]=1, h_b=1]);
```

$$(Ek) \quad \frac{Z^2}{2 a_0^2 x}$$

$$(Ep) \quad -\frac{Z \sqrt{x}}{a_0}$$

$$(E) \quad \frac{Z^2}{2 a_0^2 x} - \frac{Z \sqrt{x}}{a_0}$$

$$(Ex) \quad \frac{1}{2x} - \sqrt{x}$$

```
(%i37) wxplot2d([Ex,-0.5], [x,0.2,2])$
```

```
(%t37)
```

