1 Define Hermite polynoms

```
(%i20) kill(all);
```

(%o0) *done*

```
(%i1) H[0](y) := 1;
      H[1](y) := 2*y;
      H[2](y) := 4*y^2-2;
      H[3](y) := 8*y^3-12*y;
      H[4](y) := 16*y^4-48*y^2+12;
      H[5](y) := 32*y^5-160*y^3+120*y;
```

(%o1) $H_0(y):=1$

(%o2) $H_1(y):=2\,y$

(%o3) $H_2(y):=4\,y^2-2$

(%o4) $H_3(y):=8\,y^3-12\,y$

(%o5) $H_4(y):=16\,y^4-48\,y^2+12$

(%o6) $H_5(y):=32\,y^5-160\,y^3+120\,y$

```
(%i7) H[5](x);
```

(%o7) $32\,x^5-160\,x^3+120\,x$

```
(%i8) psi(n,y) := (m*omega/h[bar])^(1/4)/sqrt(2^n*factorial(n)*sqrt(%pi)
```

(%o8) $\Psi(n,y):=\frac{\left(\frac{m\,\omega}{h_{bar}}\right)^{1/4}}{\sqrt{2^n\,n!\,\sqrt{\pi}}}\,H_n(y)\exp\left(\frac{-y^2}{2}\right)$

```
(%i9) /* Operator matrix element with two 3D wave functions */
      Ex32(f1,op,f2) := integrate(conjugate(f1)*op*f2, x, -inf, inf);
```

(%o9) $\mathrm{Ex32}(f1,op,f2):=\int_{-\infty}^{\infty}\mathrm{conjugate}(f1)\,op\,f2\,\mathrm{d}x$

2 Orthogonality check

```
(%i10) assume(h[bar]>0, m>0, omega>0);
```

(%o10) $[h_{bar}>0,m>0,\omega>0]$

```
(%i11) y: sqrt(m*omega/h[bar])*x;
```

(%o11) $\frac{\sqrt{m}\,\sqrt{\omega}\,x}{\sqrt{h_{bar}}}$

```
(%i12) for n1: 0 thru 5 do (
          for n2: n1 thru 5 do (
             op: 1 /**sin(theta)*cos(phi)*/,
             me: radcan(Ex32(ratsimp(psi(n2,y)), op, ratsimp(psi(n1,y)))),
             /*if me # 0 then (*/
                printf (true, "n1, n2: ~2d --> ~2d:~%", n1, n2, me),
                print(me)
        ));
n1, n2:  0 -->  0:
1
n1, n2:  0 -->  1:
0
n1, n2:  0 -->  2:
0
n1, n2:  0 -->  3:
0
n1, n2:  0 -->  4:
0
n1, n2:  0 -->  5:
0
n1, n2:  1 -->  1:
1
n1, n2:  1 -->  2:
0
n1, n2:  1 -->  3:
0
n1, n2:  1 -->  4:
0
n1, n2:  1 -->  5:
0
n1, n2:  2 -->  2:
1
n1, n2:  2 -->  3:
0
n1, n2:  2 -->  4:
0
n1, n2:  2 -->  5:
0
n1, n2:  3 -->  3:
1
n1, n2:  3 -->  4:
0
n1, n2:  3 -->  5:
0
n1, n2:  4 -->  4:
1
n1, n2:  4 -->  5:
0
n1, n2:  5 -->  5:
1
(%o12) done
```

3 Transition matrix element <n2|x|n1>

```
(%i14) for n1: 0 thru 5 do (
          for n2: n1 thru 5 do (
             op: x,
             me: radcan(Ex32(ratsimp(psi(n2,y)), op, ratsimp(psi(n1,y)))),
             /*if me # 0 then (*/
                printf (true, "n1, n2: ~2d --> ~2d:~%", n1, n2, me),
                print(me)
       ))$
```

n1, n2: 0 --> 0:

0

n1, n2: 0 --> 1:

$$\frac{\sqrt{h_{bar}}}{\sqrt{2}\sqrt{m}\sqrt{\omega}}$$

n1, n2: 0 --> 2:

0

n1, n2: 0 --> 3:

0

n1, n2: 0 --> 4:

0

n1, n2: 0 --> 5:

0

n1, n2: 1 --> 1:

0

n1, n2: 1 --> 2:

$$\frac{\sqrt{h_{bar}}}{\sqrt{m}\sqrt{\omega}}$$

n1, n2: 1 --> 3:

0

n1, n2: 1 --> 4:

0

n1, n2: 1 --> 5:

0

n1, n2: 2 --> 2:

0

n1, n2: 2 --> 3:

$$\frac{\sqrt{3}\sqrt{h_{bar}}}{\sqrt{2}\sqrt{m}\sqrt{\omega}}$$

n1, n2: 2 --> 4:

0

n1, n2: 2 --> 5:

0

n1, n2: 3 --> 3:

0

n1, n2: 3 --> 4:

$$\frac{\sqrt{2}\sqrt{h_{bar}}}{\sqrt{m}\sqrt{\omega}}$$

n1, n2: 3 --> 5:

0

n1, n2: 4 --> 4:

0