One-Dimensional Quantum Harmonic Oscillator

In this note we consider 1d time independent Schrödinger equation:

$$\hat{H}\phi_n(x) = E_n\phi_n(x) \qquad (1)$$

for quantum harmonic oscillator (a particle with a mass $1/2$ in external harmonic trapping potential $V(x) = x^2$) with Hamiltonian:

$$\hat{H} = -\frac{d^2}{dx^2} + x^2. \qquad (2)$$

Below we will derive numerically and analytically exactly energy spectrum: $E_n = 2(n + 1/2)$, where $n = 0, 1, 2, 3, ...$ and energy eigen states of equation (1). Exact results will serve as a benchmark to numerical approximation.

Numerical Solution

First we study the eigenvalue problem Eq. (1) numerically, introducing 1d grid and using the simple finite difference approximation to 1d laplacian: $\frac{d^2 f(x)}{dx^2} \to \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{(\Delta x)^2}$.

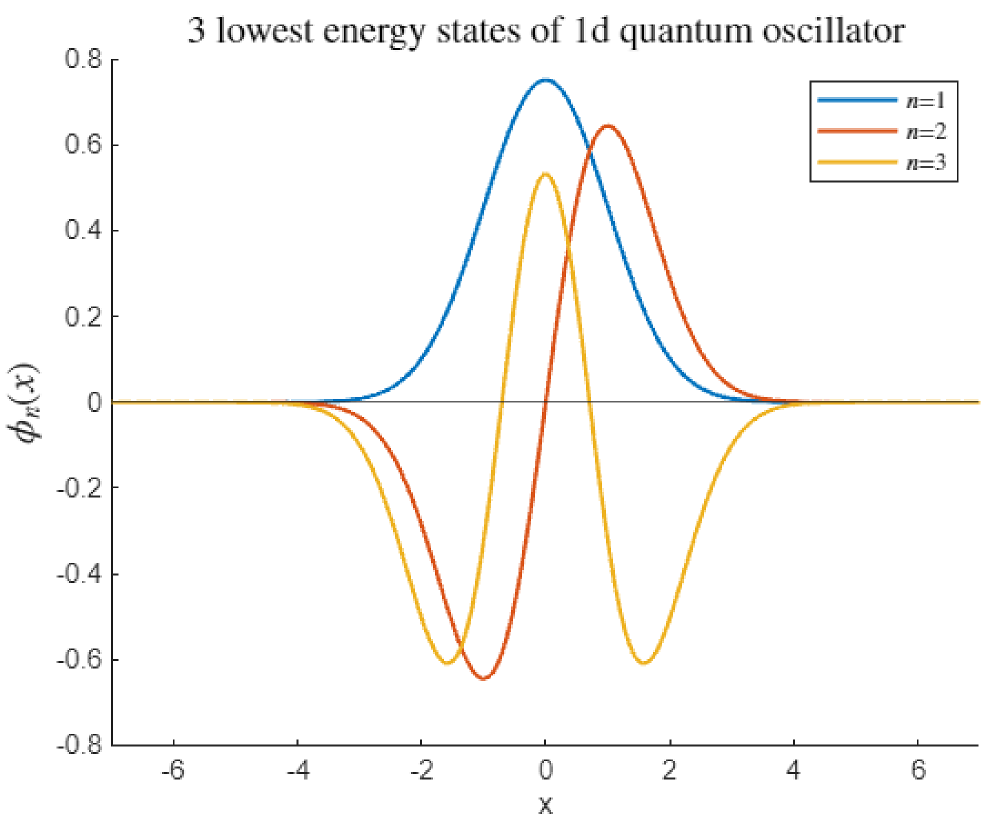
```
Rmax =70;               % half of the maximal extent of 1d simulation box
Nr = 10000;                       % number of grid points
r = linspace(-Rmax, Rmax, Nr)';   % simulation grid
dr=2*Rmax/Nr;                     % step size
d  = ones(Nr,1);
Lap_r  = spdiags([d -2*d d],[-1 0 1],Nr,Nr)/dr^2;  % second derivative as Nr x Nr
sparse matrix with -2/dr^2 on main (0) diagonal and 1/dr^2 on lower (-1) and upper
(1) diagonals
H =-Lap_r + spdiags(r.^2,0,Nr,Nr); % sparse Hamiltonian matrix
N=8;    % select number of the lowest energy eigen states and eigen values to
compute
[V,E]=eigs(H,N,'smallestreal'); % solve for N lowest eigen vectors and eigen
values
diag(E) % first N lowest energy values
```

```
ans = 8×1
    1.0001
    3.0002
    5.0003
    7.0004
    9.0004
   11.0004
   13.0003
   15.0001
```

Numerically obtained N lowest energy eigen values are N lowest positive odd integers $1, 3, 5, ..., 2N - 1$. Next, we plot obtained N lowest energy eigen functions.

```
figure
N=3;
Legend=cell(N,1);
```

```
for n=1:N
    line(r, V(:,n)./sqrt(dr));
    Legend{n}=strcat('$n$=', num2str(n));
end
legend(Legend,interpreter='Latex');
yline(0, handleVisibility='off');
xlim([-7,7]);
xlabel("x");
ylabel("$\phi_n(x)$", interpreter="Latex",fontsize=14)
title(num2str(N) + " lowest energy states of 1d quantum
oscillator",interpreter="Latex", fontsize=14 )
```



Analytical Solution

In this section we study the eigenvalue problem Eq. (1) using symbolic computation. We introduce a real number (at this moment n is not necessarily integer, but is any real number to be determined): $n = E_n/2 - 1/2$ and rewrite Eq. (1) as:

$$\phi_n'' - x^2\phi_n = -2\left(n + \frac{1}{2}\right)\phi_n. \qquad (3)$$

Next we solve Eq. (3) symbolically.

```
syms phi_n(x) n
ode = laplacian(phi_n)-x^2*phi_n+2*(n+1/2)*phi_n==0
```

```
ode(x) =
```

$$\phi_n(x)\ (2\,n+1) - x^2\,\phi_n(x) + \frac{\partial^2}{\partial x^2}\,\phi_n(x) = 0$$

```
dsolve(ode)
```

ans =

$$\frac{C_1\,\mathrm{M}_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}\left(x^2\right)}{\sqrt{x}} + \frac{C_2\,\mathrm{W}_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}\left(x^2\right)}{\sqrt{x}}$$

Hence, generic solution of second order differential Eq. (3) is given with the help of Whittaker's M and W functions as

$$\phi_n(x) = C_1\frac{M_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)}{\sqrt{x}} + C_2\frac{W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)}{\sqrt{x}}. \qquad (4)$$

Expression in Eq. (4) for real x is applicable only for $x > 0$. Now we require that $\phi_n \to 0$ for $x \to \infty$ (normalizable states), hence we have to let $C_1 = 0$, unless n is odd positive integer. If n is odd positive integer ($n = 1, 3, 5, \ldots$), then:

$$M_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2) = -\frac{\pi}{\Gamma(-n/2)\Gamma(3/2)}W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)$$

and hence for any value of n we can safely put $C_1 = 0$ in Eq. (4) to obtain the most general vanishing for $x \to \infty$ solution of Eq. (3) for $x \geq 0$ as:

$$\phi_n(x) = C_2\frac{W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)}{\sqrt{x}}. \qquad (5)$$

Whittaker's W function has a regular singularity point at $x = 0$ and to extend Eq. (5) to the region $x < 0$, where $\sqrt{x} = i\sqrt{-x}$, we have to use the following property of the Whittaker's W function, with some integer number m:

$$W_{\kappa,\mu}(ze^{2m\pi i}) = \frac{(-1)^{m+1}2\pi i\sin(2\pi\mu m)}{\Gamma(1/2-\mu-\kappa)\Gamma(1+2\mu)\sin(2\pi\mu)}M_{\kappa,\mu}(z) + (-1)^m e^{-2m\mu\pi i}W_{\kappa,\mu}(z). \qquad (6)$$

Putting in Eq. (6) values

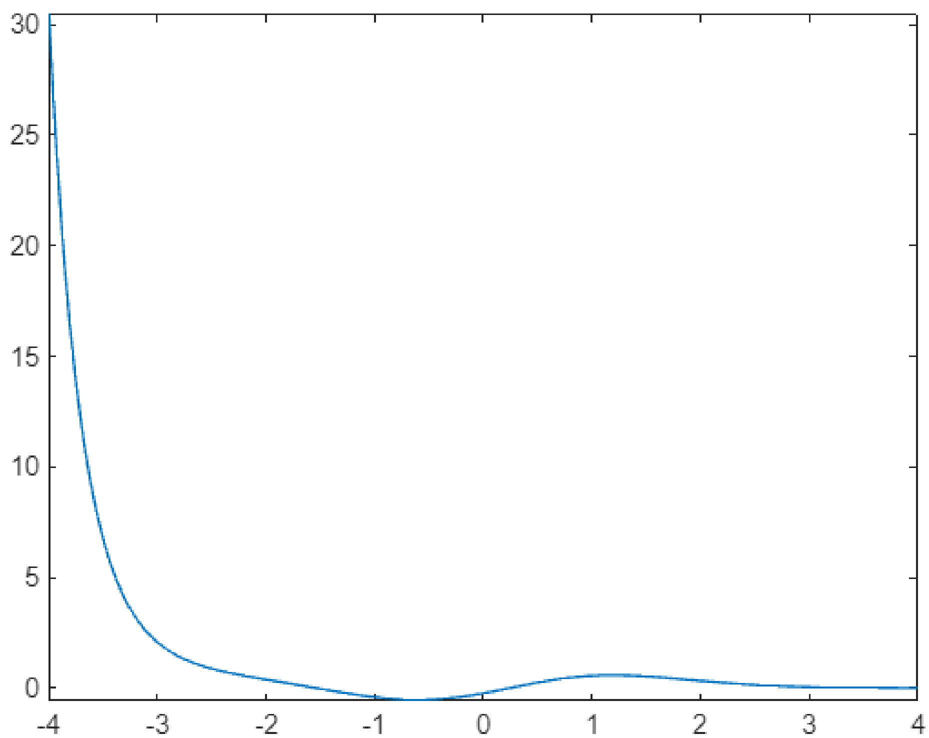
- $m = 1$
- $\kappa = n/2 + 1/4$
- $\mu = 1/4$
- $z = x^2$

we obtain

$$W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2e^{2\pi i}) = \frac{2\pi i}{\Gamma(-\frac{n}{2})\Gamma(\frac{3}{2})} M_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2) + iW_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2). \qquad (7)$$

At the end of the script we implement a function `nnps(x)` extending the expression in the right-hand-side of Eq. (5) from $x > 0$ to $x < 0$ region, using Eq. (7), for any real parameter n (for $C_2 = 1$). We call it nnps (not necessarily physical solution).

```
n=1.3;
fplot(nnps(n),[-4,4])
```



For generic values of n, if n is not a nonnegative integer number, then function `nnps(x)` (even though it is well behaved for $x > 0$) explodes for $x \to -\infty$ (due to the inevitable presence of Whittaker's M function for $x < 0$ in Eq. (7)), hence is unphysical. In order that function `nnps(x)` describes physically acceptable solutions, n **must be a nonnegative integer**. It is this step where mathematics imposes quantization of $n = 0, 1, 2, 3, \ldots$ and thus quantization of energy levels of quantum 1d harmonic oscillator $E_n = 1, 3, 5, 7, \ldots$.

- **For even nonnegative integer values** of n we have: $\Gamma(1/2 - \mu - \kappa) = \Gamma(-n/2) = \infty$, hence for even integer $n \geq 0$ we have from Eq. (7):

$$W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2e^{2\pi i}) = iW_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2) \qquad (8).$$

- **For odd positive integer values** of n the following equality holds between Whittaker's M and W functions:

$$\frac{\pi}{\Gamma(-n/2)\Gamma(3/2)} M_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2) = -W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2), \qquad (9)$$

hence for odd integer $n > 0$, using Eq. (7) and Eq. (9), we get:

$$W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2 e^{2\pi i}) = -iW_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2). \qquad (10)$$

Finally, from Eqs. (8) and (10) for any nonnegative integer n we have:

$$W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2 e^{2\pi i}) = i(-1)^n W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2). \qquad (11)$$

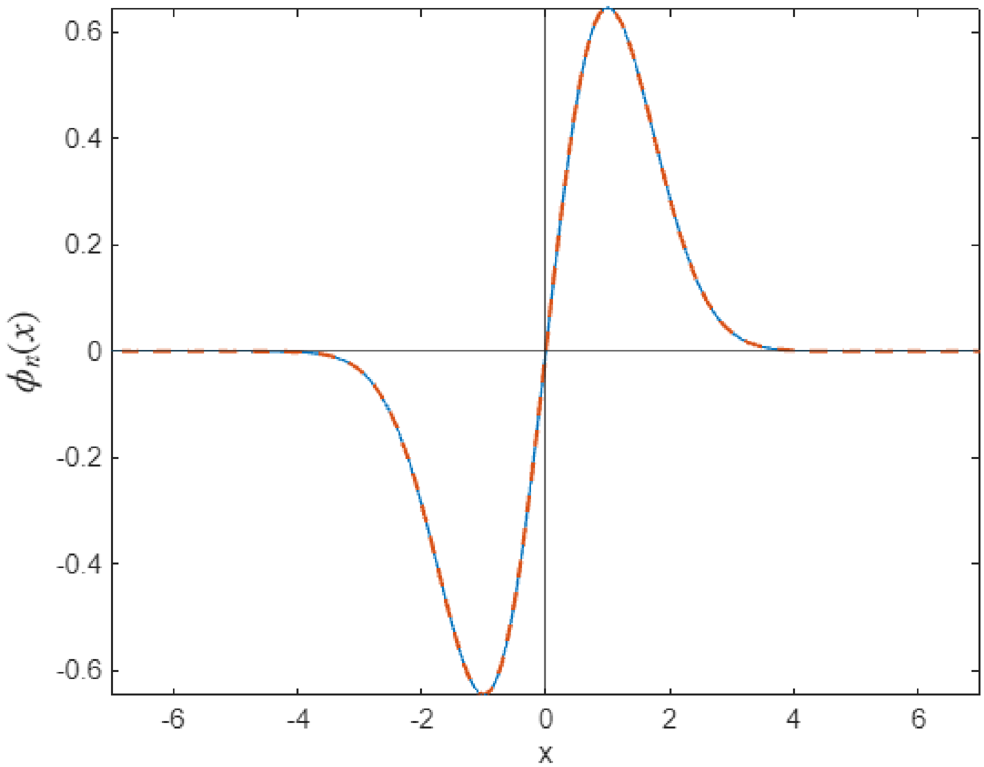
Hence 1d quantum harmonic oscillator eigen states in terms of Whittaker's W functions are given by:

$$\phi_n(x) = C_2(\mathrm{sign}(x))^n W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)/(x^2)^{1/4} = \begin{cases} C_2 W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)/\sqrt{x}, & \text{for } x \geq 0 \\ C_2(-1)^n W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)/\sqrt{-x} & \text{for } x < 0 \end{cases} \qquad (12)$$

and corresponding energies are: $E_n = 2(n + 1/2) = 2n + 1$, where $n = 0, 1, 2, 3, \ldots$

Choosing C_2 so that $\int_{-\infty}^{\infty} \phi_n^2(x)dx = 1$, at the end of the script we define symbolic function `HarmonicOscillator(n)=`$\phi_n(x)$ that implements analytically obtained eigen states using Eq. (12) for $n = 0, 1, 2, 3, \ldots$ and plot it below (continuous line), comparing with the numerically obtained eigen states (dashed line).

```
n=1;
fplot(HarmonicOscillator(n))
hold on
plot(r, V(:,n+1)./sqrt(dr),'--');  % compare to numerical solution, may need to
change sign in front of V
xlim([-7,7]);
xlabel("x");
xline(0)
yline(0)
ylabel("$\phi_n(x)$", interpreter="Latex",fontsize=14)
hold off
```




```
int(HarmonicOscillator(n)^2,-inf,inf) % check normalization
```

ans = 1

Finally, we can inspect explicit expressions of normalized eigen functions $\phi_n(x)$.

```
syms x
m=5;
phi_m(x)=HarmonicOscillator(m);
assume(x,'real')
simplify(phi_m(x))
```

ans =

$$\frac{2\sqrt{15}\,x\,e^{-\frac{x^2}{2}}\left(x^4-5\,x^2+\frac{15}{4}\right)}{15\,\pi^{1/4}}$$

We can rewite the above normalized wavefunction in Eq. (12) in terms of Hermitte-Gaussian functions $H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$ as:

$$\phi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}e^{-x^2/2}H_n(x). \qquad (13)$$

```
simplify((2^m*gamma(m+1)*sqrt(sym(pi)))^(-1/2)*exp(-x^2/2)*hermiteH(m,x))
```

ans =

$$\frac{\sqrt{15}\, x\, e^{-\frac{x^2}{2}}\, (4\, x^4 - 20\, x^2 + 15)}{30\, \pi^{1/4}}$$

Exercises

Exercise 1: In spherical coordinates solve numerically 3d harmonic oscillator and show that degeneracies of energy levels are $n(n+1)/2$, where $n = 1, 2, 3, \ldots$ and $E_1 = 3$ is non-degenerate ground state energy.

Radial equation for 3d harmonic oscillator in sector with angular momentum $\ell = 0, 1, 2, \ldots$ is:

$$-\frac{d^2\phi_{k,\ell}}{dr^2} + \left[r^2 + \frac{\ell(\ell+1)}{r^2}\right]\phi_{k,\ell} = E_{k,\ell}\phi_{k,\ell},$$

where positive integer $k = 1, 2, 3, \ldots$ enumerates energy levels in sector ℓ, with $k = 1$ corresponding to the lowest energy level in that sector.

```
Rmax =70;                         % radius of radial grid
NR = 7000;                        % number of grid points
dR=Rmax/NR;
R = linspace(dR, Rmax, NR)';      % simulation grid (radial)
d  = ones(NR,1);
l=1;
Lap_R  = spdiags([d -2*d d],[-1 0 1],NR,NR)/dR^2;  % second derivative as Nr x Nr
sparse matrix with -2/dr^2 on main (0) diagonal and 1/dr^2 on lower (-1) and upper
(1) diagonals
H =-Lap_R + spdiags(R.^2+l*(l+1)./R.^2,0,NR,NR); % sparse Hamiltonian matrix
N=6;    % select number of the lowest energy eigen states and eigen values to
compute
[V_3d,E_3d]=eigs(H,N,'smallestreal'); % solve for N lowest eigen vectors and eigen
values
diag(E_3d) % first N lowest energy values
```

```
ans = 6×1
    5.0000
    8.9998
   12.9996
   16.9993
   20.9989
   24.9984
```

$E_{k,\ell} = 2\ell + 4k - 1$, and each of these levels are $2\ell + 1$-fold degenerate, due to l^z. In addition to this degeneracy, there is a degeneracy between energy levels with different ℓ values: $E_{k,\ell} = E_{k-1,\ell+2}$, e.g. $E_{2,0} = E_{1,2}$, $E_{3,0} = E_{2,2} = E_{1,4}$ etc.

First 4 lowest energies for 4 lowest even ℓ	First 4 lowest energies for 4 lowest odd ℓ

	$\ell=0$	$\ell=2$	$\ell=4$	$\ell=6$
$k=1$	3	7	11	15
$k=2$	7	11	15	19
$k=3$	11	15	19	23
$k=4$	15	19	23	27

	$\ell=1$	$\ell=3$	$\ell=5$	$\ell=7$
$k=1$	5	9	13	17
$k=2$	9	13	17	21
$k=3$	13	17	21	25
$k=4$	17	21	25	29

Degeneracy of the energy level $E=11$, which is the 5-th lowest energy state of 3d harmonic oscillator ($n=5$) is: 1 ($\ell=0$)+5 ($\ell=2$) +9 ($\ell=4$)= $15=n(n+1)/2$.

Exercise 2: In polar coordinates solve numerically radial equation corresponding to 2d case and show that degeneracy of the energy levels is n, where $n=1$ is non-degenerate ground state level with $l^z=0$ and energy of n-th level is $2n$.

$$-\frac{d^2\phi_{k,\ell^z}}{dr^2}-\frac{1}{r}\frac{d\phi_{k,\ell^z}}{dr}+\left[r^2+\frac{(\ell^z)^2}{r^2}\right]\phi_{k,\ell^z}=E_{k,\ell^z}\phi_{k,\ell^z},$$

where $E_{k,\ell^z}=2(|\ell^z|+2k-1)$, $k=1,2,3,\ldots$ and $l^z=0,\pm1,\pm2,\ldots$

```
Rmax =70;                        % radius of radial grid
NR = 2000;                       % number of grid points
dR=Rmax/NR;
R = linspace(dR/2, Rmax, NR)';   % simulation grid (radial, avoiding R=0 point)
d  = ones(NR,1);
lz=0;
Lap_R  = spdiags([d -2*d d],[-1 0 1],NR,NR)/dR^2;  % second derivative as Nr x Nr
sparse matrix with -2/dr^2 on main (0) diagonal and 1/dr^2 on lower (-1) and upper
(1) diagonals
diff_R=spdiags([-d d],[-1 1],NR,NR)/(2*dR);        % first derivative implemented
as central finite difference (f(R+dR)-f(R-dR))/(2*dR)
H =sparse(-Lap_R-diag(1./R)*diff_R + diag(R.^2+lz.^2./R.^2)); % sparse Hamiltonian
matrix
N=6;    % select number of the lowest energy eigen states and eigen values to
compute
[V_2d,E_2d]=eigs(H,N,'smallestreal'); % solve for N lowest eigen vectors and eigen
values
diag(E_2d) % first N lowest energy values
```

```
ans = 6×1
    1.9999
    5.9997
    9.9983
   13.9956
   17.9917
   21.9865
```

Helper Functions

Symbolic function implementing analytical continuation of the right-hand-side of Eq. (5) from $x > 0$ to $x < 0$ region for $C_2 = 1$ and for any real value of parameter n,

$$\phi_n(x) = \begin{cases} W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)/\sqrt{x}, & \text{for } x \geq 0 \\ \frac{2\pi}{\Gamma(-\frac{n}{2})\Gamma(\frac{3}{2})} M_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)/\sqrt{-x} + W_{\frac{n}{2}+\frac{1}{4},\frac{1}{4}}(x^2)/\sqrt{-x}, & \text{for } x < 0 \end{cases} \tag{14}$$

```
function y = nnps(n) % implementing symbolically function in Eq. (14)
    syms x
    y =(1-heaviside(x))* (2*pi/(gamma(-n/2)*gamma(3/2))*whittakerM(n/2 + 1/4, 1/4,
x^2)/sqrt(-x) + whittakerW(n/2 + 1/4, 1/4, x^2)/sqrt(-x))...
      + heaviside(x)*whittakerW(n/2 + 1/4, 1/4, x^2)/sqrt(x);
end
```

Symbolic function implementing normalized eigen states given in Eq. (12)

```
function y = HarmonicOscillator(n)
    arguments
        n (1,1) {mustBeInteger,mustBeNonnegative}
    end
    syms x
    y =(sign(x)^mod(n,2)*whittakerW(n/2 + 1/4, 1/4, x^2)/(x^2)^(1/4));
    y=y/sqrt(int(y^2,-inf,inf));  % implementing unit normalization of probability
density
end
```