2D isotropic simple harmonics: series expansion

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Here we discuss the wavefunction of the 2D isotropic simple harmonics by solving the second-order differential equation using the series expansion method.

1. Hamiltonian and angular momentum

We consider the eigenvalue problem for the Hamiltonian of the 2D isotropic simple harmonics given by

$$\hat{H} = \frac{\hat{p}_x{}^2 + \hat{p}_y{}^2}{2\mu} + \frac{1}{2}\mu\omega_0{}^2(\hat{x}^2 + \hat{y}^2) .$$

We note that under the rotation around the *z* axis,

$$\langle \psi' | \hat{H} | \psi' \rangle = \langle \psi | \hat{H} | \psi \rangle ,$$

where

$$|\psi'\rangle = \hat{R}_z(\delta\phi)|\psi\rangle = (1 - \frac{i}{\hbar}\hat{L}_z\delta\phi)|\psi\rangle .$$

and $\hat{R}_z(\delta\phi)$ is the rotation operator around the z axis by the angle $\delta\phi$. Then we have

$$[\hat{H}, \hat{J}_z] = 0 .$$

This means that the state vector)$|\psi\rangle$ is the simultaneous eigenket of both $\hat{H}$ and $\hat{L}_z$ (orbital angular momentum).

$$\hat{H}|\psi\rangle = E|\psi\rangle , \qquad \hat{L}_z|\psi\rangle = m\hbar|\psi\rangle .$$

In the cylindrical co-ordinate, the wave function can be expressed by

$$\langle \boldsymbol{r} | \psi \rangle = \psi(\rho, \theta, z) .$$

From the symmetry of $\hat{H}$, $\psi(\rho,\theta,z)$ is independent of *z*. Here we assume that the wavefunction can be expressed by the form of separation variable

$$\psi(\rho,\phi) = R(\rho)\Phi(\phi) .$$

The differential equation for ψ can be given by

$$-\frac{\hbar^2}{2\mu}[\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\psi}{\partial\rho}) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2}] + \frac{1}{2}\mu{\omega_0}^2\rho^2 = E\psi .$$

using the cylindrical co-ordinates. The angular momentum $\hat{L}_z$ is given by

$$\langle\rho,\phi|\hat{L}_z|\psi\rangle = L_z\psi = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\psi .$$

Then we have

$$\frac{\hbar}{i}\frac{\partial}{\partial\phi}\Phi(\phi) = m\hbar\Phi(\phi) ,$$

and

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi} ,$$

where *m* is an integer; *m* = 0, ±1, ±2,…

2. Differential equation for radial wavefunction

The radial wavefunction satisfies the differential equation given by

$$-\frac{\hbar^2}{2\mu}[\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\psi}{\partial\rho}) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2}] + \frac{1}{2}\mu{\omega_0}^2\rho^2\psi = E\psi ,$$

or

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial R}{\partial\rho}) - (\frac{m^2}{\rho^2} + \frac{\mu^2{\omega_0}^2\rho^2}{\hbar^2} - \frac{2\mu E}{\hbar^2})R = 0 .$$

For convenience, we use the parameter

$$\beta = \sqrt{\frac{\hbar}{\mu\omega_0}} .$$

We also introduce a new variable x (dimensionless)

$$\rho = \beta x,$$

Then the differential equation can be rewritten as follows.

$$\frac{1}{x}\frac{\partial}{\partial x}(x\frac{\partial R}{\partial x}) - (\frac{m^2}{x^2} + x^2 - \frac{2\mu E}{\hbar^2}\beta^2)R = 0,$$

or

$$\frac{1}{x}\frac{\partial}{\partial x}(x\frac{\partial R}{\partial x}) - (\frac{m^2}{x^2} + x^2 - \lambda)R = 0,$$

or

$$R''(x) + \frac{1}{x}R'(x) - (\frac{m^2}{x^2} + x^2 - \lambda)R(x) = 0.$$

where

$$\lambda = \frac{2\mu E}{\hbar^2}\beta^2 = \frac{2E}{\hbar\omega_0} \quad \text{(eigenvalue).}$$

We now try to find the solution of this differential equation.

(a) In the limit of $x \to \infty$, we have

$$R''(x) - x^2 R(x) = 0.$$

A suitable asymptotic form of $R(x)$ is obtained as

$$R(x) \approx \exp(-\frac{x^2}{2}).$$

for which

$$R'(x) \approx -xR(x), \qquad R''(x) \approx -R(x) - xR'(x) = (x^2 - 1)R(x) \approx x^2 R(x).$$

(b) In the limit of $x \to 0$,

the dominant terms are

$$R''(x)+\frac{1}{x}R'(x)-\frac{m^2}{x^2}R(x)=0$$

We assume that

$$R(x)\approx x^s,$$

where $s\geq 0$. So we have

$$s=|m|.$$

where $|m|$ =0, 1, 2,… So $R(x)$ can be expressed by

$$R(x)\approx x^{|m|}\exp(-\frac{x^2}{2})F(x),$$

3. Series expansion I

We assume that

$$F(x)=\sum_{k=0}C_k x^k=C_0+C_1x+C_2x^2+...$$

This function $F(x)$ satisfies the differential equation,

$$xF''(x)+(1-2x^2+2|m|)F'(x)-x(2-\lambda+2|m|)F(x)=0.$$

We apply the series expansion method to find the form of $F(x)$.
From the coefficient of x,

$$(4|m|+4)C_2=(2|m|+2-\lambda)C_0,$$

From the coefficient of x^2,

$$(6|m|+9)C_3=(2|m|+4-\lambda)C_1,$$

From the coefficient of x^3,

$$(8|m|+16)C_4=(2|m|+6-\lambda)C_2,$$

From the coefficient of x^4,

$$(10|m|+25)C_5 = (2|m|+8-\lambda)C_3,$$

From the coefficient of x^5,

$$(12|m|+36)C_6 = (2|m|+10-\lambda)C_4$$

In general, we get the recursion relation between C_{k+2} and C_k,

$$(k+2)(k+2+2|m|)C_{k+2} = (2|m|+2k+2-\lambda)C_k.$$

The solution consists of even function and odd function which are independent to each other

$$F(x) = (C_0 + C_2x^2 + C_4x^4 ... + ...) + (C_1x + C_3x^3 + C_5x^5 + ...).$$

(i) Even function solution.
The series of even function must terminates at $k = 2r$, when

$$\lambda = 2|m| + 4r + 2.$$

Thus we have

$$C_0 \neq 0,\ C_2 \neq 0, ...,\ C_{2r-4} \neq 0,\ C_{2r-2} \neq 0,\ C_{2r} \neq 0,\ C_{2r+2} = 0,\ C_{2r+4} = 0, ...$$

and

$$F(x) = C_0x^0 + C_2x^2 + ... + C_{2r}x^{2r}.$$

(ii) Odd function solution.
The series of odd function must terminate at $k = 2r-1$, when

$$\lambda = 2|m| + 4r.$$

Then we have

$$C_1 \neq 0,\ C_3 \neq 0 ...,\ C_{2r-3} \neq 0,\ C_{2r-1} \neq 0,\ C_{2r+1} = 0,\ C_{2r+3} = 0, ...$$

$$F(x) = C_1x + C_3x^3 + ... + C_{2r-1}x^{2r-1}$$

In this case, when $x \to 0$,

$$R(x) = x^{|m|} F(x) \approx C_1 x^{|m|+1}$$

which is different from the predicted behavior of $R(x) \approx x^{|m|}$ in the limit of $x \to 0$. So we need to conclude that

$$C_1 = 0.$$

leading to $C_1 = C_3 = ... = 0$ from the recursion relation.

In conclusion, we have only the even function wave function given by

$$F(x) = C_0 + C_2 x^2 + ... + C_{2r} x^{2r}.$$

From the expression of λ,

$$\lambda = \frac{2E}{\hbar\omega_0} = 2|m| + 4r + 2$$

we have the energy eigenvalue as

$$E = (|m| + 2r + 1)\hbar\omega_0$$

where r = 0, 1, 2, 3, …. Here we introduce a new quantum number n as

$$n = |m| + 2r.$$

So that we have

$$E_n = (n+1)\hbar\omega_0.$$

which depends only on n.

(a) For n = 0, the degeneracy = 1 $E_1 = \hbar\omega_0$

$$r = 0 \quad |m| = 0$$

(b) For n = 1, the degeneracy = 2 $E_2 = 2\hbar\omega_0$

$r = 0 \quad |m| = 1$

(c) For $n = 2$, the degeneracy = 3, $E_2 = 3\hbar\omega_0$

$r = 0 \quad |m| = 2$

$r = 1 \quad |m| = 0$

(d) For $n = 3$, the degeneracy = 4, $E_3 = 4\hbar\omega_0$

$r = 0 \quad |m| = 3$

$r = 1 \quad |m| = 1$

(e) For $n = 4$, the degeneracy = 5, $E_4 = 5\hbar\omega_0$

$r = 0 \quad |m| = 4$

$r = 1 \quad |m| = 2$

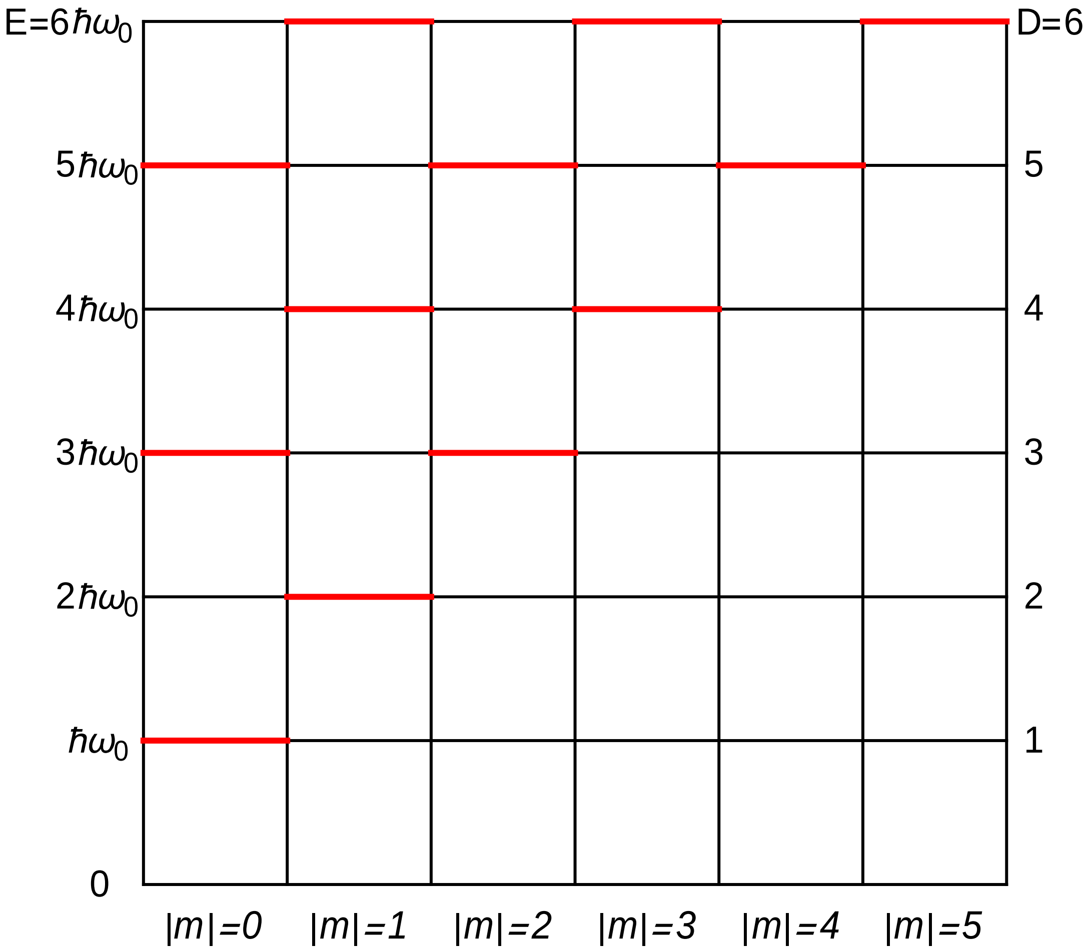
$r = 2 \quad |m| = 0$

(f) For $n = 5$, the degeneracy = 6, $E_5 = 6\hbar\omega_0$

$r = 0 \quad |m| = 5$

$r = 1 \quad |m| = 3$

$r = 2 \quad |m| = 1$



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4. Series expansion II

We start with

$$xF''(x) + (1 - 2x^2 + 2|m|)F'(x) - x(2 - \lambda + 2|m|)F(x) = 0 .$$

For simplicity we use the variable y as

$$x^2 = y , \qquad x = \sqrt{y} , \qquad F(x) = f(x^2) = f(y)$$

$$\frac{d}{dx} = \frac{dy}{dx}\frac{d}{dy} = 2x\frac{d}{dy} = 2\sqrt{y}\frac{d}{dy} ,$$

$$\frac{d^2}{dx^2} = 2\sqrt{y}\frac{d}{dy}(2\sqrt{y}\frac{d}{dy}) = 4\sqrt{y}\frac{d}{dy}(\sqrt{y}\frac{d}{dy})$$

Then we get

$$y\frac{d^2}{dy^2}f+(1-y+|m|)\frac{d}{dy}f+\frac{(\lambda-2-2|m|)}{4}f=0$$

Suppose that

$$f(y)=C_0+C_1y+...+C_ry^r+....$$

We apply the series expansion method to find the form of $f(y)$.
From the coefficient of y,

$$-\frac{1}{4}(6-\lambda+2|m|)C_1+2(2+|m|)C_2=0$$

From the coefficient of y^2,

$$-\frac{1}{4}(10-\lambda+2|m|)C_2+3(3+|m|)C_3=0$$

From the coefficient of y^3,

$$-\frac{1}{4}(14-\lambda+2|m|)C_3+4(4+|m|)C_4=0$$

From the coefficient of y^4,

$$-\frac{1}{4}(18-\lambda+2|m|)C_4+5(5+|m|)C_5=0$$

In general case, we get the recursion relation

$$-\frac{1}{4}(2+4k-\lambda+2|m|)C_k+(k+1)(k+1+|m|)C_{k+1}=0$$

or

$$C_{k+1}=\frac{(2+4k-\lambda+2|m|)}{4(k+1)(k+1+|m|)}C_k$$

The series of $f(y)$ must terminate at $k = r$, when

$$\lambda = 2 + 4r + 2|m| = 2 + 2(2r + |m|) = 2 + 2n \quad \text{(eigenvalue)}$$

with

$$n = 2r + |m| .$$

In this case, we have

$$C_0 \neq 0,\ C_1 \neq 0, \ldots,\ C_{r-2} \neq 0,\ C_{r-1} \neq 0,\ C_r \neq 0,\ C_{r+1} = 0,\ C_{r+2} = 0, \ldots$$

and

$$f(y) = C_0 + C_1 y + \ldots + C_r y^r .$$

When $\lambda = 2 + 2n$, $f(y)$ satisfies the differential equation as

$$y \frac{d^2}{dy^2} f + (1 - y + |m|) \frac{d}{dy} f + \frac{(n - |m|)}{2} f = 0 .$$

The solution of this differential equation is given by

$$f = L_{\frac{n-|m|}{2}}^{|m|}(y) = L_{\frac{n-|m|}{2}}^{|m|}(x^2)$$

Then we have

$$\psi_{n,m}(x, \phi) = \frac{1}{\sqrt{\pi}} (-1)^{\frac{n-|m|}{2}} e^{im\phi} \sqrt{\frac{[\frac{(n-|m|)}{2}]!}{[\frac{(n+|m|)}{2}]!}} \exp(-\frac{x^2}{2}) x^{|m|} L_{\frac{n-|m|}{2}}^{|m|}(x^2)$$

$$= \frac{1}{\sqrt{2\pi}} e^{im\phi} P_{n,m}(x)$$

where

$$P_{n,m}(x)=(-1)^{\frac{n-|m|}{2}}\sqrt{2\frac{[\frac{(n-|m|)}{2}]!}{[\frac{(n+|m|)}{2}]!}}\exp(-\frac{x^2}{2})x^{|m|}L_{\frac{n-|m|}{2}}^{|m|}(x^2)$$

The orthogonality takes the form as

$$\begin{aligned}\delta_{n,n'}\delta_{m,m'}&=\int dxxd\phi\psi_{n',m'}{}^*(x,\phi)\psi_{n,m}(x,\phi)\\&=\int dxxd\phi\frac{1}{\sqrt{2\pi}}e^{-im'\phi}P_{n',m'}(x)\frac{1}{\sqrt{2\pi}}e^{im\phi}P_{n,m}(x)\\&=\int_0^\infty dxxP_{n',m'}(x)P_{n,m}(x)\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i(m-m')\phi}\\&=\int_0^\infty dxxP_{n',m'}(x)P_{n,m}(x)\end{aligned}$$

which reduces to

$$\delta_{n,n'}=\int_0^\infty xdxP_{n',m}(x)P_{n,m}(x)$$

$L_{2(n-|m|)}^{|m|}(x^2)$ is the associated Laguerre function, the associated Laguerre polynomial is given

$L_\beta^\alpha(x)$ LaguerreL[β, α, x] (Mathematica)

(a) For $n = 0$, the degeneracy = 1 $E_1=\hbar\omega_0$

$r=0$ $|m|=0$ $L_{\frac{n-|m|}{2}}^{|m|}(x^2)=L_0^0(x^2)=1$

(b) For $n = 1$, the degeneracy = 2 $E_2=2\hbar\omega_0$

$r=0$ $|m|=1$ $L_{\frac{n-|m|}{2}}^{|m|}(x^2)=L_0^1(x^2)=1$

(c) For $n = 2$, the degeneracy = 3, $E_2=3\hbar\omega_0$

$r = 0 \quad |m| = 2 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^2_0(x^2) = 1$

$r = 1 \quad |m| = 0 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^0_1(x^2) = 1 - x^2$

(d) For n = 3, the degeneracy = 4, $E_3 = 4\hbar\omega_0$

$r = 0 \quad |m| = 3 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^3_0(x^2) = 1$

$r = 1 \quad |m| = 1 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^1_1(x^2) = 2 - x^2$

(e) For n = 4, the degeneracy = 5, $E_4 = 5\hbar\omega_0$

$r = 0 \quad |m| = 4 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^4_0(x^2) = 1 - x^2$

$r = 1 \quad |m| = 2 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^2_1(x^2) = 3 - x^2$

$r = 2 \quad |m| = 0 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^0_2(x^2) = \frac{1}{2}(2 - 4x^2 + x^4)$

(f) For n = 5, the degeneracy = 6, $E_5 = 6\hbar\omega_0$

$r = 0 \quad |m| = 5 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^5_0(x^2) = 1$

$r = 1 \quad |m| = 3 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^3_1(x^2) = 4 - x^2$

$r = 2 \quad |m| = 1 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^1_2(x^2) = \frac{1}{2}(6 - 6x^2 + x^4)$

(g) For n = 6, the degeneracy = 7, $E_5 = 7\hbar\omega_0$

$r = 0 \quad |m| = 6 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^6_0(x^2) = 1$

$r = 1 \quad |m| = 4 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^4_1(x^2) = 5 - x^2$

$r = 2 \quad |m| = 2 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^2_2(x^2) = \frac{1}{2}(12 - 8x^2 + x^4)$

$r = 3 \quad |m| = 0 \qquad L^{|m|}_{\frac{n-|m|}{2}}(x^2) = L^0_3(x^2) = \frac{1}{6}(6 - 18x^2 + 9x^4 - x^3)$

5. Probability density plot

$$1 = \int_0^\infty x dx [P_{n,m}(x)]^2$$

where

$$x[P_{n,m}(x)]^2 = 2(-1)^{n-|m|} \frac{[\frac{(n-|m|)}{2}]!}{[\frac{(n+|m|)}{2}]!} \exp(-x^2) x^{2|m|+1} [L^{|m|}_{\frac{n-|m|}{2}}(x^2)]^2$$

The classical limit of x is obtained from the energy conservation that

$$E = \hbar\omega_0(n+1) = K + \frac{1}{2}\mu\omega_0{}^2\rho^2 = K + \frac{1}{2}\hbar\omega_0 x^2$$

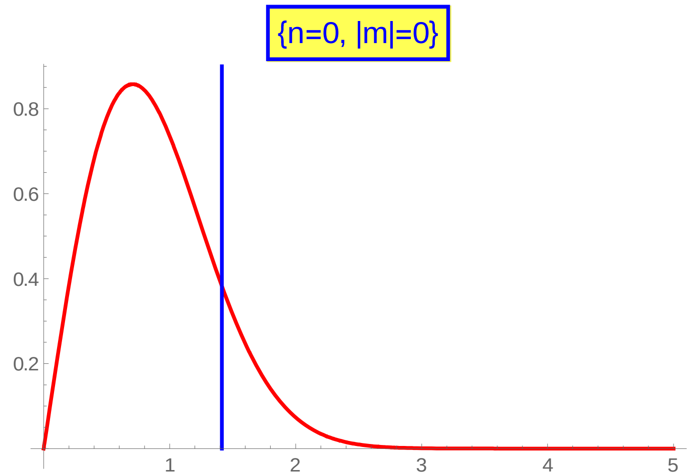
with the kinetic energy $K = 0$. Since

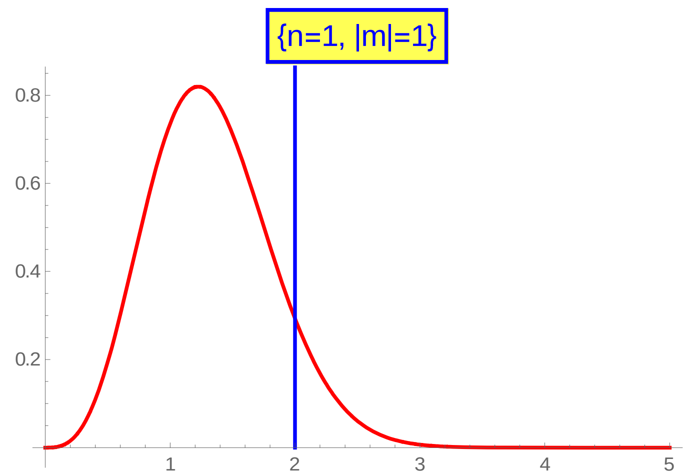
$$\hbar\omega_0(n+1) = \frac{1}{2}\hbar\omega_0 x_{cl}{}^2$$

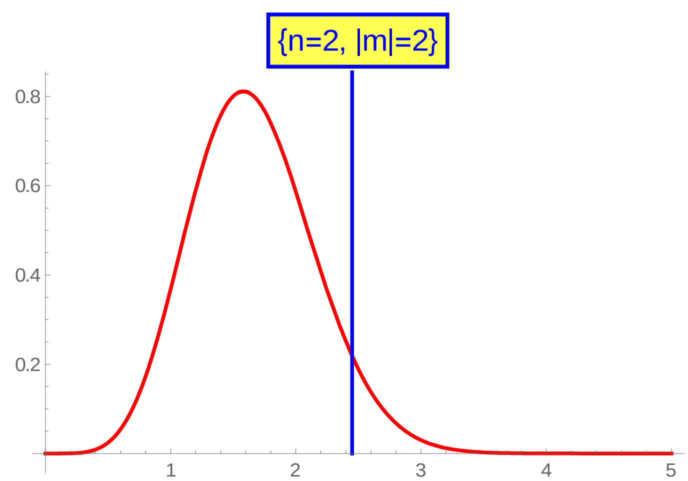
we het the classical limit x_{cl}

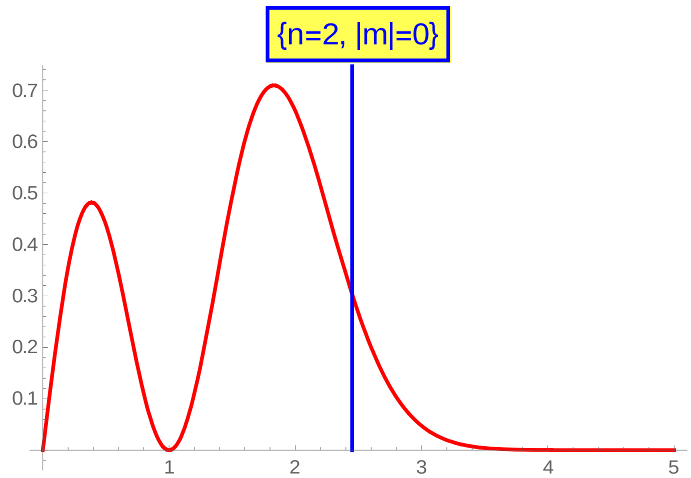
$$x_{cl} = \sqrt{2n+2}\,.$$

Here we make a plot of the probability density $x[P_{n,m}(x)]^2$ as a function of x and the line of the classical limit for each n and $|m|$ by using the Mathematica.





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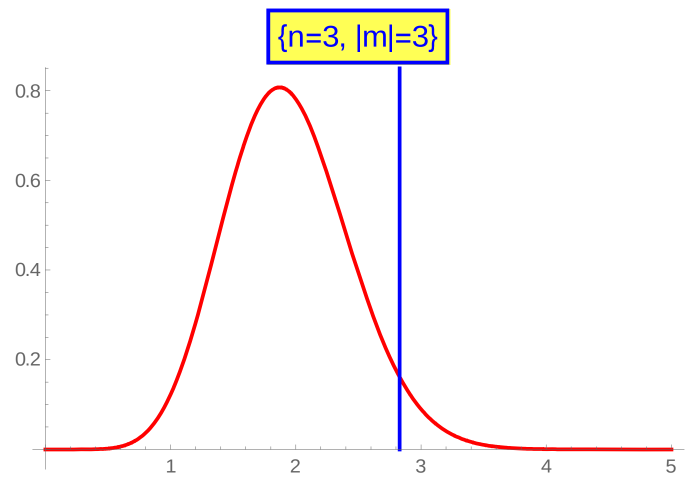
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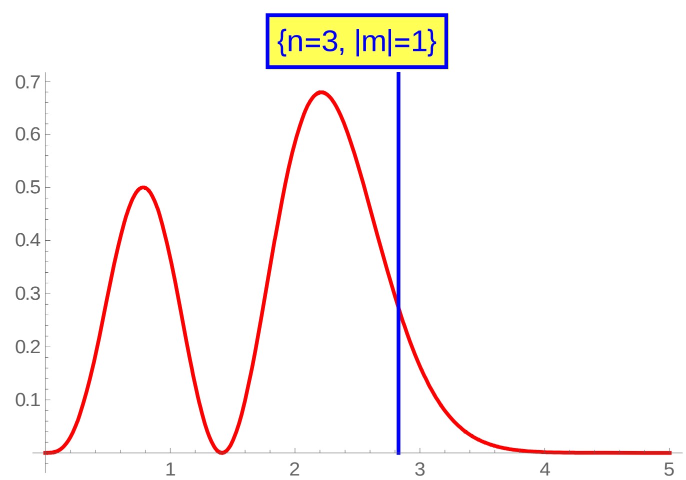
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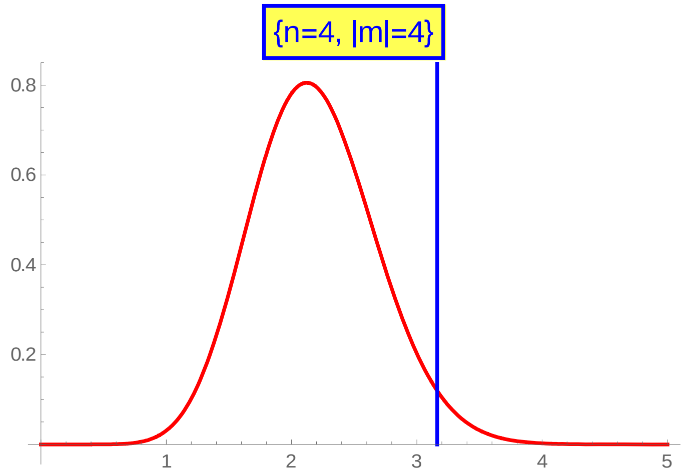
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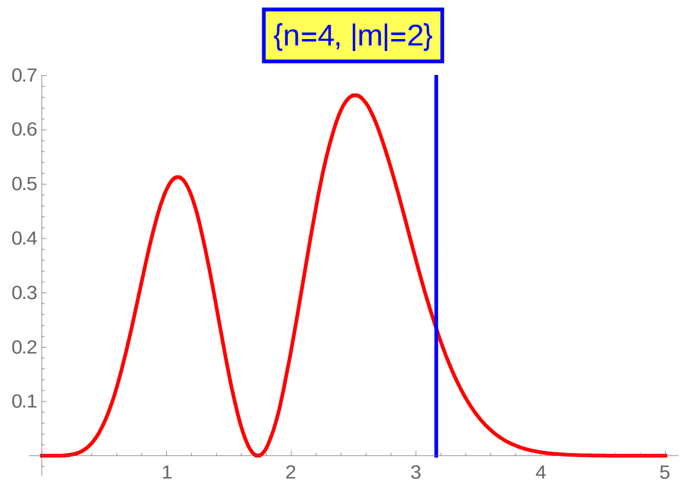
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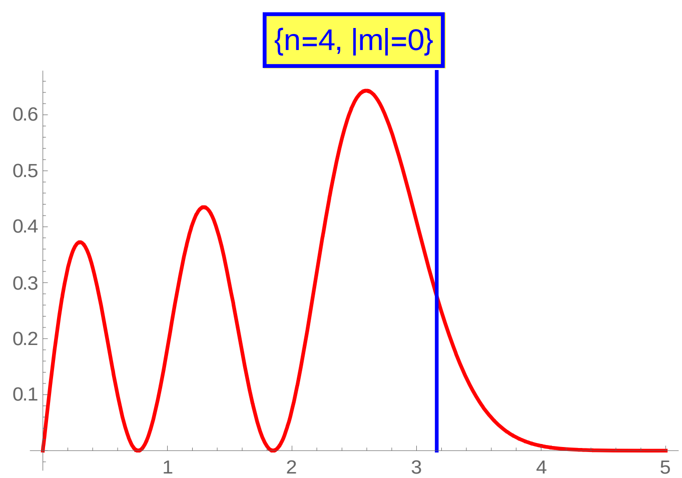
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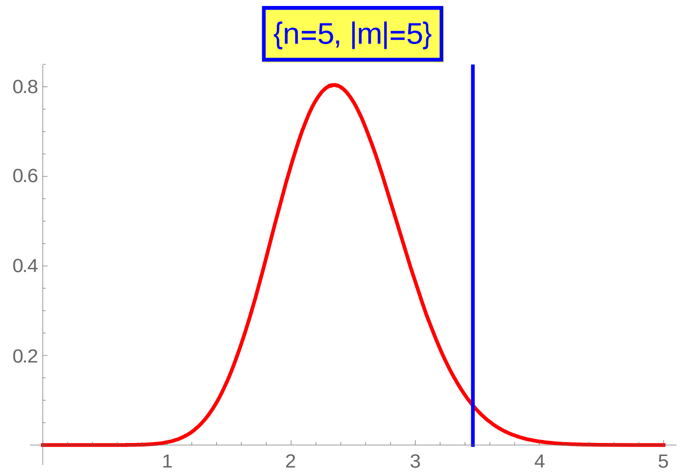
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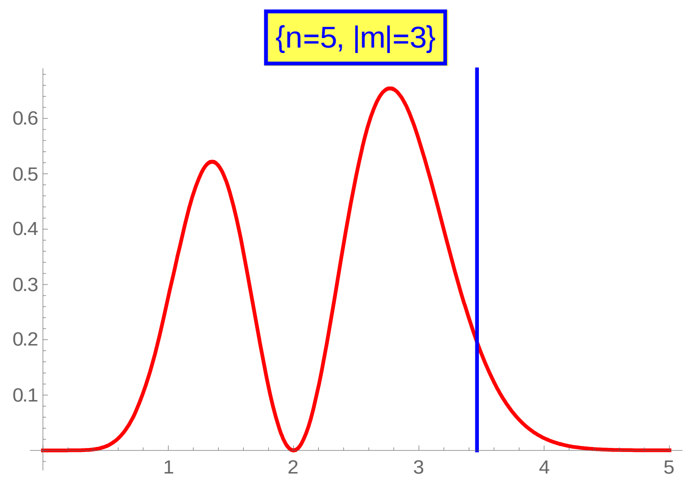
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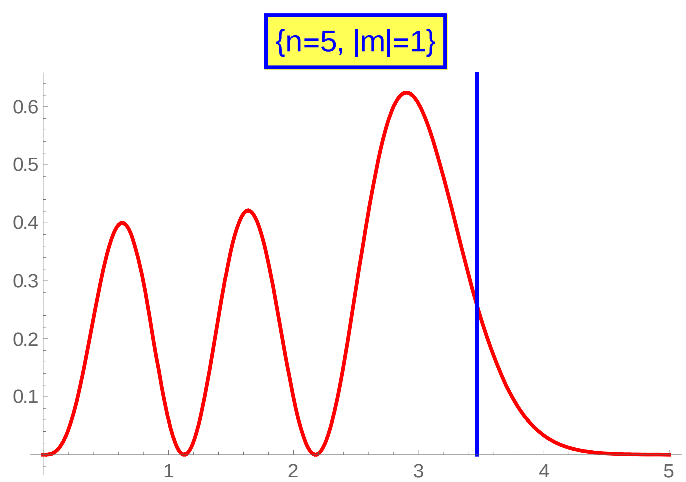
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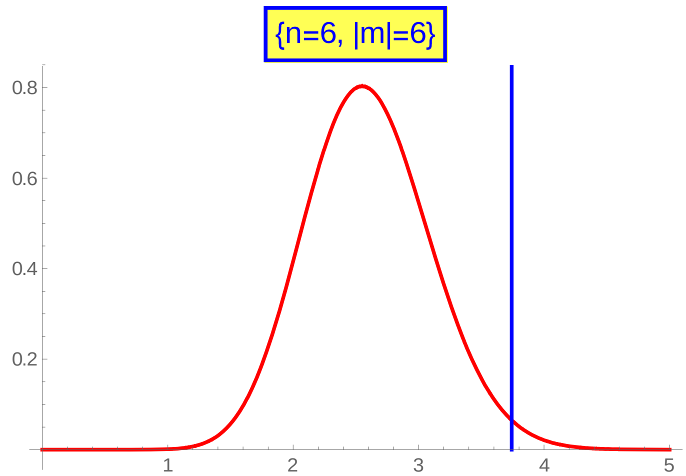
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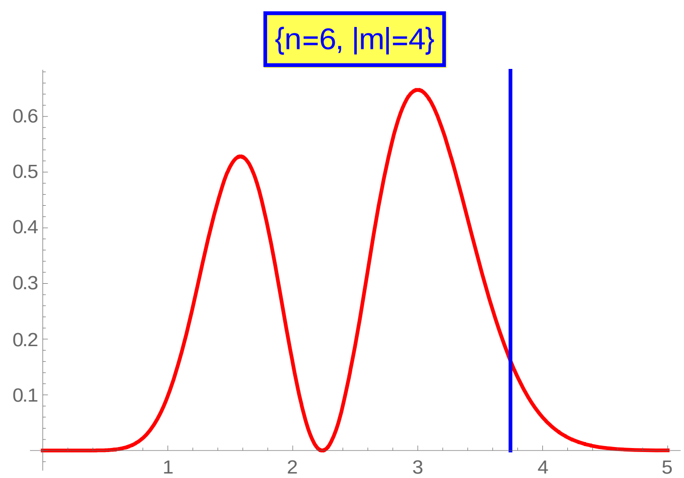
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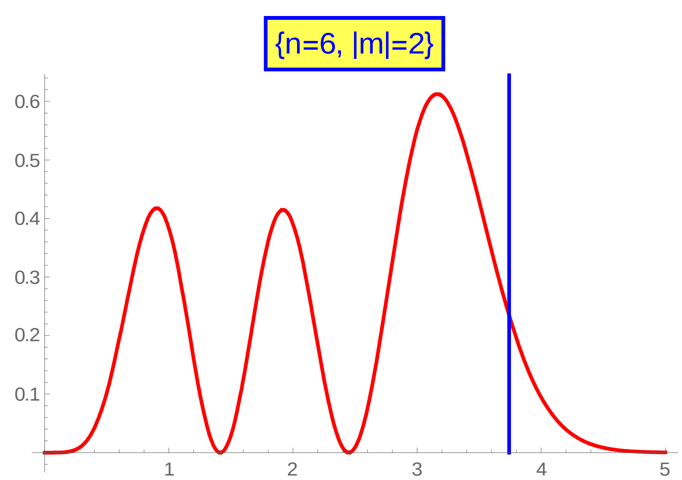
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0.4
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0.1
1
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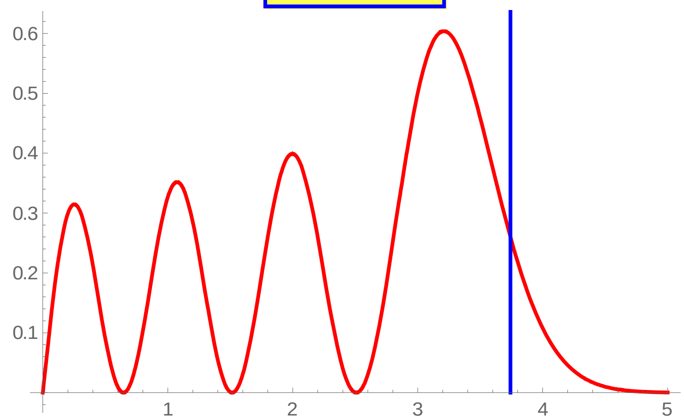
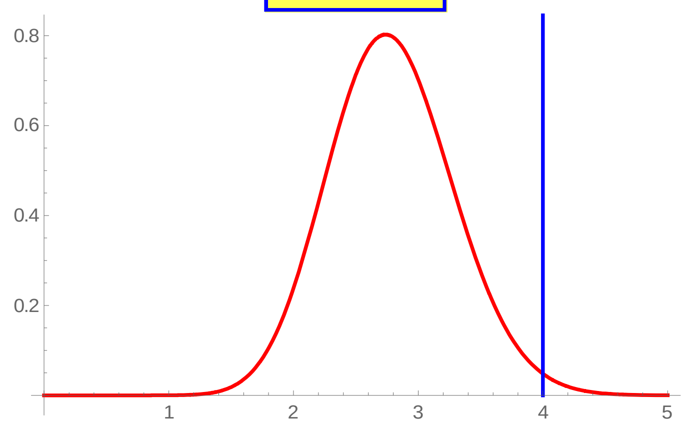
3
4
5

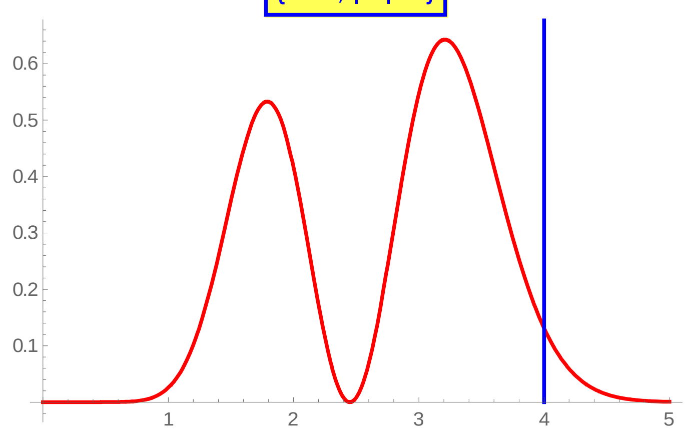
{n=6, |m|=0}

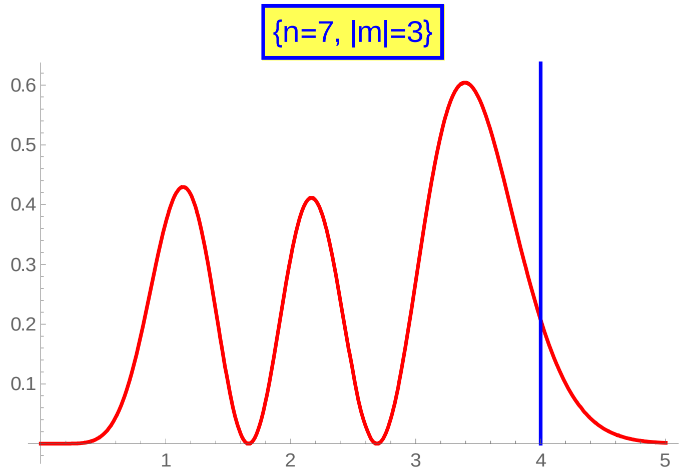


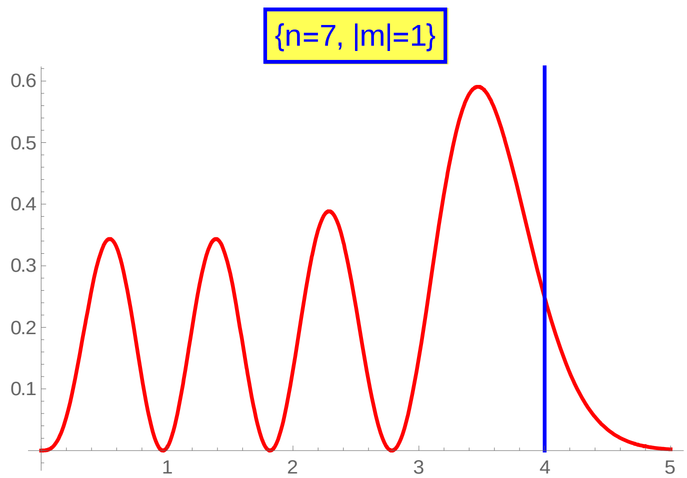
{n=7, |m|=7}



{n=7, |m|=5}







REFERENCES

R. Shankar, *Principles of Quantum Mechanics*, second edition (Springer, 1994).

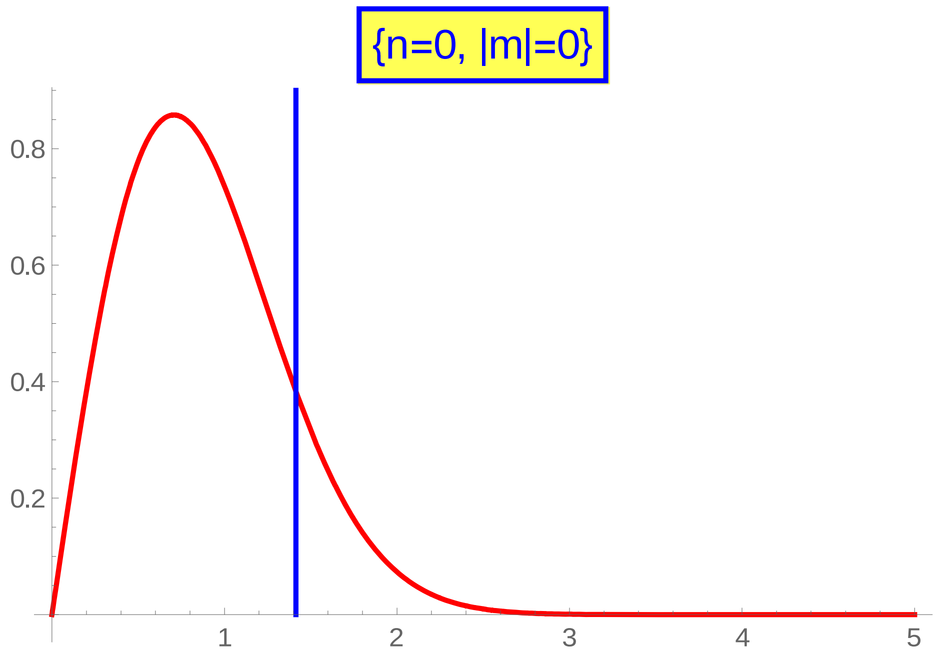
J Schwinger, *Quantum Mechanics*: Symbolism of Atomic Measurements (Springer, 2001).

APPENDIX Mathematica

```
Clear["Global`*"];
P[n_, m_, x_] := 2 (-1)^(n-Abs[m]) ((n - Abs[m])/2)!/((n + Abs[m])/2)! Exp[-x^2] x^(2 Abs[m]+1)
  (LaguerreL[(n - Abs[m])/2, Abs[m], x^2])^2;


g1[n_] := Module[{h1, h2, n1}, n1 = n;
   h1 = Graphics[{Text[Style["x", Black, 12, Italic], {4.5, 0.03}],
      Text[Style["x P^2_{n,m}", Black, 12, Italic], {0.3, 0.8}] }];
   h2 =
    Graphics[{Blue, Thick,
      Line[{{Sqrt[2 n1 + 2], 0}, {Sqrt[2 n1 + 2], 0.9}}]}]];

n = 0; m = 0;
f1 = Plot[P[n, m, x], {x, 0, 5}, PlotStyle → {Red, Thick},
  PlotLabel →
   Style[Framed[{ "n=" <> ToString[n], "|m|=" <> ToString[m]}],
    16, Blue, Background → Lighter[Yellow]]];
Show[f1, g1[n]]
```




```
n = 1; m = 1;
f1 = Plot[P[n, m, x], {x, 0, 5}, PlotStyle → {Red, Thick},
  PlotLabel →
   Style[Framed[{ "n=" <> ToString[n], "|m|=" <> ToString[m]}],
    16, Blue, Background → Lighter[Yellow]]];
Show[f1, g1[n]]
```