

# Numerical Simulations of Probability Distributions for the Hydrogen's Atom Wave Functions\*

## In Spherical, Semi-Spherical Spatial Sections and Infinite Intervals

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### ABSTRACT

**Context.** Quantum mechanics has become a fundamental pillar on which the development of humanity in modernity has take place. The hydrogen atom wave function is both, a symbol of this advance and a very complex and harmonious discovery which was brought by solving the Schrodinger equation and is written in terms of representative analytical functions.

**Aims.** The energy levels of an hydrogen atom are said to be related to the distance from the nucleus to a radial point where the electron has a probability of appearance.

**Methods.** This work will estimate the radial distances for which the integral for the probability distribution of the hydrogen atom equals one using the MonteCarlo Integral.

**Results.**

**Key words.** Wave function, Probability, Error, Integration, Interval, Monte Carlo Integration.

## 1. Theoretical Framework

### 1.1. Wave Function

The wave function of a state is commonly understood as its representation in a real vector space:

$$\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle \quad (1)$$

where if  $|\psi\rangle$  is a vector of a Hilbert space  $\mathcal{H}$  then  $\psi(\mathbf{r})$  must be both normalizable and infinitely differentiable, with the requirement of  $\langle \psi | \psi \rangle = 1$ . [1] [2]

### 1.2. Probability of the wave function

The wave function is interpreted as a probability distribution which must be equal to 1. It is:

$$\int_{-\infty}^{\infty} |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1 \quad (2)$$

where the integral is applied over  $\mathbf{r}$  and it is done such that it express the position as such in spherical coordinates. [1]

This equation make us think about the probability for continuous statistical functions, which must be 1 for some range  $[a, b]$  (here  $a = -\infty, b = \infty$ ). Now, there also exists the measurement of the probability of finding a particle in some sector of the selected space, it is:

$$P_{\mathbf{a}_i \leq \mathbf{r}_i \leq \mathbf{b}_i}(t) = \int_{\mathbf{I}} |\Psi(\mathbf{r}, t)|^2 d^n \mathbf{r}; \quad \mathbf{r}, \mathbf{I} \subset \mathcal{H} \quad (3)$$

### 1.3. Time-dependent general Schrödinger equation

The Schrödinger equation is an equality which relates the state of a system to its energy. The values for the energy which makes the equality relation hold are called eigenvalues of the wave function, the Schrödinger equation helps us to determine them when boundary conditions are given.

The time dependent general Schrödinger equation [3] is

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \quad (4)$$

Where the Hamiltonian operator  $\hat{H}^1$  is:

$$\hat{H} = \hat{T} + \hat{V} \quad (5)$$

$$\hat{T} = \frac{\hat{\mathbf{p}} \cdot \hat{\mathbf{p}}}{2m} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2; \quad \hat{\mathbf{p}} = -i\hbar \nabla \quad (6)$$

$$\hat{V} = V = V(\mathbf{r}, t) \quad (7)$$

being  $\hat{V}$  the potential energy,  $\hat{T}$  the kinetic energy and  $\hat{\mathbf{p}}$  the momentum operator. The equation can be written more completely as

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] |\Psi(t)\rangle \quad (8)$$

Now, if the basis is relative to some point in the space we use [4]

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t) \quad (9)$$

<sup>1</sup> Note that the sum of potential and kinetic energy is the total energy in the system.

where instead of a normal derivative we indicate that  $\Psi$  depends on  $\mathbf{r}$  (a position in the space) so that we present a more coherent notation.

#### 1.4. Time-independent general Schrödinger equation

When time is not being considered, the Schrödinger equation has the form

$$\hat{H} |\Psi(\mathbf{r})\rangle = E |\Psi(\mathbf{r})\rangle \quad (10)$$

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] |\Psi(\mathbf{r})\rangle = E |\Psi(\mathbf{r})\rangle \quad (11)$$

and is called time-independent Schrödinger equation. Here  $E$  is the value of the total energy. Alternatively, the notation

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E \psi(\mathbf{r}) \quad (12)$$

is also valid and does represent any different meaning, the main difference is that  $\psi$  sometimes is used for single particle systems and  $\Psi$  for multiple particle systems. [5]

Finally, it is important to mention that given suitable conditions (typically  $\Psi(\mathbf{r}, 0)$ ) the time independent Schrödinger equation determines  $\Psi(\mathbf{r}, t)$  for all value of  $t$ . [2]

#### 1.5. Hydrogen atom's wave function

The wave function for the hydrogen atom is obtained by solving the Schrodinger equation

$$\left( -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi_{n\ell m}(r, \theta, \phi) = E \psi_{n\ell m}(r, \theta, \phi) \quad (13)$$

being the following its solution (the wave function can be separated into functions of each coordinate [6])

$$\psi_{n\ell m}(r, \theta, \phi) = R(r) Y_{\ell}^m(\theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad (14)$$

$$= \sqrt{\left( \frac{2}{na_0^*} \right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]}} e^{-r/ma_0^*} \left( \frac{2r}{na_0^*} \right)^{\ell} \cdot L_{(n-\ell-1)}^{2\ell+1} \left( \frac{2r}{na_0^*} \right) \cdot Y_{\ell}^m(\theta, \phi) \quad (15)$$

this function is expressed in terms of other analytic functions which are simultaneously composed of some others as the spherical harmonic function:

$$Y_{\ell}^m(\theta, \phi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_{\ell m}(\cos(\theta)) e^{im\phi} \quad (16)$$

the associated Laguerre polynomial

$$L_n^{(\alpha)} = \frac{x^{-\alpha} e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^{n+\alpha}) \quad (17)$$

and the Legendre polynomial in the spherical harmonic

$$P_{\ell}(x) = \frac{1}{2^{\ell} \ell!} \frac{d^{\ell}}{dx^{\ell}} (x^2 - 1)^{\ell} \quad (18)$$

$$P_{\ell}^m(x) = \frac{(-1)^m}{2^{\ell} \ell!} (1 - x^2)^{m/2} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2 - 1)^{\ell} \quad (19)$$

$$P_{\ell m}(x) = (-1)^m P_{\ell}^m(x) \quad (20)$$

now, the meaning of the wave function for the electron in an hydrogen atom is that: for the coordinates  $r, \theta, \phi$ , the quantum energy level  $n = 1, 2, 3, 4, \dots$ , the quantum azimuthal number  $\ell = 0, 1, 2, 3, \dots, (n-1)$  and the quantum magnetic number  $m = -\ell, -\ell+1, -\ell+2, \dots, \ell$ . Then  $|\psi|^2$  is the probability of appearance for that electron at such given conditions and spatial point.

$$\begin{aligned} \langle \psi_{n\ell m} | \psi_{n\ell m} \rangle &= \int_{\mathbf{S}} ds \psi_{n\ell m}^* \psi_{n\ell m} = \int_{\mathbf{S}} |\psi_{n\ell m}|^2 ds \\ &= \delta_{nn} \delta_{\ell\ell} \delta_{mm} = 1 \end{aligned} \quad (21)$$

#### 1.6. Normalized hydrogen wave functions

The following table shows the wave functions for the energy levels of an hydrogen atom

$n$	$\ell$	$m$	$E_{\ell}$	$\psi_{n\ell m}(r, \theta, \phi)$
1	0	0	1s	$\left( \sqrt{\pi} a_0^{3/2} \right)^{-1} e^{-r/a_0}$
2	0	0	2s	$\left( 4\sqrt{2\pi} a_0^{3/2} \right)^{-1} \left[ 2 - \frac{r}{a_0} \right] e^{-r/2a_0}$
2	1	0	2p	$\left( 4\sqrt{2\pi} a_0^{3/2} \right)^{-1} \frac{r}{a_0} e^{-r/2a_0} \cos(\theta)$
2	1	$\pm 1$	2p	$\left( 8\sqrt{\pi} a_0^{3/2} \right)^{-1} \frac{r}{a_0} e^{-r/2a_0} \sin(\theta) e^{\pm i\phi}$
3	0	0	3s	$\left( 81\sqrt{3\pi} a_0^{3/2} \right)^{-1} \left[ 27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2} \right] e^{-r/3a_0}$
3	1	0	3p	$\left( 81\sqrt{\pi} a_0^{3/2} \right)^{-1} \sqrt{2} \left[ 6 - \frac{r}{a_0} \right] \frac{r}{a_0} e^{-r/3a_0} \cos(\theta)$
3	1	$\pm 1$	3p	$\left( 81\sqrt{\pi} a_0^{3/2} \right)^{-1} \left[ 6 - \frac{r}{a_0} \right] \frac{r}{a_0} e^{-r/3a_0} \sin(\theta) e^{\pm i\phi}$
3	2	0	3d	$\left( 81\sqrt{6\pi} a_0^{3/2} \right)^{-1} \frac{r^2}{a_0^2} e^{-r/3a_0} (3\cos^2(\theta) - 1)$
3	2	$\pm 1$	3d	$\left( 81\sqrt{\pi} a_0^{3/2} \right)^{-1} \frac{r^2}{a_0^2} e^{-r/3a_0} \sin(\theta) \cos(\theta) e^{\pm i\phi}$
3	2	$\pm 2$	3d	$\left( 162\sqrt{\pi} a_0^{3/2} \right)^{-1} \frac{r^2}{a_0^2} e^{-r/3a_0} \sin^2(\theta) e^{\pm i2\phi}$

Where  $a_0 = \hbar^2/me^2 \approx 0.0529\text{A}$ . [7]

#### 1.7. Monte Carlo integration method

Monte Carlo integration is a numerical integration method using random elements in the domain of a function, the Monte Carlo integral has better accuracy than successively applied Simpson's Rule or Trapezoidal method. The Monte Carlo numerical integral is defined taking as basis the integration of the following quadrature rule: [11]

$$I(f) = \sum_{i=1}^N c_i f(x^{(i)}); \quad x^{(i)} \equiv \left( x_d^{(i)} \right) \in \mathbf{E}^d \quad (22)$$

where we can reshape the notation and fix the weights  $c_i$  expressing those as  $V/N$  (equal weights  $\forall f(x^{(i)})$ ):

$$I(f) = \int_{\Omega} f(\bar{\mathbf{x}}) d\bar{\mathbf{x}}; \quad \Omega \subset \mathbb{R}^n \quad (23)$$

where  $\Omega$  is a region of  $\mathbb{R}^n$ . The value of the integral  $I$  can be approximated by

$$V = \int_{\Omega} d\bar{\mathbf{x}} \quad (24)$$

$$I \approx Q_N \equiv V \frac{1}{N} \sum_{i=1}^N f(\bar{\mathbf{x}}_i) = V \langle f \rangle; \quad \bar{\mathbf{x}}_i \in \Omega \quad (25)$$

$$\lim_{N \rightarrow \infty} Q_N = I \quad (26)$$

which for  $N$  tending to infinity is equal to the analytical integral due the law of large numbers.

### 1.7.1. Monte Carlo integral Error

The weighted Monte Carlo method has an estimated error

$$|\bar{\xi}_N - I| \leq x_{\beta} \sqrt{\frac{D\xi}{N}} \quad (27)$$

Where  $\bar{\xi}_N$  is an estimation,  $I$  the analytical integral value,  $x_{\beta}$  a value which establishes a measure,  $D\xi$  denotes the variance of  $\xi$  (a set of random samples) and  $N$  the number of samples. [11] For our current notation it is:

$$\text{Var}(f) \equiv \sigma_N^2 = \frac{1}{N-1} \sum_{i=1}^N \left( f(\bar{\mathbf{x}}_i) - \left( \frac{1}{N} \sum_{i=1}^N f(\bar{\mathbf{x}}_i) \right) \right)^2 \quad (28)$$

$$= \frac{1}{N-1} \sum_{i=1}^N (f(\bar{\mathbf{x}}) - \langle f \rangle)^2 \quad (29)$$

$$\therefore \text{Var}(Q_N) = \frac{V^2}{N^2} \sum_{i=1}^N \text{Var}(f) = V^2 \frac{\sigma_N^2}{N} \quad (30)$$

Being the following the error estimator of  $Q_n$

$$\delta Q_N \approx \sqrt{\text{Var}(Q_n)} = V \frac{\sigma_N}{\sqrt{N}} \quad (31)$$

## 2. Probability of the Hydrogen Wave Function in a Closed Spatial Section

The Monte Carlo integration method applied over the general wave function of the hydrogen atom is

$$I \approx \int_{\Omega} \Upsilon(v) dv \frac{1}{N} \sum_{i=1}^N |\psi_{n\ell m}(r_i, \theta_i, \phi_i)|^2 \quad (32)$$

where the integral of  $\Upsilon$  is an spatial volume section of a sphere as follows

$$\int_{\Omega} \Upsilon(v) dv = \int_{\phi_a}^{\phi_b} \int_{\theta_a}^{\theta_b} \int_{r_a}^{r_b} r^2 \sin(\phi) dr d\theta d\phi \quad (33)$$

$$= \int_{r_a}^{r_b} r^2 dr \int_{\phi_a}^{\phi_b} \sin(\phi) d\phi \int_{\theta_a}^{\theta_b} d\theta \quad (34)$$

$$= \left( \frac{r^3}{3} \Big|_{r_a}^{r_b} \right) \left( -\cos(\phi) \Big|_{\phi_a}^{\phi_b} \right) \left( \theta \Big|_{\theta_a}^{\theta_b} \right) \quad (35)$$

for  $v = (r, \theta, \phi)$ ,  $dv = dr d\theta d\phi$ ,  $\Upsilon \mapsto r^2 \sin(\phi)$ .

The Monte Carlo integral of the wave function can be expressed as

$$I \approx \left( \frac{r^3}{3} \Big|_{r_a}^{r_b} \right) \left( -\cos(\phi) \Big|_{\phi_a}^{\phi_b} \right) \left( \theta \Big|_{\theta_a}^{\theta_b} \right) \cdot \frac{1}{N} \sum_{i=1}^N |\psi_{n\ell m}(r_i, \theta_i, \phi_i)|^2 \quad (36)$$

being then

$$I \approx \Delta r \Delta \theta \Delta \phi \frac{1}{N} \sum_{i=1}^N |\psi_{n\ell m}(r_i, \theta_i, \phi_i)|^2 \quad (37)$$

the numerical integral, where

$$\Delta r = \left( \frac{r^3}{3} \Big|_{r_a}^{r_b} \right); \quad \Delta \theta = \left( \theta \Big|_{\theta_a}^{\theta_b} \right); \quad \Delta \phi = \left( -\cos(\phi) \Big|_{\phi_a}^{\phi_b} \right) \\ r_i \in [r_a, r_b]; \quad \theta_i \in [\theta_a, \theta_b]; \quad \phi_i \in [\phi_a, \phi_b] \quad (38)$$

and if we compress terms the integral can be denoted by

$$I_{\rho_a}^{\rho_b}(\psi_{n\ell m}) \approx V \Big|_{\rho_a}^{\rho_b} \frac{1}{N} \sum_{i=1}^N |\psi_{n\ell m}(r_i, \theta_i, \phi_i)|^2 \quad (39)$$

if we consider the spatial boundaries  $\rho_a = (r_a, \theta_a, \phi_a)$ ,  $\rho_b = (r_b, \theta_b, \phi_b)$  as embedded arguments in the integral.

Finally, as we would expect of a normalized wave function the following relationship holds

$$0 \leq I \left( |\psi_{n\ell m}|^2 \right) \cong 1 \quad (40)$$

because due the numerical error and that the integral of any squared normalized wave function is expected to be equal to one.

### 2.1. Numerical simulation for the first hydrogen's atom wave function

Considering the first wave function

$$\psi_{1,0,0}(r, \theta, \phi) = \left( \sqrt{\pi} a_0^{3/2} \right)^{-1} e^{-r/a_0} \quad (41)$$

It represents the probability of finding the electron at a distance  $r$  for any angular directions  $\theta, \phi$  (azimuthal and polar angles respectively). Replacing it on the previous derived formula we obtained, the finite numerical distribution probability of appearance for an electron in the hydrogen atom of electronic configuration 1s is

$$I \approx V \Big|_{\rho_a}^{\rho_b} \frac{1}{N} \sum_{i=1}^N |\psi_{1,0,0}|^2 \quad (42)$$

$$\approx V \Big|_{\rho_a}^{\rho_b} \frac{1}{N} \sum_{i=1}^N \left| \left( \sqrt{\pi} a_0^{3/2} \right)^{-1} e^{-r_i/a_0} \right|^2 \quad (43)$$

$$\approx V \Big|_{\rho_a}^{\rho_b} \frac{1}{N} \sum_{i=1}^N \frac{1}{\pi a_0^3} e^{-2r_i/a_0} \quad (44)$$

so, this is the simplified form for the hydrogen 1s wave function.

### 3. Integral Representations for Real Valued Wave Functions

Due the complexity of graphing complex valued vector functions those to be implemented won't involve complex values as result.

$\psi_{nlm}$	MonteCarlo Integral
1s	$V \left[ \frac{1}{N} \sum_{i=1}^N \left  \left( \sqrt{\pi} a_0^{3/2} \right)^{-1} e^{-r_i/a_0} \right ^2 \right]$
2s	$V \left[ \frac{1}{N} \sum_{i=1}^N \left  \left( 4\sqrt{2\pi} a_0^{3/2} \right)^{-1} \left[ 2 - \frac{r}{a_0} \right] e^{-r/2a_0} \right ^2 \right]$
2p	$V \left[ \frac{1}{N} \sum_{i=1}^N \left  \left( 4\sqrt{2\pi} a_0^{3/2} \right)^{-1} \frac{r}{a_0} e^{-r/2a_0} \cos(\theta) \right ^2 \right]$
3s	$V \left[ \frac{1}{N} \sum_{i=1}^N \left  \left( 81\sqrt{3\pi} a_0^{3/2} \right)^{-1} \left[ 27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2} \right] e^{-r/3a_0} \right ^2 \right]$
3p	$V \left[ \frac{1}{N} \sum_{i=1}^N \left  \left( 81\sqrt{\pi} a_0^{3/2} \right)^{-1} \sqrt{2} \left[ 6 - \frac{r}{a_0} \right] \frac{r}{a_0} e^{-r/3a_0} \cos(\theta) \right ^2 \right]$
3d	$V \left[ \frac{1}{N} \sum_{i=1}^N \left  \left( 81\sqrt{6\pi} a_0^{3/2} \right)^{-1} \frac{r^2}{a_0^2} e^{-r/3a_0} (3 \cos^2(\theta) - 1) \right ^2 \right]$

### 4. Stochastic Sampling

This section contains iterative searches for suitable values of  $r_b$  in the MonteCarlo integral of the real eigenfunctions of the hydrogen atom.

The initial value for  $r_b$  is taken as the first Bohr radius  $a_0$ , the step size for  $r_b$  is 1E-13 and the sampling size is 1E+3. (Note that  $E \pm N = 10^{\pm N}$ )

H <sub>1s</sub> ( $\psi_{1,0,0}$ )			
Iteration	$\int_0^{r_b}  \psi ^2 dV$	$r_b$	$\delta Q_N$
130	0,9457019	6,5817721E-11	2,1031176%
131	0,9595269	6,5917721E-11	2,0185508%
132	0,9176160	6,6017721E-11	2,0389192%
133	0,9829230	6,6117721E-11	2,1481853%
134	1,0025933	6,6217721E-11	2,1479737%

H <sub>2s</sub> ( $\psi_{2,0,0}$ )			
Iteration	$\int_0^{r_b}  \psi ^2 dV$	$r_b$	$\delta Q_N$
1311	0,9091722	1,8391772E-10	5,0342333%
1312	0,8510967	1,8401772E-10	4,7661942%
1313	0,9406232	1,8411772E-10	5,2906420%
1314	0,9496419	1,8421772E-10	5,0903240%
1315	1,0151406	1,8431772E-10	5,4509201%

H <sub>2p</sub> ( $\psi_{2,1,0}$ )			
Iteration	$\int_0^{r_b}  \psi ^2 dV$	$r_b$	$\delta Q_N$
2171	0,9631911	2,6991772E-10	2,6748278%
2172	0,9848947	2,7001772E-10	2,6065623%
2173	0,9567920	2,7011772E-10	2,6329902%
2174	0,9284070	2,7021772E-10	2,6330210%
2175	1,0221785	2,7031772E-10	2,8217323%

H <sub>3s</sub> ( $\psi_{3,0,0}$ )			
Iteration	$\int_0^{r_b}  \psi ^2 dV$	$r_b$	$\delta Q_N$
2719	0,8474818	3,2471772E-10	6,1158473%
2720	0,8570234	3,2481772E-10	6,4824615%
2721	0,9295840	3,2491772E-10	6,3611570%
2722	0,8450058	3,2501772E-10	6,0798280%
2723	1,0280992	3,2511772E-10	7,2012712%

H <sub>3p</sub> ( $\psi_{3,1,0}$ )			
Iteration	$\int_0^{r_b}  \psi ^2 dV$	$r_b$	$\delta Q_N$
4519	0,9095951	5,0471772E-10	4,5325230%
4520	0,9494293	5,0481772E-10	4,5971247%
4521	0,8962857	5,0491772E-10	4,3819209%
4522	0,8631052	5,0501772E-10	4,3409817%
4523	1,0376629	5,0511772E-10	4,8082404%

H <sub>3d</sub> ( $\psi_{3,2,0}$ )			
Iteration	$\int_0^{r_b}  \psi ^2 dV$	$r_b$	$\delta Q_N$
5476	0,9643382	6,0041772E-10	3,7983305%
5477	0,9714497	6,0051772E-10	3,6970124%
5478	0,9762733	6,0061772E-10	3,8403023%
5479	0,9468050	6,0071772E-10	3,5944818%
5480	1,0085111	6,0081772E-10	3,8450384%

### 5. Conclusions

1. The Monte Carlo integration method is cleverly useful, it can be adjusted or used to be suitable enough in complex problems such as multivariate probability integrals.
2. The values of  $r_b$  obtained in each wave function matches an increasing pattern in radial distance for the energy levels. As we know, for higher energy levels the electrons in the hydrogen atom will be able to locate in greater radial distances from the nucleus. Hence, the evaluation via MonteCarlo Integration is correct and matches experimental results.

3. The values of  $\int_0^{r_b} |\psi|^2 dV$  (probabilities) may suggest experimental areas where the likely to find the electron of a wave function is considerably higher than in other locations. Because the material to realize empirical sampling isn't at disposition this hypothesis cannot be verified.
4.  $\delta Q_N$  representing the error estimation due the standard deviation is related to the geometrical form given by the specter of the wave function once it's plotted in the three dimensional space, because the points of data where the probability augments will be closer depending on the specter of it.
5. In addition,  $\delta Q_N$  reinforces the accuracy of the results. Due to the geometrical shape of the wave function, a high error estimate indicates that the probability is relatively sparse in the space as well a low error estimator indicates that it's located on dense spatial sections.

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