

# Approximating the Radial Distribution Function of the Electron in a Hydrogen Atom by a Normal Distribution Suggests That Magnetic Confinement Fusion Would Be Less Energy Efficient than Inertial Confinement Fusion

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## Abstract

Since the position of the electron in a hydrogen atom cannot be determined, the region in which it resides is said to be determined stochastically and forms an electron cloud. The probability density function of the single electron in 1s orbit is expressed as  $\varphi^2$ , a function of distance from the nucleus. However, the probability of existence of the electron is expressed as a radial distribution function at an arbitrary distance from the nucleus, so it is estimated as the probability of the entire spherical shape of that radius. In this study, it has been found that the electron existence probability approximates the radial distribution function by assuming that the probability of existence of the electron being in the vicinity of the nucleus follows a normal distribution for arbitrary  $x$ -,  $y$ -, and  $z$ -axis directions. This implies that the probability of existence of the electron, which has been known only from the distance information, would follow a normal distribution independently in the three directions. When the electrons' motion is extremely restricted in a certain direction by the magnetic field of both tokamak and helical fusion reactors, the probability of existence of the electron increases with proximity to the nucleus, and as a result, it is less likely to be liberated from the nucleus. Therefore, more and more energy is required to free the nucleus from the electron in order to generate plasma.

## Keywords

Electron Cloud, Radial Distribution Function, Nuclear Fusion, Tokamak, Laser

## 1. Introduction

According to the uncertainty principle, the motion of the single electron in the 1s orbit of a hydrogen atom cannot be known, but can only be known as the magnitude of the probability that the electron could exist at a certain location in quantum space [1]. Therefore, the state of existence of the electron is described as looking like a cloud surrounding the nucleus in terms of quantum mechanical probability.

The physical significance of the fact that the electron of a hydrogen atom is under the influence of the Coulomb force on the nucleus, yet its location can only be estimated probabilistically, is immense. In this study, the possibility of approximating the existence probability by a normal distribution, which is universally observed in natural phenomena, has been examined [2]-[4]. If a mass point moves independently in the  $x$ - and  $y$ -axis directions according to normal distribution of  $\mathcal{N}(0, \sigma^2)$ , the distance of this point from the origin follows the famous Rayleigh probability distribution [5]. Surprisingly, the point has a maximum probability of being at the origin in the  $x$ - and  $y$ -axis directions, but in two dimensions, the maximum probability of the existence of the point is not at the origin, but on the circumference of a certain radius from the origin. In this study, we have tried to extend this to three dimensions. The maximum probability of the existence of the point is also found to be on the circumference of a certain radius from the origin. It has been found that the probability density function of the point at any distance from the origin is very similar to the radial distribution function of the single electron in the 1s orbit of a hydrogen atom, which is a famous result from the Schrödinger equation [6]. The radial distribution function is a function of distance from the nucleus and does not provide information on how the electron moves in arbitrary directions, but the present study suggests that it exists in arbitrary directions according to a normal distribution.

The structure of this paper is as follows: 1) Introduction, 2) Derivation of the probability density function for a mass point following a normal distribution in any direction centered at the origin, 3) Derivation of the radial distribution function for the single electron in the 1s orbit of a hydrogen atom, which has been already known [6], 4) Showing that these density functions are quite similar, 5) Application of the results obtained in this study to fusion reactions, 6) Discussion, and 7) Conclusion.

## 2. Derivation of the Probability Density Function for a Mass Point

### 1) In two dimensions

It is assumed that the mass point moves independently in the  $x$ - and  $y$ -directions according to a normal distribution of  $\mathcal{N}(0, \sigma^2)$ . In other words,  $X$  and  $Y$  are independent random variables each obeying a normal distribution of  $\mathcal{N}(0, \sigma^2)$ . The distance from the origin,  $U = \sqrt{x^2 + y^2}$ , is also a random variable following the joint probability density function being given by

$$f(x, y) = \left( \frac{1}{\sigma\sqrt{2\pi}} \right)^2 e^{-(x^2+y^2)/2\sigma^2} = \frac{1}{2\pi\sigma^2} e^{-(x^2+y^2)/2\sigma^2}. \quad (1)$$

In order to find the probability density function of  $U$ , polar coordinates are used:

$$x = u \cos \theta, \quad y = u \sin \theta; \quad 0 \leq u < \infty, \quad 0 \leq \theta < 2\pi. \quad (2)$$

The Jacobian of the transformation is  $|u|$ , and the joint probability density function of  $u$  and  $\theta$  becomes

$$f(u, \theta) = \frac{u}{2\pi\sigma^2} e^{-u^2/2\sigma^2}. \quad (3)$$

Then, the marginal probability density function  $f(u)$  becomes

$$f(u) = \int_0^{2\pi} f(u, \theta) d\theta = \frac{u}{\sigma^2} e^{-u^2/2\sigma^2}. \quad (4)$$

This is the famous Rayleigh probability distribution [5].  $f(u)$  is at its maximum value when  $df/du = 0$ .

$$\frac{df}{du} = \frac{1}{\sigma^2} e^{-u^2/2\sigma^2} \left( 1 - \frac{u^2}{\sigma^2} \right) = 0. \quad (5)$$

Hence,  $f(u)$  is maximal when  $u = \sigma$ . The results show that in two dimensions, the probability that the mass point is on the circumference of the radius of  $u = \sigma$  from the origin is maximum.

## 2) In three dimensions

These results can be extended to three dimensions in the same way as two dimensions. The distance from the origin,  $U = \sqrt{x^2 + y^2 + z^2}$ , is also a random variable following the joint probability density function being given by

$$f(x, y, z) = \left( \frac{1}{\sigma\sqrt{2\pi}} \right)^3 e^{-(x^2+y^2+z^2)/2\sigma^2}. \quad (6)$$

In order to find the probability density function of  $U$ , polar coordinates are used:

$$\begin{aligned} x &= u \sin \theta \cos \varphi, \quad y = u \sin \theta \sin \varphi, \quad z = u \cos \theta; \\ 0 &\leq u < \infty, \quad 0 \leq \theta < \pi, \quad 0 \leq \varphi < 2\pi. \end{aligned} \quad (7)$$

The Jacobian of the transformation is  $|u^2 \sin \theta|$ , and the joint probability density function of  $u$ ,  $\theta$  and  $\varphi$  becomes

$$f(u, \theta, \varphi) = \left( \frac{1}{\sigma\sqrt{2\pi}} \right)^3 u^2 e^{-u^2/2\sigma^2} \sin \theta. \quad (8)$$

Then, the marginal probability density function  $f(u)$  becomes

$$f(u) = \int_0^{2\pi} d\varphi \int_0^\pi \left( \frac{1}{\sigma\sqrt{2\pi}} \right)^3 u^2 e^{-u^2/2\sigma^2} \sin \theta d\theta = \frac{1}{\sigma^3} \sqrt{\frac{2}{\pi}} u^2 e^{-u^2/2\sigma^2}. \quad (9)$$

$f(u)$  is at its maximum value when  $df/du = 0$ .

$$\frac{df}{du} = \frac{1}{\sigma^3} \sqrt{\frac{2}{\pi}} 2ue^{-u^2/2\sigma^2} \left( 1 - \frac{u^2}{2\sigma^2} \right) = 0. \quad (10)$$

Hence,  $f(u)$  is maximal when  $u = \sqrt{2}\sigma$ . The results show that in three dimensions, the probability that the mass point is on the sphere of the radius of  $u = \sqrt{2}\sigma$  from the origin is maximum.

Appendix: Similarly, these results can be easily extended beyond  $n$  ( $n > 3$ ) dimensions. The maximum probability of the existence of a mass point is on a hypersphere of radius  $u = \sqrt{(n-1)}\sigma$  from the origin.

### 3. Derivation of the Radial Distribution Function for the Single Electron in the 1s Orbit of a Hydrogen Atom

The wave function of the electron,  $\varphi$ , in the 1s orbit modeled as a hydrogen atom is expressed as a function of the distance  $r$  from the hydrogen nucleus:

$$\varphi = \sqrt{\frac{2}{a_0}} e^{-r/a_0}; \quad a_0 = \frac{\varepsilon_0 h^2}{\pi m e^2}. \quad (11)$$

$a_0$  ( $=5.3 \times 10^{-11}$  m) is said to be a Bohr radius;  $\varepsilon_0$ : vacuum dielectric constant,  $h$ : Planck's constant,  $m$ : electron mass, and  $e$ : unit charge [6]. Probability density functions and distribution functions calculated based on the wave function are denoted by Greek letters, while probability density functions and distribution functions of a mass point derived from the normal distribution function are denoted by alphabetic letters.

The square of the wave function,  $\varphi^2$ , is a probability density function for existence of the electron at any point of distance  $r$  from the hydrogen nucleus:

$$\varphi^2 = \frac{2}{a_0} e^{-2r/a_0}. \quad (12)$$

The probability that the electron exists on a spherical surface at a distance  $r$  from the hydrogen nucleus is expressed as a radial distribution function  $\Phi(r)$  (Figure 1).

$\Phi(r)$ : radial distribution function,  
probability that the electron exists on a spherical surface at a distance  $r$   
from the hydrogen nucleus

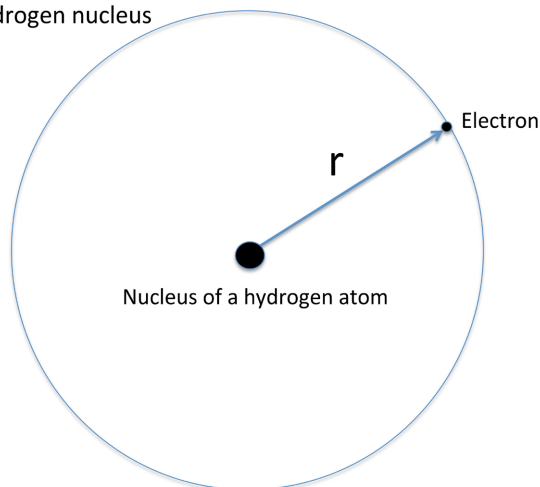


Figure 1. Radial distribution function.

If  $\Phi = Br^2\varphi^2$ ,  $B$  must satisfy the following conditions because  $\varphi^2$  is a probability density function:

$$\int_0^\infty \Phi dr = \int_0^\infty Br^2\varphi^2 dr = 1. \quad (13)$$

Hence,

$$\Phi(r) = \frac{4}{a_0^3} r^2 e^{-2r/a_0}. \quad (14)$$

$r$  when  $\Phi$  is at its maximum satisfies the following equation:

$$\frac{d\Phi}{dr} = 0. \quad (15)$$

Hence,  $r = a_0$ .

#### 4. Showing That These Density Functions Are Quite Similar

The probability of a mass point existing at a distance  $u$  from the origin can be expressed by Equation (9) when the position of each coordinate independently follows a normal distribution of  $N(0, \sigma^2)$  in three dimensions.  $f(u)$  is maximized at  $u = \sqrt{2}\sigma$ , so the following equation is obtained by replacing  $R \equiv u/(\sqrt{2}\sigma)$  and  $a_0 \equiv \sqrt{2}\sigma$ :

$$f(u) = \frac{1}{\sigma^3} \sqrt{\frac{2}{\pi}} u^2 e^{-u^2/2\sigma^2} \rightarrow F(R) = \frac{4}{a_0 \sqrt{\pi}} R^2 e^{-R^2}. \quad (16)$$

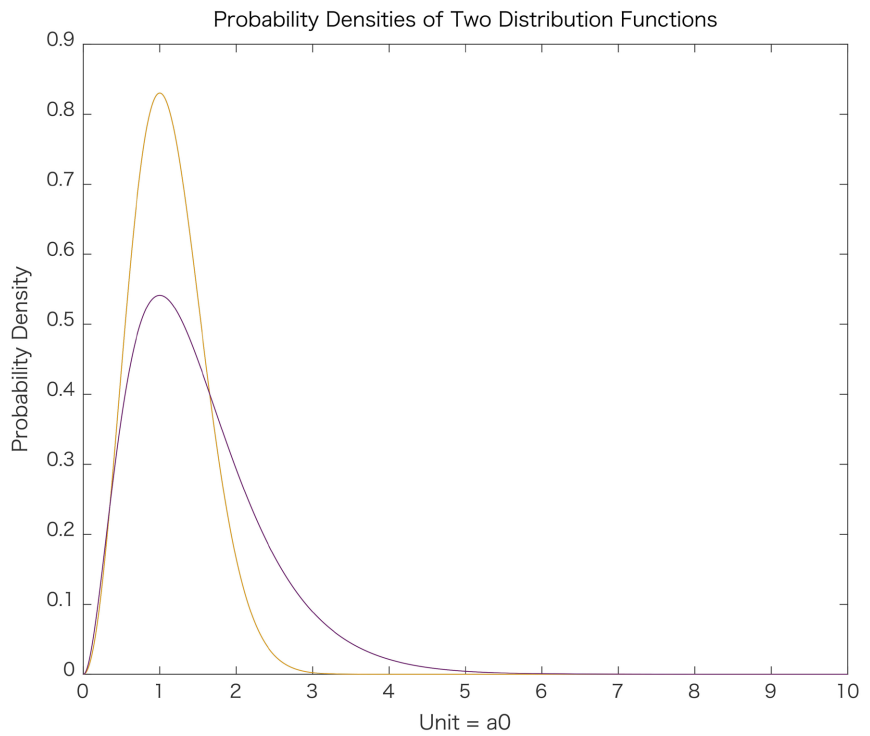
$\Phi(r)$  is maximized at  $r = a_0$ , so the following equation is obtained by replacing  $R \equiv r/a_0$  for Equation (14):

$$\Phi(r) = \frac{4}{a_0^3} r^2 e^{-2r/a_0} \rightarrow \psi(R) = \frac{4}{a_0} R^2 e^{-2R}. \quad (17)$$

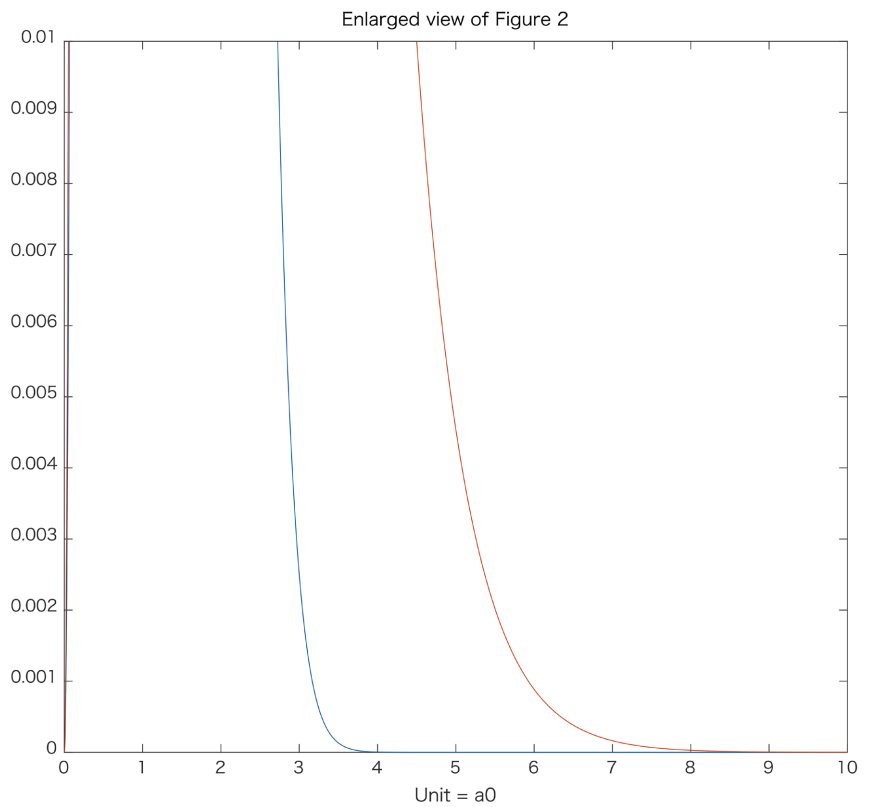
**Figure 2** shows the probability densities of  $F(R)$  and  $\psi(R)$  with  $a_0$  as the unit of distance from the origin or the nucleus. It can be seen that these probability density functions are quite similar. **Figure 3** is an enlarged version of **Figure 2**. The probability of the electron being at a distance of  $6a_0$  or more from the nucleus is about 0.0005. If 2 kg of hydrogen are enclosed in a spherical pellet, about 1 g of hydrogen would have the electron at a distance of  $6a_0$  or more from the nucleus.

#### 5. Application of the Results Obtained to Fusion Reactions

The position of the electron in a hydrogen atom can only be estimated probabilistically, which is expressed as a radial distribution function of distance from the nucleus. In other words, the probability of the existence of the electron is estimated only on a sphere at an arbitrary distance from the nucleus. In this study, it has been shown that the radial distribution function approximates the probability density function obtained by assuming that the coordinates of the electron are normally distributed with the nucleus as the origin. This shows that the existence of the electron follows a normal distribution in arbitrary directions. If the electron is restricted to move in one direction, the probability of its existence will follow a normal distribution in this direction, and the probability of its existence will be maximum not at  $a_0$  but at the origin, *i.e.*, at the nucleus.



**Figure 2.** Probability density (PD) (purple line) of radial distribution function of existence of the electron in a hydrogen atom and PD (brown line) for a mass point following a normal distribution in any direction centered at the origin.



**Figure 3.** Enlarged view of **Figure 2**.

It is unknown how far away from the nucleus the electron is likely to be released from the nucleus under certain conditions (heat, pressure, etc), but let us assume, for example, that the electron existing at a distance of more than  $6 a_0$  from the nucleus is likely to be released from it. **Figure 2** shows that the probability of the electron being at a distance of  $6 a_0$  or more from the nucleus is about 0.0005. If 2 kg of hydrogen is enclosed in a spherical pellet, about 1 g of hydrogen would have the electron at a distance of  $6 a_0$  or more from the nucleus. If this pellet were used as fuel for a laser fusion reactor and a fusion reaction occurred, we would get  $6.5 \times 10^{11}$  J in energy [7].

## 6. Discussion

When the probability distribution of the existence of a one-dimensional mass point follows a normal distribution centered at the origin, the maximum probability of the existence of the mass point is naturally at the origin, and nothing unusual happens. However, the situation changes drastically when this is located in two dimensions. In the  $x$ -axis direction, the maximum probability of existence of a mass point is at the origin, and similarly in the  $y$ -axis direction, the maximum probability of existence of the point is at the origin, but in the  $x$ - $y$  two-dimensional case, even if the  $x$ -coordinate of the point is at the origin, the origin is not necessarily also at the  $y$ -coordinate. Therefore, in two dimensions, the probability of existence of the point at the origin is not maximum. Similarly, in three dimensions, even if the  $x$ -coordinate of a mass point is the origin, the  $y$ -coordinate or  $z$ -coordinate may not also be the origin at the same time. Therefore, in three dimensions, the probability of existence of the point at the origin is not maximized, but the probability of existence of the point at a certain distance further away from the origin than in two dimensions is maximized.

Let us apply these results to tokamak and helical fusion reactors, which are currently considered promising [8]. Nuclear fusion is the process by which lighter nuclei, such as hydrogen, are brought together (fused) and converted into heavier nuclei, such as helium. To do this, hydrogen is heated to several thousand degrees Celsius or more, creating a plasma state in which the protons and electrons of the hydrogen nuclei are free to fly around. However, these nuclei are subject to repulsive forces that must be overcome and the nuclei must collide with each other at a high speed in order to overcome these repulsive forces. Therefore, the plasma must be heated to over 100 million degrees Celsius. The magnetic confinement fusion reactors such as Tokamak and helical fusion reactors use intense magnetic fields to confine such high-temperature plasma. However, since the nuclei follow the magnetic field lines in Larmor motion, collisions between nuclei are not likely to occur. The results of this study suggest that when electron motion is restricted to a certain direction (that is, this spiral motion is a linear one-dimensional motion when viewed on a very small scale), the probability of existence of the electron increases with proximity to the nucleus, and as a result, it is less likely to be liberated from the nucleus. Therefore, more and more energy is required to

free the nucleus from the electron.

In the inertia confinement fusion reactors such as the laser fusion reactor, which is completely different from these types of reactors, the spherical fuel is uniformly irradiated by high-power laser pulses. The outside of the irradiated fuel is heated to a high temperature, and pressure of tens of millions of atmospheres is generated, which compresses the spherical fuel toward its center (implosion). In this way, a nuclear fusion reaction is induced instantaneously. The present study shows that the probability of existence of the electron decreases rapidly as the electron move away from the nucleus. In fact, it is unknown how far away from the nucleus the electron is likely to be released from the nucleus by external conditions (heat, pressure, etc.), but let us assume that the electrons at a distance  $6 a_0$  or more from the nucleus are likely to be released from the nucleus. Based on the results of this study, if 2 kg of hydrogen was sealed in a spherical pellet, there would be about 1 g of hydrogen with the electron at a distance  $6 a_0$  or greater from the nucleus. When this amount of hydrogen undergoes a fusion reaction, it produces  $6.5 \times 10^{11}$  J in energy.

## 7. Conclusion

It has been shown that the radial distribution function approximates the probability density function obtained by assuming that the coordinates of the electron are normally distributed with the nucleus as the origin. This shows that the existence of the electron follows a normal distribution in arbitrary one-dimensional direction. The maximum probability of existence of the electron in a hydrogen atom is on a sphere of radius  $a_0$  from the nucleus, but if the motion of the electron is restricted to one-dimensional direction, it exists very close to the nucleus and would require higher energy to free it from the nucleus.

## Conflicts of Interest

The author declares that there is no conflict of interests regarding the publication of this paper.

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