5) Find Out The Expectation Values : , , , For An Electron In Ground State Of Hydrogen Atom?

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Understanding the quantum mechanical behavior of electrons in atoms is fundamental to modern physics and chemistry. One of the key concepts in quantum mechanics is the idea of expectation values, which provide the average results of measurements of certain physical quantities in a given quantum state. Specifically, for the hydrogen atom, calculating the expectation values of position $\langle r \rangle$, $\langle r^2 \rangle$, and related quantities in the ground state offers profound insights into the electron's distribution and behavior. This article delves into how to determine these expectation values for an electron in the ground state of the hydrogen atom, explaining the underlying theory, the mathematical methods used, and their physical significance.

Understanding Expectation Values in Quantum Mechanics

What Are Expectation Values?

In quantum mechanics, the expectation value of an observable quantity corresponds to its average measured value over many identical systems prepared in the same quantum state. Mathematically, for an operator $\hat{A}$, the expectation value $\langle A \rangle$ in a state described by the wavefunction ψ is given by:

$$
\langle A \rangle = \int \psi^(\mathbf{r}) \hat{A} \psi(\mathbf{r}) \, dV
$$

where:
- $\psi(\mathbf{r})$ is the wavefunction of the system,
- $\psi^(\mathbf{r})$ is its complex conjugate,
- dV is the volume element in the relevant coordinate system.

This concept allows us to connect the probabilistic nature of quantum mechanics with measurable physical quantities like position, momentum, and energy.

Relevance to Hydrogen Atom

For the hydrogen atom, the wavefunctions are solutions to the Schrödinger equation with Coulomb potential. The ground state, characterized by quantum numbers $n=1$, $l=0$, and $m=0$, exhibits a spherically symmetric probability distribution. Calculating expectation values such as $\langle r \rangle$ and $\langle r^2 \rangle$ helps in understanding the average location and spread of the electron relative to the nucleus.

Wavefunction of the Ground State of Hydrogen Atom

Hydrogen Ground State Wavefunction ψ_{100}

The normalized wavefunction for the ground state (also called the 1s orbital) of hydrogen is:

$$
\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}
$$

where:
- a_0 is the Bohr radius ($\approx 0.529 \times 10^{-10}$ m),
- r, θ, ϕ are spherical coordinates.

Since the wavefunction is spherically symmetric, calculations involving expectation values of r, r^2, etc., are simplified by integrating over the radial coordinate with the appropriate probability density.

Calculating Expectation Values for the Ground State

General Approach

The expectation value of a radial quantity r^k (where k is any real number) in the ground state of hydrogen is given by:

$$
\langle r^k \rangle = \int_0^{\infty} r^k |R_{10}(r)|^2 r^2 dr
$$

where:
- $R_{10}(r)$ is the radial part of the wavefunction,
- the angular parts integrate to 1 due to symmetry.

The radial wavefunction for the ground state is:

$$
R_{10}(r) = 2 \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}
$$

and the probability density becomes:

$$
|R_{10}(r)|^2 = 4 \left(\frac{1}{a_0^3} \right) e^{-2r/a_0}
$$

Expectation Value of r: $\langle r \rangle$

Calculation:

$$
\langle r \rangle = \int_0^{\infty} r \times 4 \left(\frac{1}{a_0^3} \right) e^{-2r/a_0} r^2 dr
$$

which simplifies to:

$$
\langle r \rangle = 4 \left(\frac{1}{a_0^3} \right) \int_0^{\infty} r^3 e^{-2r/a_0} dr
$$

Using the integral:

$$
\int_0^{\infty} r^n e^{-br} dr = \frac{n!}{b^{n+1}}
$$

\]

for \(n=3 \), \(b=2/a_0 \), we get:

\[
\int_0^{\infty} r^3 e^{-2r/a_0} dr = \frac{3!}{(2/a_0)^4} =
\frac{6}{(2/a_0)^4} = 6 \times \left(\frac{a_0^4}{16} \right) =
\frac{6a_0^4}{16} = \frac{3a_0^4}{8}
\]

Plugging back into the expectation value:

\[
\langle r \rangle = 4 \times \frac{1}{a_0^3} \times \frac{3a_0^4}{8} =
\frac{4 \times 3 a_0^4}{8 a_0^3} = \frac{12 a_0^4}{8 a_0^3} = \frac{3 a_0}{2}
\]

Result:

\[
\boxed{
\langle r \rangle = \frac{3}{2} a_0
}
\]

Physical Significance:

This indicates that on average, the electron is located at a distance of \(
1.5 \, a_0 \) from the nucleus in the ground state.

Expectation Value of \(r^2 \): \(\langle r^2 \rangle \)

Calculation:

\[
\langle r^2 \rangle = \int_0^{\infty} r^2 \times 4 \left(\frac{1}{a_0^3}
\right) e^{-2r/a_0} r^2 dr
\]

which simplifies to:

\[
\langle r^2 \rangle = 4 \left(\frac{1}{a_0^3} \right) \int_0^{\infty} r^4
e^{-2r/a_0} dr
\]

Using the integral:

$$
\int_0^{\infty} r^n e^{-br} dr = \frac{n!}{b^{n+1}}
$$

for $n=4$, $b=2/a_0$:

$$
\int_0^{\infty} r^4 e^{-2r/a_0} dr = \frac{4!}{(2/a_0)^5} = \frac{24}{(2/a_0)^5} = 24 \times \frac{a_0^5}{32} = \frac{24 a_0^5}{32} = \frac{3 a_0^5}{4}
$$

Plugging into the expectation value:

$$
\langle r^2 \rangle = 4 \times \frac{1}{a_0^3} \times \frac{3 a_0^5}{4} = \frac{4 \times 3 a_0^5}{4 a_0^3} = 3 a_0^2
$$

Result:

$$
\boxed{
\langle r^2 \rangle = 3 a_0^2
}
$$

Physical Significance:

This value relates to the spread or variance of the electron's position, giving a measure of how far the electron is likely to be found from the nucleus squared, on average.

Other Expectation Values and Physical Quantities

Expectation Value of $1/r$: $\langle 1/r \rangle$

This expectation value is important for calculating the potential energy of the electron:

```
\[
\langle \frac{1}{r} \rangle = \int_0^{\infty} \frac{1}{r} \times 4 \left(
\frac{1}{a_0^3} \right) e^{-2r/a_0} r^2 dr
\]
```

which simplifies to:

```
\[
\langle \frac{1}{r} \rangle = 4 \left( \frac{1
```

Frequently Asked Questions

What are the expectation values of position ($\langle r \rangle$), momentum ($\langle p \rangle$), and energy ($\langle E \rangle$) for an electron in the ground state of a hydrogen atom?

For the ground state of hydrogen (1s orbital), the expectation value of position $\langle r \rangle$ is approximately 1.5 a_0 (where a_0 is the Bohr radius), the expectation value of momentum $\langle p \rangle$ is zero due to symmetry, and the expectation value of energy $\langle E \rangle$ is -13.6 eV, which is the ground state energy.

How is the expectation value of the electron's radius ($\langle r \rangle$) in the ground state of hydrogen calculated?

The expectation value $\langle r \rangle$ in the ground state (1s orbital) is calculated using the hydrogen atom wavefunction and is approximately 1.5 times the Bohr radius (a_0). Specifically, $\langle r \rangle \approx 1.5a_0$.

What is the significance of the expectation value of momentum, $\langle p \rangle$, for an electron in the hydrogen atom's ground state?

Due to the spherical symmetry of the ground state wavefunction, the expectation value of momentum $\langle p \rangle$ is zero, indicating no preferred direction of momentum for the electron in this state.

Can you explain the expectation value of the energy ($\langle E \rangle$) for the electron in the ground state of hydrogen?

Yes, the expectation value of energy $\langle E \rangle$ for the ground state is equal to the energy eigenvalue of the 1s orbital, which is approximately -13.6 eV, indicating a bound state with negative energy.

Are the expectation values of position and momentum for the ground state of hydrogen consistent with the Heisenberg uncertainty principle?

Yes, the non-zero ⟨r⟩ and zero ⟨p⟩ (on average) are consistent with the uncertainty principle, as the electron's position is localized around the nucleus but its momentum has uncertainty, preventing both from being precisely determined simultaneously.

How do the expectation values change if the hydrogen atom is in an excited state instead of the ground state?

In excited states, the expectation values of ⟨r⟩ increase, indicating the electron on average is farther from the nucleus, while ⟨p⟩ may have non-zero values depending on the state's symmetry, and the energy ⟨E⟩ becomes less negative.

Why are expectation values important in understanding the behavior of an electron in the hydrogen atom?

Expectation values provide average measurable quantities like position, momentum, and energy, offering insights into the electron's probabilistic distribution and physical properties without requiring exact knowledge of its exact state.

Additional Resources

Find Out The Expectation Values: , , , and for An Electron In Ground State Of Hydrogen Atom

Understanding the expectation values of various physical quantities is fundamental in quantum mechanics, especially when analyzing atomic systems such as the hydrogen atom. These expectation values provide vital insights into the average behavior of an electron within an atom and serve as the bridge between the probabilistic wavefunction description and classical observable quantities. In the context of the hydrogen atom's ground state, computing expectation values like , , , and not only deepens our understanding of atomic structure but also highlights the symmetry and spatial distribution of the electron cloud. This article thoroughly explores these expectation values, detailing their calculations, significance, and implications in quantum theory.

Introduction to Expectation Values in Quantum Mechanics

In quantum mechanics, the expectation value of an observable corresponds to the average result one would obtain after many measurements of that observable on identically prepared systems. Mathematically, for an operator $\hat{A}$, the expectation value is given by:

$$
\langle A \rangle = \int \psi^(\mathbf{r}) \hat{A} \psi(\mathbf{r}) \, dV
$$

where $\psi(\mathbf{r})$ is the wavefunction of the system, and the integration is over all space.

For the hydrogen atom's ground state, the wavefunction possesses spherical symmetry, which significantly simplifies the calculation of expectation values. The ground state wavefunction is known as the 1s orbital, described by the quantum numbers $n=1, l=0, m=0$, and is given by:

$$
\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}
$$

where a_0 is the Bohr radius (~0.529 Å).

Expectation Value of , , and

The expectation values of the position coordinates x, y, z give insight into the average position of the electron in space.

Symmetry Considerations

Due to the spherical symmetry of the ground state wavefunction, the expectation values of these Cartesian coordinates have specific properties:

- $\langle x \rangle = \langle y \rangle = \langle z \rangle = 0$

This stems from the fact that the probability distribution is symmetric about the origin, leading to equal average displacements in any direction, which cancel out over many measurements.

Calculation of , , and

For the ground state wavefunction:

$$
\langle x \rangle = \int \psi^(\mathbf{r}) \, x \, \psi(\mathbf{r}) \, dV
$$

Given the symmetry, and the form of the wavefunction, the expectation value of x (or y or z) is zero:

$$
\boxed{
\langle x \rangle = \langle y \rangle = \langle z \rangle = 0
}
$$

Features and Implications:

- These zero values indicate that, on average, the electron doesn’t favor any particular direction.
- The symmetry simplifies the analysis of many quantum systems, emphasizing the importance of symmetry considerations.

Expectation Value of

The quantity $r = \sqrt{x^2 + y^2 + z^2}$ represents the radial distance from the nucleus. Its expectation value, $\langle r \rangle$, gives the average distance of the electron from the nucleus in the ground state.

Significance of

- Provides a measure of the "size" of the electron cloud.
- Reflects the average spatial extent of the electron in the ground state.
- Useful in understanding the scale of atomic interactions and the effective size of the atom.

Calculation of

The expectation value $\langle r \rangle$ is calculated as:

$$
\langle r \rangle = \int \psi^(r) \, r \, \psi(r) \, dV
$$

Expressed in spherical coordinates, the volume element is:

$$
dV = r^2 \sin \theta \, dr \, d\theta \, d\phi
$$

For the 1s orbital:

$$
\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}
$$

The expectation value becomes:

$$
\langle r \rangle = \int_0^{\infty} \int_0^\pi \int_0^{2\pi} r \left| \psi_{100}(r) \right|^2 r^2 \sin \theta \, dr \, d\theta \, d\phi
$$

Integrating over angular variables:

$$
\int_0^\pi \sin \theta \, d\theta = 2, \quad \int_0^{2\pi} d\phi = 2\pi
$$

The radial integral:

$$
\langle r \rangle = 4\pi \int_0^{\infty} r^3 \left| \psi_{100}(r) \right|^2 dr
$$

Substituting $\left| \psi_{100}(r) \right|^2$:

$$
\left| \psi_{100}(r) \right|^2 = \frac{1}{\pi a_0^3} e^{-2r/a_0}
$$

Thus,

$$
\langle r \rangle = 4\pi \times \frac{1}{\pi a_0^3} \int_0^{\infty} r^3 e^{-2r/a_0} dr = \frac{4}{a_0^3} \int_0^{\infty} r^3 e^{-2r/a_0} dr
$$

Change variable:

\[
x = \frac{2r}{a_0} \Rightarrow r = \frac{a_0 x}{2}, \quad dr = \frac{a_0}{2}
dx
\]

Integral becomes:

\[
\langle r \rangle = \frac{4}{a_0^3} \times \left(\frac{a_0}{2} \right)^4
\int_0^{\infty} x^3 e^{-x} dx
\]

Simplify:

\[
\langle r \rangle = \frac{4}{a_0^3} \times \frac{a_0^4}{16} \times 6
\]

since:

\[
\int_0^{\infty} x^3 e^{-x} dx = 3! = 6
\]

Final calculation:

\[
\boxed{
\langle r \rangle = \frac{a_0}{2} \times 6 = 3a_0
}
\]

Result:

\[
\boxed{
\langle r \rangle = 1.5 \times a_0
}
\]

(Note: The standard textbook result for the ground state expectation value of
\(r \) in hydrogen is \(\langle r \rangle = \frac{3}{2} a_0 \).)

Features and Significance:

- The average radius of the electron cloud in the ground state is 1.5 times
the Bohr radius.
- This measure is crucial in estimating atomic sizes and understanding
electron distributions.

Summary of Expectation Values for the Ground State of Hydrogen

Expectation Quantity	Value	Remarks
$\langle x \rangle$	0	Due to symmetry
$\langle y \rangle$	0	Due to symmetry
$\langle z \rangle$	0	Due to symmetry
$\langle r \rangle$	$\frac{3}{2} a_0$ (~0.793 Å)	Average distance from nucleus

---

Conclusion and Implications

The expectation values of position and radial distance for an electron in the ground state of hydrogen exemplify the profound symmetry and probabilistic nature of quantum systems. The zero expectation values of x, y, z underscore the spherical symmetry of the 1s orbital, indicating that, on average, the electron does not favor any particular spatial direction. Meanwhile, the expectation value $\langle r \rangle = \frac{3}{2} a_0$ provides a tangible measure of the atom's size, reflecting the spread of the electron's probability density.

These calculations are more than mere mathematical exercises; they form the foundation for understanding atomic behavior, spectral lines, and chemical bonding. They also serve as benchmarks for more complex systems, where symmetry considerations and expectation values guide approximations and computational methods.

Pros of Expectation Value Calculations:

- Offer a quantitative measure of quantum states.
-

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