True Nature of Potential Energy of a Hydrogen Atom

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Abstract

In considering the potential energy of a hydrogen atom, we offered the hypothesis that this physical quantity corresponds to the decrease in the electron's rest mass energy. It is not possible to establish the ground state energy of a hydrogen atom without quantum mechanics. However, for the atom's stability only, this can be explained even without using quantum mechanics.

Our discussion reveals that there exists an off-limit boundary r_c within the electron inside a hydrogen atom.

I. Introduction

According to the Rutherford atomic model, one or more electrons orbit around the nucleus. If we assume that electrons are moving in circles around the atomic nucleus, then we know that an electron must emit electromagnetic waves through that acceleration and will fall into the nucleus after a period of about 10^{-10} seconds. Classical mechanics cannot currently be used to explain the stability of an atom, and we consider that this problem was solved for the first time by the appearance of Bohr's classical quantum theory.

By assuming quantum conditions, Bohr derived the orbit radius of a hydrogen atom. He further explained that there is a minimum value of the total energy of a hydrogen atom, and that electron is not absorbed into the atomic nucleus.

In this paper, though, we consider the potential energy of a hydrogen atom and attempt to explain the stability of a hydrogen atom. However, "stability" in this paper is used not to refer to the stability of an atom that has been successfully described by Bohr, but instead refers to the condition of an electron not falling into the atomic nucleus.

II. Electron energy as described according to classical mechanics

Let us review the energy of an electron inside a hydrogen atom. Let us suppose that an atomic nucleus is at rest because it is heavy, and consider the situation where an electron (electric charge $-e$, mass m) is orbiting at speed v along an orbit (radius r) with the atomic nucleus as its center. An equation describing the motion is as follows:

$$\frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r^2}. \tag{II.1}$$

From this, we obtain:

$$\frac{1}{2}mv^2 = \frac{1}{2} \cdot \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}. \tag{II.2}$$

Meanwhile, the potential energy of the electron is:

$$V(r) = -\frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r}. \tag{II.3}$$

Since the right side of (II.2) is –1/2 times the potential energy, (II.2) indicates:

$$V(r) = -2\left(\frac{1}{2}mv^2\right). \tag{II.4}$$

Therefore, the total electron energy:

$$E = \frac{1}{2}mv^2 + V(r) \tag{II.5a}$$

$$= -K. \tag{II.5b}$$

Also, the total energy of the electron is equal to half its potential energy.

$$E = \frac{1}{2}V(r). \tag{II.6}$$

The reason for the difference in potential energy and kinetic energy (K) in (II.4) is thought to be the photon energy $\hbar\omega$ released by the electron.

Accordingly, we can establish the following law of energy conservation.

$$V(r) + K + \hbar\omega = 0, \qquad V(r) \le 0. \tag{II.7}$$

III. An absolute definition of the total energy of a hydrogen atom

Referring to classical quantum theory and (II.5b), the relationship between the total energy and kinetic energy of an electron inside a hydrogen atom is:

$$E_n = -\frac{1}{2}\left(\frac{1}{4\pi\varepsilon_0}\right)^2 \frac{me^4}{\hbar^2} \cdot \frac{1}{n^2} \tag{III.1a}$$

$$= \frac{E_1}{n^2} \tag{III.1b}$$

$$= -\frac{K_1}{n^2}, \qquad n = 1, 2, \cdots. \tag{III.1c}$$

Here, n is a principal quantum number. In this case, the total energy of a hydrogen atom has a negative value.

When describing the total energy of a hydrogen atom according to classical mechanics, we must know the atom's potential energy and kinetic energy. However, discussing the energy of a hydrogen atom according to quantum mechanics, we are only concerned with the increase or decrease in total energy.

Additionally, the classical quantum radius r_n is represented as follows:

$$r_n = \frac{4\pi\varepsilon_0 \hbar^2 n^2}{me^2} \tag{III.2a}$$

$$= a_{\mathrm{B}} n^2, \qquad n = 1, 2, \cdots. \tag{III.2b}$$

Here, the value n=1 is the Bohr radius a_{B}, which corresponds to the ground state of the hydrogen atom. According to classical quantum theory, the total energy and the potential energy of a hydrogen atom are considered to be zero when the electron is separated from the atomic nucleus by a distance of infinity and remains at rest in that location. The total energy of (III.1a) is the value obtained from this perspective.

In classical quantum theory, we emphasize the difference in energy, not the absolute energy. However, according to quantum mechanics textbooks, the eigenvalue of the energy of a hydrogen atom as obtained from the Dirac equation, which is a relativistic wave equation, is as follows [1].

$$E = mc^2 \left[1 - \frac{\gamma^2}{2n^2} - \frac{\gamma^4}{2n^4} \left(\frac{n}{|k|} - \frac{3}{4} \right) \right]. \tag{III.3}$$

It is important to note that energy here is defined on an absolute scale. Because Z = 1 in the case of a hydrogen atom, $\gamma = e^2/\hbar c$, (γ is the fine structure constant). If we ignore for the third term of this equation and define it as an approximation, (III.3) can be written as follows.

$$E = mc^2 - \frac{1}{2} \left(\frac{1}{4\pi\varepsilon_0} \right)^2 \frac{me^4}{\hbar^2} \cdot \frac{1}{n^2} \tag{III.4a}$$

$$= mc^2 + E_n. \tag{III.4b}$$

Moreover, E of (A.5) defines an absolute quantity, which includes the electron's rest mass energy (See Appendix).

From this fact, in this paper, the total energy in absolute terms, $E_{\text{ab},n}$ for a hydrogen atom is defined as below.

$$E_{\text{ab},n} = E_0 + K_n + V(r_n) \qquad \text{(III.5a)}$$

$$= E_0 + \frac{V(r_n)}{2} \qquad \text{(III.5b)}$$

$$= E_0 + E_n, \qquad n = 1, 2, \cdots, E_n < 0. \qquad \text{(III.5c)}$$

Here, $E_{\text{ab},n}$ is the total energy as defined in absolute terms when the principal quantum number is *n*.

To agree with *n* on the left side, *n* is added to *K* and *r* on the right side.

When defined on an absolute scale, the total energy of a hydrogen atom is less than the electron's rest mass energy.

IV. True nature of potential energy of a hydrogen atom

The case of a single electron, at rest in free space, is considered. According to Einstein, the only energy of an electron in this state is its rest mass energy, or E_0, which is $m_e c^2$ [2].

Although a particle cannot exist in a certain location with zero momentum according to the uncertainty principle, we shall set that problem aside for the moment and proceed with our consideration.

If this electron absorbs photon energy, the photon energy absorbed is transferred into kinetic energy of the electron. We know that the following Einstein's relationship is true for the total energy *E* and the momentum *p* of the electron that begins moving:

$$E^2 = c^2 p^2 + E_0^2. \qquad \text{(IV.1)}$$

Of course, $E > E_0$ in this case.

However, what happens if this electron at rest is attracted to the nucleus of a hydrogen atom, a proton, and is drawn into the atom?

The electron emits a photon from itself without absorbing external energy, and at the same time gains an amount of kinetic energy equivalent to the photon energy.

Even if the electron which was at rest begins moving in free space, and even if it is absorbed into an atom, the starting point of the electron's energy for either case is its rest mass energy.

The electron's energy *E* for the former state is $E > E_0$ and for the latter state is $E < E_0$.

Meanwhile, in order to maintain the law of energy conservation in the latter case, an energy source is needed to supply the increased kinetic energy and released photon energy.

According to the explanation based on classical mechanics in Chapter II of this paper, the reduction comes from potential energy.

However, potential energy has no fundamental substance and is considered a concept introduced by classical mechanics to maintain the law of energy conservation.

Meanwhile, the energy gained by the hydrogen atom, as obtained using the Dirac equation, includes the electron's rest mass energy.

The energy here is measured on an absolute scale. Because $E < E_0$ in this case, Einstein's relationship does not apply to an electron in this state.

However, the energy of a hydrogen atom, obtained through classical quantum theory or the Schrödinger equation, is negative. This can be considered to be a measurement on an absolute scale which excludes the electron's rest mass energy. However, it appears that we have failed to notice this exclusion.

Let us imagine an electron transported an infinite distance from the proton of a hydrogen atom and placed at rest. The energy of a hydrogen atom in this state, as obtained from classical quantum mechanics or the Schrödinger equation, is zero. This zero energy is sometimes described as the total energy and sometimes described as the potential energy.

However, the Dirac equation predicts that the potential energy for this case will be zero but that the total energy will be $m_e c^2$. When describing the total energy of a hydrogen atom on an absolute scale, the energy in this case equals the electron's rest mass energy.

If we define the single photon energy and kinetic energy now being released as $-E_n$, the energy transfer in the initial state could be written as follows.

$$[E_0 + V(r_n)] + K_n + \hbar\omega = (E_0 + 2E_n) - E_n - E_n \qquad \text{(IV.2a)}$$

$$= E_0. \qquad \text{(IV.2b)}$$

Because the photon is emitted externally, if we omit that energy here, the total energy of a hydrogen atom can be expressed as:

$$E_{\mathrm{ab},n} = [E_0 + V(r_n)] + K_n \qquad \text{(IV.3a)}$$

$$= (E_0 + 2E_n) - E_n \qquad \text{(IV.3b)}$$

$$= E_0 + E_n. \qquad \text{(IV.3c)}$$

$2E_n$, which corresponds to the potential energy $V(r_n)$ of a hydrogen atom from Eq. (IV.3b), is thought to be the reduction in the electron's rest mass energy.

The potential energy of a hydrogen atom is usually related to the distance between the proton and the electron. However, when considering that Eq. (III.4b), which predicts the energy of a hydrogen atom, includes the electron's rest mass energy, it is possible to surmise that the potential energy of a hydrogen atom is related to the energy of the electron.

This paper predicts that the rest mass energy of the electron is the source of the kinetic energy obtained by the electron and of the photon energy emitted by the electron.

Let us summarize the points covered until now. Under classical mechanics, the following equation is true.

$$V(r) + K + \hbar\omega = 0, \qquad V(r) \le 0. \tag{II.7}$$

Meanwhile, from the perspective of this manuscript, if we represent the reduction in rest mass energy of the electron as $-\Delta E_0$, then the following equation is true.

$$-\Delta E_0 + K + \hbar\omega = 0. \tag{IV.4}$$

Thus, in our discussion, in dealing with the potential energy of a hydrogen atom, we offer the hypothesis that this physical quantity corresponds to the reduction of the electron's rest mass energy:

$$V(r) = -\Delta E_0. \tag{IV.5}$$

If this relationship is accepted to be true, then it is possible for potential energy, which did not exist when the electron was at rest, to decrease.

V. Discussion

In the central field inside a hydrogen atom, the amount of reduced potential energy can be thought to be equivalent to the sum of increase in the kinetic energy of an electron and the energy of photons emitted by the electron. Accordingly, we can establish the following law of energy conservation.

$$-\Delta V(r) + \Delta K + \hbar\omega = 0. \tag{V.1}$$

According to (IV.2a), half decrease in rest mass energy was released outside the atom as photon energy, while the other half was converted into the electron's kinetic energy. When each of photon energy and electron's kinetic energy reach $m_e c^2/2$, the electron cannot obtain more kinetic energy than this, and it is also unable to decrease its potential energy. Thus, the value $V(r)$ must satisfy the following inequality.

$$-m_e c^2 \le V(r) \le 0. \tag{V.2}$$

Therefore, there exists a minimum value of potential energy, whereupon the following relationship is established.

$$-\left(\frac{1}{4\pi\varepsilon_0}\right)\frac{e^2}{r_e} = -m_e c^2. \tag{V.3}$$

The location that satisfies this relationship is the distance of closest approach r_e, which indicates how close the electron comes to the center of the atom. From (V.3), r_e is the following value.

$$r_e = \frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{m_e c^2} \qquad \text{(V.4a)}$$

$$= r_c . \qquad \text{(V.4b)}$$

Here, r_c is the classical electron radius.

Thus, it becomes clear that an electron is not absorbed in an atomic nucleus. Furthermore, the distance r_c agrees with the distance of closest approach of α-particle in Rutherford scattering [4,5].

Even though we could explain the reason why an electron is not absorbed into a nucleus without waiting for the appearance of Bohr's classical quantum theory, we remained oblivious to this fact for the past century.

VI. Conclusion

1. In considering the potential energy of a hydrogen atom, we offered the hypothesis that this physical quantity corresponds to the decrease in the electron's rest mass energy. Thus,

$$V(r) = -\Delta E_0 .$$

2. The stability of a hydrogen atom was first explained according to Bohr's classical quantum theory. However, it becomes clear that within the electron inside a hydrogen atom, there exists an off-limits boundary r_c. Furthermore, this distance of closest approach corresponds to the classical electron radius. (See Table. 1)

Distance from nucleus	∞	a_B	r_c
Photonic energy (total) $\hbar\omega$	0	$-E_1$	$\frac{mc^2}{2}$
Kinetic energy K	0	$-E_1$	$\frac{mc^2}{2}$
Potential energy $V(r) = -\Delta E_0$	0	$2E_1$	$-mc^2$
Total energy $E_0 + V(r) + K$	mc^2	$mc^2 + E_1$	$\frac{mc^2}{2}$
Rest mass energy $E_0 + V(r)$	mc^2	$mc^2 + 2E_1$	0

Table.1 Energy of electrons at distances ∞, a_B and r_c from an atomic nucleus.

This value is different from the value predicted by classical quantum theory, or the Bohr radius, but the atom's stability can be explained even by our approach. However, this does not necessarily mean that our discussion has casts doubt onto quantum mechanics. Our discussion shows only that it is possible to explain the stability of a hydrogen atom according to theories other than quantum mechanics.

The conclusion of this paper is a common sense conclusion based on classical mechanics logic.

Even so, it has been intentionally highlighted because this fact is not commonly known by all current physicists.

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Appendix

One of the important relationships in the Special Theory of Relativity is as follows.

$$E^2 = c^2 p^2 + E_0^2. \tag{A.1}$$

Here, E is the total energy of an object or a particle.

Gasiorowicz discusses the relativistic analog of Schrödinger for a bound (scalar) electron inside a hydrogen atom, which does include the rest mass energy of the electron in an attractive, central potential [3].

This equation is

$$\left(\frac{E}{\hbar c} + \frac{Ze^2}{4\pi\varepsilon_0 \hbar c}\frac{1}{r}\right)^2 \psi = -\nabla^2\psi + \left(\frac{mc}{\hbar}\right)^2 \psi. \tag{A.2}$$

which is the operator version of (A.1) when a potential is included,

$$(E - V)^2 = c^2 p^2 + E_0^2. \tag{A.3}$$

The solution by solving for this (A.2) did not agree with the actual energy level of the hydrogen atom. The reason proposed is that electrons are 1/2 spin particles and do not follow the Klein-Gordon equation. However, as a remaining problem, the left side of (A.3) is as follows.

$$E - V = (K + V) - V \quad \text{(A.4a)}$$

$$= K. \quad \text{(A.4b)}$$

Thus, $K^2 > E_0^2$, or $(p^2/2m)^2 > (mc^2)^2$, but this kind of inequality should normally not be possible. Here, let us surmise that *E* of (A.3) is defined not as the *E* of (II.5b) but instead as:

$$E = E_0 - K. \quad \text{(A.5)}$$

By substituting this *E* into (A.3) and considering the relation to (II.4), we obtain:

$$(E_0 + K)^2 = c^2 p^2 + E_0^2. \quad \text{(A.6)}$$

This equation is identical to Einstein's relationship. In the end, the total energy *E* of (A.3) is the energy as defined by (A.5). *E* of (A.3) includes the electron's rest mass energy and is defined on an absolute scale.

References

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