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A Simple Remark Leading to a Basic Precision Estimate for Non-Relativistic (NR) Real Values of Quantum Mechanics Operators

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Abstract

Starting with a very basic statement that any physical constants cannot be written with an infinite precision, it is shown how to introduce this uncertainty into the Hamiltonian of non-relativistic atomic (NR) physics and how to estimate errors on quantum operators (energy, frequency, momenta) when an uncertainty $\delta\hbar$ is assigned to $\hbar = \frac{h}{2\pi}$. The Schrödinger equation is written and the kinetic energy term $T_c = \frac{p^2}{2m_e}$ is transformed into a Laplacian: $T_c = -\frac{\hbar^2}{2m_e}\Delta_r$. This transformation leads (as known since 1926) to the wave equation, whose solutions are wave functions. The relativity correction to the kinetic energy term is introduced and its effect is discussed. ($\hbar$ constant has an uncertainty $\frac{\delta\hbar}{\hbar} \approx 10^{-8}$ value taken from CODATA.)

Keywords

Atomic Physics, Planck Constant, Schrödinger Equation

1. Introduction

It is customary in almost all text books on Quantum Mechanics that all physical quantities, as m_e electron mass, e electric charge, and $\hbar$ are not given with an infinite precision leaving the physicist to ask the following question.

Will a small uncertainty on the fundamental nature constant h or $\hbar = \frac{h}{2\pi}$, (leaving outside electric charge e and electron mass m_e) blur the expected results that one finds using $\hbar$, such as energy levels for most electron systems constrained to a Hamiltonian? Just because this basic uncertainty ($\delta\hbar$) exists! The purpose of this letter is to show how a small variation $\delta\hbar$, that one introduces in the NR Hamiltonian H_0 can produce an effect on numerical quantum observable such as energy levels. This work puts forward a way to calculate analytically the uncertainty of a quantum datum, such as I_H the ionization energy of hydrogen, when one pays attention to the slight modification of the Hamiltonian H_0, inserting $\hbar \pm \delta\hbar$ rather than $\hbar$ in the kinetic energy $T_c = -\frac{\hbar^2}{2m_e}\Delta_r$.

2. Non-Relativistic Hamiltonian

This atomic unit system serves to simplify numerical coefficients to establish the Hamiltonian H_0 and to solve the Schrödinger equation and find the wave function. In the end, the numerical results are obtained restoring the numerical values of m_e, e electric charge and $\hbar$. The simple equations written below hint at a way to show how to estimate the error on of quantum observables, such as impulse p or energy E when making the assumption that the Planck constant $\hbar$ is known within the experimental precision:

$$H_0 = -\frac{\hbar^2}{2m}\Delta_r + V(r) = E \tag{1}$$

$$H_{\delta\hbar} = -\frac{(\hbar \pm \delta\hbar)^2}{2m}\Delta_r + V(r) = E \pm \Delta E \tag{2}$$

subtracting (3) from (2)

$$H_{\delta\hbar} - H_0 = \pm\Delta E \tag{3}$$

Taking the positive sign for the correction term: $(\hbar + \delta\hbar)$
then:

$$H_{\delta\hbar} - H_0 = +\Delta E \tag{4}$$

Neglecting terms $O(\delta\hbar^2)$ in the subtraction $H_{\delta\hbar} - H_0 = \Delta E$. We arrive simply to:

$$\Delta E = \frac{\delta\hbar}{\hbar}.\frac{\hbar^2}{m}\Delta_r \tag{5}$$

$$\frac{\hbar^2}{2m}\Delta_r = \frac{\Delta E}{2}.\frac{\hbar}{\delta\hbar} \tag{6}$$

There is the kinetic energy term:

$$T_c = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\Delta_r \tag{7}$$

Let'us use the virial theorem:

$$2\langle T_c \rangle + \langle U \rangle = 0 \tag{8}$$

Replacing:

$$\langle T_c \rangle = -\left\langle \frac{U}{2} \right\rangle = \frac{\Delta E}{2} \cdot \frac{\hbar}{\delta \hbar} \tag{9}$$

3. Relativity Correction

At this point I will show that the relativity term that appears below (that is *H*) compared to H_0 is indeed negligible, for what are correction terms order of $\delta\hbar^2$ and greater. Using the relativity energy correction term [1] to the H_0 Hamiltonian:

$$H = m_e c^2 \left(\sqrt{1 + \frac{p^2}{m_e^2 c^2}} - 1 \right) - \frac{e^2 Z}{r} \tag{10}$$

The quantity $\frac{p^2}{m_e^2 c^2}$ is dimensionless so that the hamiltonian *H* is indeed an energy. (Mechanics of the atom pp 202-204)

$$H = H_0 + H_1 \tag{11}$$

Considering $\alpha = \frac{p^2}{m_e^2 c^2}$, a small quantity, and proceeding to a Taylor expansion order of α^2 for the square root term, the correction H_1 is given by:

$$H_1 = -\frac{p^4}{8 m_e^3 c^2} \tag{12}$$

$H_1 = E_1$ with:

$$E_1 = -\frac{p^4}{8 m_e^3 c^2} \tag{13}$$

$$p^2 = -\hbar^2 \Delta_r \tag{14}$$

$$E_1 = -\frac{1}{2 m_e c^2} \frac{\hbar^4}{4 m_e^2} (\Delta_r)^2 \tag{15}$$

Replacing the square impulse operator in H_1 lead to a p^4 term that is :

$$-\frac{\hbar^2}{2m} \Delta_r + V(r) - \frac{p^4}{8 m_e^3 c^2} = E + E_1 \tag{16}$$

$$T_c = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \Delta_r \tag{17}$$

As before, one adds the relativity term H_1 to both Equations (1) and (2) to give:

$$-\frac{\hbar^2}{2m} \Delta_r + V(r) - \frac{p^4}{8 m_e^3 c^2} = E + E_1 \tag{18}$$

$$-\frac{\hbar^2}{2m} \Delta_r + V(r) - \frac{1}{8 m_e c^2} \frac{(\hbar \Delta_r)^2}{4 m_e^2} = E + E_1 \tag{19}$$

The same is perfomed as in Equations (2) and (3). That is:

$$-\frac{\hbar^2}{2m}\Delta_r+V(r)-\frac{1}{2m_ec^2}\frac{\hbar^4\Delta_r^2}{4m_e^2}=E+E_1 \tag{20}$$

$$-\frac{(\hbar\pm\delta\hbar)^2}{2m}\Delta_r+V(r)-\frac{1}{2m_ec^2}\frac{(\hbar\pm\delta\hbar)^4\Delta_r^2}{4m_e^2} \tag{21}$$

$$=E\pm\Delta E+E_1\pm\Delta E_1 \tag{22}$$

Using symbolic Mathematica, it is easy to develop the product $(\hbar\pm\delta\hbar)^4$ and to subtract Equation (22) from Equation (21). It is shown that leaving out all orders $\geq O(\delta\hbar^2)$ in the subtraction there is only one term order $O(\delta\hbar)$ coming from the relativity correction:

$$\Delta E_1=-\frac{\Delta_r^2\hbar^3\delta\hbar}{2c^2m_e^3} \tag{23}$$

This corrected term ΔE_T can be evaluated with the NR ΔE (or T_c) term as:

$$\Delta E_T=\Delta E+\Delta E_1=\Delta E\left(1-\frac{\Delta E}{2m_ec^2}\right) \tag{24}$$

Numerical Effect on Physical Constants

To check this on the value of the ionization potential I_H of hydrogen: $I_H=13.606\text{ eV}$ we can use the ionization energy of hydrogen I_H to give a value to $\left\langle\frac{U}{2}\right\rangle$ neglecting the irrelevant sign:

$$\Delta E=I_H\cdot\frac{\delta\hbar}{\hbar} \tag{25}$$

$$\Delta I_H=I_H\cdot\frac{\delta\hbar}{\hbar} \tag{26}$$

It is enough to define $m_ec^2=511\text{ keV}$ for the rest mass of the electron. The result is:

$$\Delta E_T=I_H\left(1-\frac{I_H}{2m_ec^2}\right)\frac{\delta\hbar}{\hbar} \tag{27}$$

The quantity $-\left(\frac{I_H}{2m_ec^2}\right)$ is numerically:

$$E_{cor}=1.81138\times10^{-4} \tag{28}$$

That uctuating energy is on the order of the uncertainty:

$$\frac{\delta\hbar}{\hbar}=10^{-8} \tag{29}$$

$$\Delta I_H=13.606\times10^{-8}\text{ eV} \tag{30}$$

$$\Delta E_T=13.6058\times10^{-8}\text{ eV} \tag{31}$$

Equivalent energies in quantum mechanics are found in [2] Mécanique Quantique and can be linked to an equivalent temperature T_k:

$$T_k = 1.36 \times 11605 \times 10^{-7} \approx 0.00157\ \text{K} \tag{32}$$

$$1\ \text{eV} \approx 11605\ \text{K} \tag{33}$$

4. Conclusions and Suggestions

I can define the temperature T_T with the corrected value $\Delta E_T = 13.6058 \times 10^{-8}\ \text{eV}$. It will give an uncertainty on $\delta T_k = \pm 2.321\ \text{nK}$. The relativity correction gives an uncertainty 10^{-3} compared to the fluctuation caused by the basic uncertainty $\frac{\delta \hbar}{\hbar} = 10^{-8}$. I can conclude that an uncertainty such as $\delta \hbar$ on the Planck constant can produce an important (in se) fluctuation for energy in atomic systems enough to be experimentally seen. Elsewhere an ultra cold temperature obtained by ultra cold atoms could detect this effect, and can be used to determine an ultra precise $\hbar$ Planck constant. Recalling that ultra cooled atoms can be cooled to a temperature $T = 1\ \mu\text{K}$ well under the temperature T_k [3].

$$T_k = 157\ \mu\text{K} \tag{34}$$

obtained with the newly uncertainty on Planck constant used for S.I. units system [4]:

$$\frac{\delta \hbar}{\hbar} = 10^{-8} \tag{35}$$

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