# On the bound energies of the hydrogen atom with a more general uncertainty relation

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RÉSUMÉ. On considère la possibilité présentée de l'existence d'états atomiques de l'hydrogène avec une énergie plus basse que la valeur habituelle de −13.6 eV, en profitant d'une forme nouvelle et plus générale des relations d'incertitude.

ABSTRACT. We consider the proposed possibility of the existence of hydrogen atomic states with an energy lower than the usual −13.6 eV ground state energy, taking advantage of a newly proposed more general form of the uncertainty relations.

P.A.C.S.: 03.65.-w; 03.65.Ge; 03.65.Ta

## 1 Mill's claims and criticisms

The reported observations, by R. L. Mills and his collaborators ([1], [2], [3], [4]), of release of energy in devices in which hydrogen atoms interact with catalytic substances, lead this author to propose the existence of induced electronic transitions from the ground state of −13.6 eV to even lower energy states, the so-called hydrino states. The theoretical basis for such an explanation would be provided by a new description of quantum phenomena, to be called Classical Quantum Mechanics, of which basic tenets are a classical wave equation and the non-radiation condition for distributions of electric current densities.

The underlying interpretation of the published experimental results has been criticized by several authors [5], [6], [7], based on the fact that such states are not admissible in standard quantum mechanics (or even in Mills own theory, see [5]), either non-relativistic or relativistic, even though the Klein-Gordon equation for a Coulomb potential shows a lower energy state, as does the Dirac equation in two dimensions; in fact, consideration of a small but nonzero radius for the atomic nucleus reveals ([7]) the unphysical character of those solutions.

Mills, in turn [8], criticizes standard quantum mechanics, taking issue, in particular, with an estimate by Feynman [9] of the radius of the ground state of the hydrogen atom, based on a qualitative, semi-classical use of the Heisenberg uncertainty relations for the position and momentum of a particle. It seems to us that his observations are, in general, sound, but it must be kept in mind that the argument was originally presented in a pedagogical context, with no pretense of quantitative, or even physical, rigour.

Our aim in the present work is to show that Feynman's deduction does allow for the ocurrence of hydrogen states more tightly bound then the usual electronic ground state, if one employs a more general set of uncertainty relations, recently proposed.

## 2 Generalized uncertainty relations

All of the above criticisms are based on the acceptance of the traditional linear quantum mechanical equations for the electron, either nonrelativistic or relativistic. However, several other authors (among others, [10], [11],[12], [13]) have proposed the introduction of some forms of nonlinear Klein-Gordon and Schrödinger equations. One such equation was used to deduce, from a new type of acceptable solutions based on wavelet analysis, a more general expression for the uncertainty relations, allowing an extension of the available measurement space, in line with modern advances in microscopy techniques [13]. This was done in the context of de Broglie's theory of the double solution, where a real physical wave $\Phi(\mathbf{r}, t)$ will be given by the addition of an extended yet finite guiding wave, $\Theta(\mathbf{r}, t)$, with a very much localized $\xi(\mathbf{r}, t)$ wave representing the particle itself, both waves being in phase and in such a way that the particle will most probably be in the small region where the $\Theta$ wave is most intense. In the linear approximation, this $\Theta$ wave becomes the $v$ wave in de Broglie´s linear version of the double solution theory, such that both this $v$ wave and the usual $\Psi$ wave satisfy the traditional Schrödinger equation. However, here $\Psi$ is, as usual, a probability amplitude wave, whereas $v$ is a real physical, non-normalizable, wave, both related by $\Psi = Cv$, $C$ being a normalization constant. As a consequence, it will be the extended $\Theta$ wave that will be ultimately responsible for the usual, observable, linear superposition, interference and confinement effects [14]. We will use in what follows a general form for these $\Theta$ waves, specifically an integral over Morlet wavelets, obeying a nonlinear Schrödinger equation of the form

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + \frac{\hbar^2}{2m}\frac{\nabla^2(\Psi\Psi^*)^{1/2}}{(\Psi\Psi^*)^{1/2}}\Psi(\mathbf{r},t) + V(\mathbf{r},t)\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}. \tag{1}$$

In fact, starting from a spatial Morlet mother wavelet represented by

$$f_0(x) = e^{-\frac{x^2}{2\sigma^2}+ikx}, \tag{2}$$

of width $\sigma$ and wavelength $2\pi/k$, one builds up the extended part (for $t = 0$) of the free particle guiding wave, $\Theta$, solution of the nonlinear equation above in one spatial dimension, as

$$\Theta(x) = \int\int\int\int g(k,\sigma,b,e)e^{-\frac{(x-b)^2}{2\sigma^2}+ik(x-e)}dk\,d\sigma\,db\,de, \tag{3}$$

where $b$ and $e$ are the translational parameters of the mother wavelet. Now three possible approaches are introduced, *viz.*,

### *2.1 first*

$e = b$, $\sigma$=const., $g(k,b) = g(k)\delta(b)$ and $g(k) = A\,e^{-\frac{(k-k_0)^2}{2\sigma_k^2}}$, where $A$ and $\sigma_k$ are also constants. Then, one obtains

$$\Theta(x) = \sqrt{2\pi}A\,\sigma_k e^{-\frac{x^2}{2\sigma_x^2}+ik_0x}, \tag{4}$$

where

$$\sigma_x^2 = \frac{1}{\sigma_k^2 + \frac{1}{\sigma^2}}, \tag{5}$$

that is

$$(\Delta x)^2 = \frac{\hbar^2}{(\Delta p_x)^2 + \frac{\hbar^2}{\sigma^2}}. \tag{6}$$

### 2.2 *second*

$e = 0$, $\sigma =$ const., $g(k, b) = g(k)e^{-\frac{b^2}{2\sigma_b^2}}$, with $\sigma_b =$ const., and $g(k) = A\,e^{-\frac{(k-k_0)^2}{2\sigma_k^2}}$, leading to

$$\Theta(x) = 2\pi A \left(\frac{1}{\sigma^2 + \sigma_b^2}\right)^{-1/2} \sigma_k \; e^{\frac{-x^2}{2/\left(\sigma_k^2 + \frac{1}{\sigma^2+\sigma_b^2}\right)} + ik_0 x} \tag{7}$$

and

$$\sigma_x^2 = \frac{1}{\sigma_k^2 + \frac{1}{\sigma^2+\sigma_b^2}} \tag{8}$$

or

$$(\Delta x)^2 = \frac{\hbar^2}{(\Delta p_x)^2 + \frac{\hbar^2}{\sigma^2+\sigma_b^2}} \tag{9}$$

### 2.3 *third*

$e = b$, $\sigma = M\lambda$ — i.e., now the extended part of the particle is proportional, through the parameter $M$, to the wavelength $\lambda = 2\pi/k$ — such that the exponential $e^{-\frac{(x-b)^2}{2\sigma^2}}$ in the integral expression for $\Theta(x)$ above becomes $e^{-\frac{k^2(x-b)^2}{8\pi^2 M^2}}$, $g(k, b) = g(k)\delta(b)$ and $g(k) = A\,e^{-\frac{(k-k_0)^2}{2\sigma_k^2}}$, and then

$$\begin{aligned}\Theta(x) &= \int_{-\infty}^{+\infty} A\,e^{-\frac{(k-k_0)^2}{2\sigma_k^2}}\, e^{-\beta^2 k^2 x^2 + ikx} dk \\ &= \sqrt{2\pi} A\, \frac{\sigma_k}{\sqrt{2\sigma_k^2\beta^2 x^2 + 1}} e^{-\frac{x^2}{2\sigma_x^2} + i\frac{k_0}{2\sigma_k^2\beta^2 x^2+1} x}\end{aligned} \tag{10}$$

where $\beta^2 = 1/(8\pi^2 M^2)$ and

$$\sigma_x^2 = \frac{2\sigma_k^2\beta^2 x^2 + 1}{\sigma_k^2 + 2\beta^2 k_0^2}. \tag{11}$$

Representative values for the parameters above are $k_0 = 10$ and $M \simeq 100$, that is $\beta \simeq 10^{-3}$, for a free particle. However, as we will see below, they may attain different values for bounded particles. Nevertheless, for these values, one can take $2\sigma_k^2\beta^2 x^2 \ll 1$ [13] and then

$$\Theta(x) = \sqrt{2\pi} A\, \sigma_k e^{-\frac{x^2}{2\sigma_x^2} + ik_0 x} \tag{12}$$

and also

$$\sigma_x^2 \simeq \frac{1}{\sigma_k^2 + 2\beta^2 k_0^2} = \frac{1}{\sigma_k^2 + \frac{k_0^2}{4\pi^2 M^2}}, \tag{13}$$

or

$$(\Delta x)^2 \simeq \frac{\hbar^2}{(\Delta p_x)^2 + \frac{\hbar^2}{\sigma_0^2}}, \tag{14}$$

where $\sigma_0 = 1/(\sqrt{2}\beta k_0) = M\lambda_0$ is the width of the central wavelet.

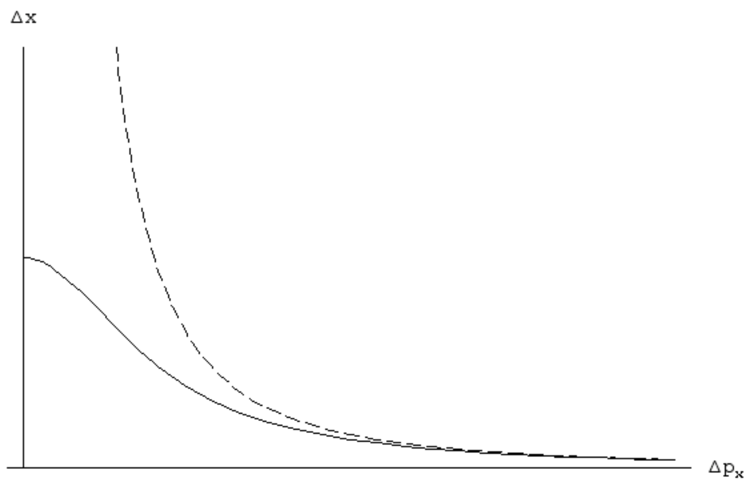


Figure 1: Heisenberg and generalized measurement spaces

It is now obvious, from these more general forms of the uncertainty relations, that the simultaneous precisions of position and momentum measurements are no longer limited by the hyperbola $\Delta x \Delta p_x = \hbar$ (dashed line in Fig.1 below), but that this product can in fact come closer to the origin (full line in the same figure), depending on the chosen value for the various parameters $\sigma$ such as, in this last case, $\sigma_0$, the width of the central wavelet.

## 3 Minimizing the orbital electron energy

### *3.1 Feynman's argument*

We briefly review Feynman's qualitative argument [9], leading to an estimate of the Bohr radius from the uncertainty relations. Taking the classical expression for the total energy of the orbital electron in a hydrogen atom, $E = p^2/2m - (4\pi\epsilon_0)^{-1}e^2/r$, we consider $p \sim \Delta p$ and $r \sim \Delta r$, with $\Delta p \Delta r \sim \hbar$. Then,

$$E = \frac{\hbar^2}{2mr^2} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} \tag{15}$$

and the equilibrium condition $dE/dr = 0$ leads to

$$r_{eq.} = \frac{\hbar^2}{m}\frac{4\pi\epsilon_0}{e^2}, \tag{16}$$

the well known minimum radius $a_B$ of 0.53 Å for the hydrogen ground state $|1s\rangle$ orbital, with a binding energy

$$E_1(r = a_B) = -\frac{1}{2}\frac{m}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \tag{17}$$

of $-13.6$ eV. A similar qualitative reasoning had been previously presented by D. Bohm [15].

### *3.2 The new equilibrium condition*

We now turn to the computation of an estimate of the possible orbital radii, taking advantage of the generalized uncertainty relations, obtained above from the wavelet solutions of the nonlinear Schrödinger equation. From equation (14) above we get $\Delta p^2 = \hbar^2(1/\Delta x^2 - 1/\sigma_0^2)$, and still with $\Delta p \sim p$, $\Delta x \sim r$, the total orbital energy acquires an additional negative term

$$E(r) = \frac{\hbar^2}{2m}\frac{1}{r^2} - \frac{\hbar^2}{2m}\frac{1}{\sigma_0^2(r)} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}. \tag{18}$$

Since $\sigma_0$ represents the width of the central wavelet, it is natural to suppose that its value will depend on the dimensions of the available space for the motion of the electron, in the present case of the order of the radius $r$ of its orbit. Then the equilibrium condition gives us

$$\frac{dE}{dr} = -\frac{\hbar^2}{mr^3} + \frac{\hbar^2}{m}\frac{1}{\sigma_0^3(r)}\frac{d\sigma_0(r)}{dr} + \frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2} = 0. \tag{19}$$

The simplest dependence will be linear, $\sigma_0(r) = Mr$, where the value of the parameter $M > 1$ is to be specified. The condition above for the smallest, equilibrium radius now gives

$$r_{eq.} = a_B \times \left(1 - \frac{1}{M^2}\right) \leq a_B. \tag{20}$$

### *3.3 Checking the more general relation*

We note that even if we use the more general relation (11), our results are not significantly altered. In fact, taking $x \sim \sigma_x$ in the spirit of the present approach, we obtain

$$\sigma_x^2 = \frac{1}{\sigma_k^2(1-2\beta^2) + 2\beta^2 k_0^2} \tag{21}$$

that is,

$$(\Delta p_x)^2 = \frac{\hbar^2}{1-2\beta^2}\left(\frac{1}{(\Delta x)^2} - \frac{1}{\sigma_0^2}\right). \tag{22}$$

The equilibrium condition now reads

$$\frac{dE}{dr} = 0 = -\frac{\hbar^2}{m}\frac{1}{1-2\beta^2}\frac{1}{r^3} + \frac{\hbar^2}{m}\frac{1}{1-2\beta^2}\frac{1}{\sigma_0^3(r)}\frac{d\sigma_0(r)}{dr} + \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}, \tag{23}$$

and the corresponding radius, with, as before, $\sigma(r) = Mr$, becomes

$$r_{eq.} = a_B \times \frac{1}{1-2\beta^2}\left(1 - \frac{1}{M^2}\right) \leq a_B, \tag{24}$$

or, with $\beta = 1/(2\pi\sqrt{2}M)$,

$$r_{eq.} = a_B \times \frac{M^2 - 1}{M^2 - 0.025} \sim a_B \times \left(1 - \frac{1}{M^2}\right) \leq a_B \tag{25}$$

once more.

### *3.4 Resulting energies*

Now it is obvious that the radii of one or more possible states with lower energy, i.e., more tightly bound than the usual ground state, will depend on the actual numerical values for the parameter $M > 1$, a computation that is beyond the scope of the present work. Nevertheless, we can immediately plug in this result in the expression (18) above for the orbital electron energy, resulting in

$$\begin{aligned} E(r_{eq.}) &= \frac{\hbar^2}{2m}\left(\frac{1}{r_{eq.}^2} - \frac{1}{M^2 r_{eq.}^2}\right) - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r_{eq.}} \\ &= \left(1 - \frac{1}{M^2}\right)^{-1} \times E_1 < E_1, \end{aligned} \tag{26}$$

where $E_1$ is, as in (17) above, the traditional ground state binding energy of $-13.6$ eV.

## 4 Conclusions

The fundamental recourse to the nonlinear Schrödinger equation above seems to allow for the ocurrence of additional solutions to the Coulomb problem for a single electron orbiting a proton. The use of integral wavelet solutions avoids some well known paradoxes of traditional quantum mechanics [13], constituting a promising approach which has been developed recently, aimed at a realistic description of quantum phenomena by extension of the theory of the double solution, in particular through the application of wavelet analysis. One of the main outcomes of this new approach, here applied, is a renewed, generalized form of the basic position-momentum uncertainty relation which seems to permit, if applied to an orbiting electron, the recovery of Feynman's reasoning criticized by Mills and the existence of energy states below −13.6 eV.

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