Basic quantum Hamiltonian’s relativistic corrections

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Abstract

After analyzing Dirac’s equation, one can suggest that a well-known quantum-mechanical momentum operator is associated with relativistic momentum, rather than with non-relativistic one. Consideration of relativistic energy and momentum expressions allows us to define the non-relativistic, relativistic and pseudo-relativistic (present in Schrödinger equation) kinetic energy operators. Consequences of kinetic energy operator’s correction for spectra of basic quantum Hamiltonians are investigated. In some cases this correction can produce remarkable spectra modifications.

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I. INTRODUCTION

The many-particle Schrödinger equation is the best tool for quantum systems low-energy phenomena investigation. The existing powerful approximate methods enable successful description of such systems as electrons in solid state, molecules, atoms and even the atomic nuclei. The Hamiltonian is defined as a non-relativistic operator, hence relativistic modifications are among the most important. However, the solution of this problem is very problematic due to the complex relativistic kinetic energy operator and the undefined many-particle Dirac equation. This problem has been solved only in weakly relativistic approximation for systems with Coulomb potential, such as an atom. The main points of this solution are based on Hamiltonian’s corrections, saving the usual form of kinetic energy operator and introducing new potentials like spin-orbit, following from corresponding Dirac equation. For systems with strong interaction these Hamiltonian corrections are not sufficient in order to obtain acceptable result. New ways need to be investigated in order to solve this problem.

Let us take a new look at relativistic modifications for basic quantum-mechanical Hamiltonians describing particle, moving in spherically-symmetric external fields, created by deep well, harmonic oscillator and Coulomb potentials. These Hamiltonians consist of one-particle kinetic energy operator and external field potential operator, and can be presented as:

$$h_0 = -\frac{(\hbar c)^2}{2mc^2} \Delta + \mathbf{v}(r, \tau),$$  \hspace{1cm} (1)

where $mc^2$ is particle’s rest energy, given in GeV, $\hbar c = 0.197 \text{ GeV \, fm}$. $r$ is absolute value of it’s radius-vector and $\tau$ marks the set of intrinsic variables, such as mass, charge, spin, isospin and possible others. Such operators are the essential parts of many-particle Hamiltonian, hence relativistic corrections are necessary for further investigation of this problem.

II. DIRAC EQUATION TRANSFORMATIONS

Dirac equation \cite{1, 2} is the basic for Hamiltonian’s relativistic corrections:

$$\left(1 - \frac{1}{c} \frac{\partial}{\partial t} + \sum_{k=1}^{3} \alpha_k \frac{\partial}{\partial x_k} + \beta \frac{i mc^2}{\hbar c}\right) \Psi = 0,$$  \hspace{1cm} (2)

where $\alpha_k$ and $\beta$ are Dirac matrices and wave-function $\Psi$ is defined as set of four functions - components. Modified stationary equation for free particle with spin, equal $\hbar/2$ can be
written in Pauli matrices as system of two equations:

\[
\begin{align*}
(\epsilon - mc^2) \varphi + i\hbar c (\sigma \cdot \nabla) \chi &= 0, \\
(\epsilon + mc^2) \chi + i\hbar c (\sigma \cdot \nabla) \varphi &= 0.
\end{align*}
\]  

Here \(\epsilon\) is relativistic particle’s energy operator, and \(\sigma\) - spin operator. \(\varphi\) and \(\chi\) are two-component spinors composing entire wave-function

\[
\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}.
\]

Let us define \(\Psi\) as eigenfunction of operator \(\epsilon\) corresponding to eigenvalue, equal \(\epsilon\). Having in mind that commutator of operators \(\epsilon\) and \(\nabla\) equals zero, the eigenfunction of \(\epsilon\) is also eigenfunction of momentum operator \(p = -i\hbar \nabla\) with eigenvalue, equal \(p\), one obtains that

\[
\epsilon^2 = (mc^2)^2 + (pc)^2 = (\gamma mc^2)^2.
\]

This is the well-known expression for energy of the relativistic particle with momentum \(p = \gamma mv\), where Lorentz factor

\[
\gamma = \left(1 - (v/c)^2\right)^{-1/2}.
\]

This leads to the conclusion that quantum-mechanical momentum operator \(p = -i\hbar \nabla\) is associated with relativistic momentum \(p = \gamma mv\) rather than with non-relativistic one \(p_0 = mv\).

The non-relativistic momentum operator can be defined in a following way. From Eq. (5), written in operators form, it follows that

\[
p^2 = (\gamma^2 - 1) (mc)^2,
\]

where the operator

\[
\gamma^2 = \left(1 - (p_0/mc)^2\right)^{-1}.
\]

Defining this classical Lorentz factor as quantum-mechanical operator, gives us the possibility to introduce non-relativistic momentum operator, non-relativistic, relativistic and pseudo-relativistic (present in Schrödinger equation) kinetic energy operators. As well as analyze relations between them and investigate spectrum modifications when different kinetic energy operators are present in Hamiltonian.
Applying the definition of the non-relativistic kinetic energy operator

\[ t_n = \frac{p_0^2}{2m} \]  

one obtains the expression:

\[ p^2 = p_0^2 \gamma^2 = 2mt_n \left(1 - 2t_n/mc^2\right)^{-1}. \]  

Let us introduce the operator present in Schrödinger equation and call it pseudo-relativistic kinetic energy operator:

\[ t_0 = \frac{p^2}{2m} = -\frac{(\hbar c)^2}{2mc^2} \Delta. \]  

It can be present in terms of \( t_n \):

\[ t_0 = t_n \left(1 - 2t_n/mc^2\right)^{-1}. \]  

From last expression it follows that

\[ t_n = \frac{p^2}{2m} \left(1 + \left(p/mc^2\right)^2\right)^{-1} = t_0 \left(1 + 2t_0/mc^2\right)^{-1}, \]  

or

\[ t_n = t_0 \left[1 - 2t_0/mc^2 + (2t_0/mc^2)^2 - ...\right]. \]  

Therefore, the non-relativistic kinetic energy operator \( t_n \) is far more complex than pseudo-relativistic one \( t_0 \).

Having kinetic energy definition in classical relativity \( t = \varepsilon - mc^2 \) in mind, one can present the system of Dirac equations [3] in the form of quantum-mechanical operators

\[
\begin{align*}
\{ \begin{align*}
t \varphi &= c(\sigma \cdot p) \chi, \\
(t + 2mc^2) \chi &= c(\sigma \cdot p) \varphi
\end{align*} \}
\end{align*}
\]

and after usual manipulations

\[ \chi = (t + 2mc^2)^{-1} c(\sigma \cdot p) \varphi, \]  

\[ t \varphi = c(\sigma \cdot p) (t + 2mc^2)^{-1} c(\sigma \cdot p) \varphi, \]  

can obtain the relativistic kinetic energy operator:

\[ t = \sqrt{(mc^2)^2 + (pc)^2} - mc^2. \]
In terms of \( t_0 \) it can be presented as

\[
\begin{align*}
t &= mc^2 \left[ \sqrt{1 + 2t_0/mc^2} - 1 \right]. \\
\end{align*}
\]  

This can be written as a series expansion:

\[
\begin{align*}
t &= t_0 \left[ 1 - t_0/2mc^2 + \left( t_0/mc^2 \right)^2/2 - \ldots \right],
\end{align*}
\]  

or

\[
\begin{align*}
t &= t_0 \sum_{k=0}^{\infty} \frac{(-1)^k}{2^k (k+1)} \binom{2k}{k} \left( t_0/mc^2 \right)^k.
\end{align*}
\]  

The first term of all operators equals \( t_0 \), see (14), (20), hence at non-relativistic energies, when \( t_0 \ll mc^2 \), all operators have the same form.

The expression of relativistic kinetic energy operator in terms of non-relativistic one is

\[
\begin{align*}
t/mc^2 &= (1 - 2t_n/mc^2)^{-1/2} - 1.
\end{align*}
\]  

The commutators of all pairs of presented kinetic energy operators equal zero, all of them are differential operators of the same argument - radius vector of particle - hence relations between eigenvalues can be defined as relations between operators, and can be considered in terms of classic relativity. The eigenvalues, corresponding to the same eigenfunction, are distributed in a following way:

\[
t_n < t < t_0.
\]  

Thus, the pseudo-relativistic operator produces the largest eigenvalue in comparison with other two for the same eigenfunction. All operators are positively defined, so it follows that at non-relativistic kinetic energy, corresponding to the maximum possible velocity \( v = c \), when \( t_n/mc^2 = 1/2 \), both (relativistic (22) and pseudo-relativistic (12)) kinetic energy operator’s eigenvalues approach, as necessary, the infinite values.

Therefore, the Schrödinger equation is not completely non-relativistic. Some relativistic corrections have already been taken into account applying relativistic momentum operator instead of the non-relativistic one. In first approximation, i.e. at negligible in comparison with \( mc^2 \) kinetic energy, all operators coincide.

Dirac equation (3) can be transformed into Schrödinger equation form also for particle moving in external field, which scalar potential is \( v \). It is necessary to introduce the expression \( t = h - v \), where \( h \) is the Hamiltonian instead of kinetic energy operator \( t \). The
equation (15) can be rewritten in following form

\[
\mathbf{h} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \mathbf{v} & c(\mathbf{\sigma} \cdot \mathbf{p}) \\ c(\mathbf{\sigma} \cdot \mathbf{p}) & \mathbf{v} - 2mc^2 \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix}.
\]  

(24)

Now let’s assume that present wave-function is an eigenfunction of Hamiltonian

\[
\mathbf{h} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = e \begin{pmatrix} \varphi \\ \chi \end{pmatrix},
\]  

(25)

where \(e\) is corresponding eigenvalue. The system of equations now is:

\[
\begin{align*}
(e - \mathbf{v}) \varphi &= c(\mathbf{\sigma} \cdot \mathbf{p}) \chi, \\
(e - \mathbf{v} + 2mc^2) \chi &= c(\mathbf{\sigma} \cdot \mathbf{p}) \varphi.
\end{align*}
\]  

(26)

As usual, the following operation eliminates the wave-function component \(\chi\). The equation for component \(\varphi\) appears in form:

\[
e \varphi = \mathbf{v} \varphi + c(\mathbf{\sigma} \cdot \mathbf{p}) \left( e - \mathbf{v} + 2mc^2 \right)^{-1} c(\mathbf{\sigma} \cdot \mathbf{p}) \varphi.
\]  

(27)

The commutator of potential energy operator \(\mathbf{v}\) and momentum operator \(\mathbf{p}\) does not equal zero. This makes the expression complex enough, so it can be successfully developed only at fulfilled condition \(e - \mathbf{v} \ll 2mc^2\), known as weakly relativistic approach [3], [2]. After the simple manipulations it can be presented as

\[
\mathbf{h} = \mathbf{h}_0 + \mathbf{v}_T + \mathbf{v}_S + \mathbf{v}_D,
\]  

(28)

where apart the standard Hamiltonian \(\mathbf{h}_0 = \mathbf{t}_0 + \mathbf{v}\), the additional potentials appear.

\[
\mathbf{v}_T = -\frac{(e - \mathbf{v} (r))^2}{2mc^2},
\]  

(29)

equals relativistic kinetic energy second order term [20], converted to potential operator form.

\[
\mathbf{v}_S = \frac{1}{2} \left( \frac{\hbar c}{mc^2} \right)^2 (\mathbf{s} \cdot \mathbf{l}) \frac{1}{r} \frac{d\mathbf{v} (r)}{dr}
\]  

(30)

is the spin-orbit potential (here \(\mathbf{s}\) and \(\mathbf{l}\) are dimensionless spin and orbital momenta operators) and

\[
\mathbf{v}_D = \frac{1}{8} \left( \frac{\hbar c}{mc^2} \right)^2 \Delta \mathbf{v} (r)
\]  

(31)

is the Darwin potential.
This investigation shows that potential’s weakly relativistic modification has to be considered only as some approximation for complete kinetic energy conversion to relativistic form.

Dirac equation for particle, moving in external field, transformation into Schrödinger equation form was very attractive years ago. Namely because kinetic energy expression is like one, present in Schrödinger equation, $e$ is characteristic for Schrödinger equation energy of particle’s bound state in given potential (equal binding energy with negative sign) and additional terms of a potential have a well-defined structure, appearing because of the nonzero spin and associated magnetic momentum.

However nucleons or constituent quarks besides of spin have additional intrinsic degrees of freedom, such as isospin and color and the realistic potentials contain all operators, allowed by symmetry considerations, these weakly relativistic modifications of strong interaction potentials are not necessary.

**III. BASIC QUANTUM HAMILTONIAN’S RELATIVITY**

Let us now investigate bound-states spectrum of basic quantum-mechanical Hamiltonian (1) when relativistic kinetic energy operator is applied instead of pseudo-relativistic one. The Schrödinger equation for these Hamiltonians is

$$\left[ -\frac{(\hbar c)^2}{2mc^2} \Delta + \mathbf{v}(r, \tau) - e \right] \varphi(r) = 0. \quad (32)$$

The spherically-symmetric potential provides the possibility to reduce this equation to ordinary differential equation for radial function, defined in a following way:

$$\varphi(r) = R_{nl}(r) Y_{l\mu}(\theta, \varphi), \quad (33)$$

where $Y_{l\mu}(\theta, \varphi)$ is spherical harmonic and $n = 1, 2, ...$ equals the number of bound state, counted from the lowest one. The radial equation after some transformations can be presented as

$$\left[ \frac{1}{r} \frac{d}{dr} r \frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2mc^2}{(\hbar c)^2} (e_{nl} - \mathbf{v}(r)) \right] R_{nl}(r) = 0. \quad (34)$$

Here the function $u_{nl}(r) = r R_{nl}(r)$ is more acceptable than the radial function. Radial Schrödinger equation for this function has the form

$$\left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2mc^2}{(\hbar c)^2} (e_{nl} - \mathbf{v}(r)) \right] u_{nl}(r) = 0. \quad (35)$$
The attracting points of this radial function are as follows: it is normalized by condition
\[ \int_0^\infty |u_{nl}(r)|^2 \, dr = 1, \quad (36) \]
so \( |u_{nl}(r)|^2 \) equals the radial probability density. Moreover, this function satisfies a condition
\[ \lim_{r \to 0} u_{nl}(r) = 0. \quad (37) \]
Next, the equation is transformed into dimensionless form. Introducing dimension-free energy and potential, one obtains an equation, where each member has dimension that equals \( 1/ (\text{length})^2 \):
\[
\left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2\frac{mc^2\epsilon (e_{nl} - v(r))}{(hc)^2 \epsilon} \right] u_{nl}(r) = 0, \quad (38)
\]
where \( \epsilon \) is combination of Hamiltonian parameters with energy dimension. For deep well and Coulomb potentials this parameter equals \( mc^2 \). For Harmonic Oscillator potential
\[
v(r) = m\omega^2 r^2 / 2 \quad (39)
\]
parameter \( \epsilon = \hbar \omega \) is the best choice. It follows that parameter with length dimension for our problem is
\[
b^2 = \frac{(hc)^2}{mc^2 \epsilon}. \quad (40)
\]
Taking new radial variable
\[
\xi = r/b, \quad (41)
\]
the equation converts to form
\[
\left[ \frac{d^2}{d\xi^2} - \frac{l(l+1)}{\xi^2} + 2\frac{(e_{nl} - v(b\xi))}{\epsilon} \right] u_{nl}(\xi) = 0. \quad (42)
\]
The discrete spectrum eigenfunctions of this equation form the orthonormal set:
\[
\int_0^\infty u_{nl}^+(\xi) u_{nl}(\xi) \, d\xi = \delta_{n',n}. \quad (43)
\]
The kinetic energy expectation value is
\[
\langle t_0 \rangle_{nl} = -\frac{1}{2} \int_0^\infty u_{nl}^+(\xi) \left[ \frac{d^2}{d\xi^2} - \frac{l(l+1)}{\xi^2} \right] u_{nl}(\xi) \, d\xi. \quad (44)
\]
The potential energy expectation value equals
\[
\langle v \rangle_{nl} = \int_0^\infty u_{nl}^+(\xi) v(b\xi) u_{nl}(\xi) \, d\xi. \quad (45)
\]
Let us now compare bound eigenvalues spectra of two Hamiltonians - one with pseudo-relativistic kinetic energy operator, i.e.

$$h_0 = t_0 + v$$  \hspace{1cm} (46)

and second - with relativistic kinetic energy operator

$$h = t + v,$$ \hspace{1cm} (47)

defined in (19). Let us mark the eigenvalue of the first Hamiltonian as $e_{nl}$. The eigenvalue of the second Hamiltonian in first perturbation theory approximation equals

$$\langle h \rangle_{nl} = e_{nl} + \langle \Delta h \rangle_{nl},$$ \hspace{1cm} (48)

where, according to given above expressions, the eigenvalue correction due to kinetic energy relativistic expression is

$$\langle \Delta h \rangle_{nl} = \langle t - t_0 \rangle_{nl} = mc^2 \left[ \sqrt{1 + 2 \langle t_0 \rangle_{nl} / mc^2} - 1 - \langle t_0 \rangle_{nl} / mc^2 \right]$$ \hspace{1cm} (49)

The first basic potential, which is going to be analyzed, is spherically symmetric well of infinite depth. This potential describes free particle, moving inside of sphere with no probability to find particle penetrated to outer region and equals:

$$v(r) = \begin{cases} 0, & \text{if } r \leq d \\ \infty, & \text{if } r > d \end{cases},$$ \hspace{1cm} (50)

where $d$ is sphere radius. The solution of corresponding Schrödinger equation (42) at $v(b\xi) \equiv 0$ is

$$u_{nl}(\xi) = \xi j_l(\xi),$$ \hspace{1cm} (51)

where $j_l(\xi)$ is the spherical Bessel function (5, § 10.1). The quantum number $n = 1, 2, \ldots$ is defined according to the boundary condition

$$u_{nl}(d/b) = 0.$$ \hspace{1cm} (52)

This equation has an infinite number of solutions, defined by different values of $b = b_n$. For $l = 0$

$$u_{n0}(\xi) = N_{n0} \sin \xi,$$ \hspace{1cm} (53)
hence
\[ b_n = d/n\pi, \quad N_{n0} = \sqrt{2/n\pi}. \quad (54) \]

Thus, the eigenvalues of Schrödinger equation (42) equal to:
\[ e_{n0}/mc^2 = z(n\pi)^2/2, \quad (55) \]

where \( z \) is the dimensionless well parameter
\[ z = \left( \frac{\hbar c}{d\; mc^2} \right)^2. \quad (56) \]

Potential equals zero in an inside region, hence the kinetic energy expectation value for this potential equals eigenvalue \( e_{n0} \). The perturbation due to relativistic corrections is
\[ \langle \Delta h \rangle_{n0}/mc^2 = \sqrt{1 + z(n\pi)^2} - 1 - z(n\pi)^2/2. \quad (57) \]

This equals one percent of eigenvalue (55) at
\[ z(n\pi)^2 \approx 0.083. \quad (58) \]

For nucleon \((mc^2 \approx 1\; GeV)\), moving in well, which radius equals 1 \( fm \), the parameter
\[ z \approx \left( \frac{0.2\; GeV \; fm}{1\; fm \; 1Gev} \right)^2 = 0.04, \quad (59) \]

so this kinetic energy correction give a remarkable effect even for ground state \( (n = 1) \) of corresponding strong process model. After kinetic energy correction, the spectrum of spherical well will change in comparison with the well-known levels distribution, whose energies are proportional to \( n^2 \). The distances between pairs of neighboring levels will be smaller than in spectrum without relativistic kinetic energy correction.

Three-dimensional Harmonic Oscillator potential is next on the list. As previously defined, the parameters of the equation equal:
\[ \epsilon = \hbar\omega, \quad \epsilon b^2 = (hc)^2/mc^2, \quad b^2 = \hbar/m\omega. \quad (60) \]

So,
\[ v(b\xi) = \epsilon\xi^2/2, \quad (61) \]

and the dimensions-free equation is
\[ \left[ \frac{d^2}{d\xi^2} - \frac{l(l+1)}{\xi^2} - \xi^2 + \frac{2enl}{\hbar\omega} \right] u_{nl}(\xi) = 0. \quad (62) \]
The eigenvalues of this equation are
\[ e_{nl} = \hbar \omega (2n + l - 1/2). \] (63)

The eigenfunctions, normalized by condition (43) are defined as in ([4], § 22.6.18):
\[ u_{nl}(\xi) = N_{nl}\xi^{l+1} e^{-\xi^2/2} L_{n-1}^{l+1/2}(\xi^2). \] (64)

Here normalization constant
\[ N_{nl}^2 = \frac{2^{n+l+1} (n-1)!}{\sqrt{\pi} [2 (n+l) - 1]!!}. \] (65)

Laguerre polynomial is defined as
\[ L^\lambda_k(x) = \sum_{j=0}^{k} (-1)^j \binom{k + \lambda}{k} x^j \frac{j!}{j!}, \] (66)

where
\[ \binom{\beta}{j} = \frac{\Gamma(\beta + 1)}{j! \Gamma(\beta - j + 1)} \] (67)

is a binomial coefficient and \( \Gamma(\beta) \) – Gamma function \([\Gamma(\beta + 1) = \beta \Gamma(\beta), \Gamma(1/2) = \sqrt{\pi}]\).

The potential expectation value equals the kinetic energy expectation value and both are defined as
\[ \langle v \rangle_{nl}/mc^2 = \langle t_0 \rangle_{nl}/mc^2 = e_{nl}/2mc^2 = z (2n + l - 1/2)/2, \] (68)

where dimensionless parameter
\[ z = \left( \frac{hc}{b mc^2} \right)^2 = \hbar \omega/mc^2. \] (69)

The Hamiltonian eigenvalue relativistic correction, defined in ([49] is:
\[ \langle \Delta h \rangle_{nl}/mc^2 = \sqrt{1 + z (2n + l - 1/2)} - 1 - z (2n + l - 1/2)/2. \] (70)

As in square well case, this correction again will produce one percent of bound state energy at
\[ z (2n + l - 1/2) \approx 0.083. \] (71)

As in earlier evaluation, at \( z \approx 0.04 \), this correction will be remarkable even in ground state of strong interaction models with such Harmonic Oscillator potential, i.e. at \( n = 1, l = 0. \)
The spectrum of corrected Hamiltonian will not consist of equidistant levels. The levels will be distributed closer than in the well-known Harmonic Oscillator spectrum with usual pseudo-relativistic kinetic energy operator.

The last basic Hamiltonian is for Hydrogen-like atom with infinitely heavy nucleus. The Coulomb potential equals

\[ v(r) = -\alpha Z \hbar c \frac{1}{r}, \]  

where \( \alpha \approx 1/137.036 \) is fine structure constant, \( Ze \) - nucleus charge and \( \hbar c \approx 0.197 \) keV \( nm \). The length parameter of this problem equals Bohr radius:

\[ a = \frac{\hbar c}{\alpha Z mc^2}, \]  

the dimensionless problem parameter

\[ z = \left( \frac{\hbar c}{a \cdot mc^2} \right)^2 = (\alpha Z)^2. \]  

After the new variable definition

\[ \xi = r/a, \]  

the dimensions-free equation looks as

\[ \left[ \frac{d^2}{d\xi^2} - \frac{l(l+1)}{\xi^2} + \frac{2}{\xi} + \frac{2e_{nl}}{zm^2} \right] u_{nl} (\xi) = 0. \]  

The eigenvalue equals

\[ e_{nl}/m^2 = -z/2n^2. \]  

The corresponding eigenfunction is \([4, \S \, 22.6.17]\):

\[ u_{nl} (\xi) = N_{nl} \rho^{l+1} e^{-\rho/2} L_{n-l-1}^{2l+1} (\rho), \]  

where

\[ \rho = 2\xi/n \]  

and normalization factor

\[ N_{nl}^2 = \frac{(n - l - 1)!}{n^2 (n + l)!}. \]  

The potential energy expectation value for this problem is two times larger than the eigenvalue

\[ \langle v \rangle_{nl} /m^2 = 2e_{nl}/m^2 = -z/n^2, \]  

\[ 12 \]
so the kinetic energy mean value is

\[
\langle t_0 \rangle_{nl}/mc^2 = -e_{nl}/mc^2 = z/2n^2.
\]  

(82)

The expression for eigenvalue correction now is:

\[
\langle \Delta h \rangle_{nl}/mc^2 = \sqrt{1 + z/n^2} - 1 - z/2n^2.
\]  

(83)

This equals one percent of energy eigenvalue when

\[
Z/n \approx 39.48.
\]

(84)

It happens only at extremely hard conditions. It reaches maximum value for ground state only at large nucleus charge. This corresponds to the known character of relativistic effects, significant mainly for heavy atoms \([5], \S 11.7\).

IV. CONCLUSIONS

Our consideration of relativistic corrections for basic quantum Hamiltonian has shown that the well-known momentum operator is not completely non-relativistic, as it has been widely believed. Pseudo-relativistic kinetic energy operator, present in Schrödinger equation produces larger kinetic energy expectation values than the relativistic operator. It appears that relativistic kinetic energy correction can produce remarkable Schrödinger equation spectrum transformations. The further consideration of Dirac equations transformation into Schrödinger form has shown that kinetic energy modification, known as weakly relativistic potential correction, can not be useful for actual problems, because modern strong interaction realistic potentials have already all the possible potential members, allowed by symmetry consideration.

V. REFERENCES

[1] P. A. M. Dirac, The Principles of Quantum Mechanics (Clarendon Press, Oxford, 1958)

[2] A. S. Davydov, Quantum Mechanics (Pergamon Press, Oxford, 1965)
[3] C. Cohen-Tannoudji, B. Diu, F. Laloë, Quantum Mechanics (Wiley-VCH, Paris, 2005)

[4] M. Abramowitz, I. A. Stegun, Handbook of Mathematical Functions (National Bureau of Standards, New York, 1964)

[5] I. N. Levine, Quantum Chemistry, 6th edition (PEARSON Prentice Hall, London, 2009)