



Original article

Hydrogen atom mass spectrum in the excited states

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ABSTRACT

Calculation and analysis of energy spectrum in Coulomb potential of atomic systems, and hadrons in relativistic conditions due to requirements of using higher grades of relativistic corrections have attracted physics theoreticians. The ability to create mono-electron ions of heavy, semi-heavy, strange atoms and/or hadrons atoms in laboratory conditions has boomed the need of more precise and meticulous corrections. One of these factors is to determine electron mass and recoil effect of core in this system. Perturbative and variation theories, regardless of recoil effect, have been calculated in this way so far. The method presented in this paper considers recoil effect intervening and without considering that it researches energy spectrum, mass, and constituent mass in the system. To make more sense of the calculations, hydrogen atomic system has been studied to pave calculation methods for other atoms and systems including quarks, glueball, and pomeron which can be over-generalized using the intended potential.

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1. Introduction

The description of the bound states of atoms is one of the classical problems in quantum mechanics. This problem has been studied by many scholars who have made it well known. At present, the study of the mechanism of interaction of colored objects has widely adapted the phenomenological potential model of quarks

(Quigg, Rosner, 1979), built by analogy of the theory of atomic structures. This model describes precisely spectrum and characteristics of charmonium and bottomium (Martin, 1981) which consist of heavy quarks. It is necessary to consider the relativistic nature of interaction, during the study of the properties of hadrons, which are formed by lightweight quarks. However, the conventional prescription of the calculation of the relativistic nature interaction within the framework of the phenomenological potential model of quarks is absent at the moment. On the other hand, the calculation of different corrections of higher order is required for describing the last experimental data along with the atomic spectrum. In particular, in the last ten years, transition frequency $1s - 2s$ levels in hydrogen atom have changed to three orders, i.e. from $3 \cdot 10^{-10}$ (Boshier, 1989) to $3,4 \cdot 10^{-13}$ (Udem, Huber, 1947). The relative uncertainty in measurement of the muonium hyperfine splitting has reduced recently by the factor three from $3,6 \cdot 10^{-8}$ (Mariam, Beer, 1982) to $1,2 \cdot 10^{-8}$ (Liu, Boshier, 1999). Thus, the definition of relativistic corrections to the energy spectrum for both atomic and hadrons structures is one of the urgent problems for todays. Corrections in atomic physics can be classified as relativistic, radiation and bonded by return. Numerous experimental and theoretical works are dedicated to the evaluation of these corrections. At the present time, the technical achievements of experimental studies have made it possible to obtain the ions of heavy elements with one electron. In this case, the coupling constant of electromagnetic interaction becomes the order of one so that electromagnetic interactions are strengthened and the calculation of relativistic corrections becomes necessary. However, the theoretical models, intended for describing the relativistic corrections to the spectrum, are limited to the lowest order on the coupling constant. We will consider this problem, according to the asymptotic behaviour of the loop function in the scalar electrodynamics field and method oscillator representation in quantum physics. The mass of the bound state analytical is calculated with Coulomb interaction. The result is in full supplement with the result of other theories.

2. General formalism

Nowadays, calculating energy spectrum with coulomb potential and considering relativistic features of bound state system has attracted many researchers. That is due to the fact that it is essential to involve various higher order relativistic corrections to describe the results of atomic spectrum experiments. Coulomb return spectrum has been calculated by using perturbative and variation theories in papers(Lucha, Schoberl, 1997), (Brambilla, Vairo,1995) and (Erickson, Crotch, 1988) respectively. However, this paper aims at using method oscillator representation of energy spectrum and hydrogen atom mass.

We determine the mass of a bound state in asymptotical behaviour of the polarization loop function for two scalar particles in external electromagnetic field. The polarization operator in an external electromagnetic field looks like (Dineykhana et al, 2009).

$$\Pi(x - y) = \langle G_{m_1}(x, y | A_\alpha) G_{m_2}^*(x, y | A_\alpha) \rangle_{A_\alpha} \quad (1)$$

Here is taking the average on external statistical field $A_\alpha(x)$. The Green function $G_m(y, x | A)$ of a scalar particle in external gauge field looks like:

$$\left[\left(i \frac{\partial}{\partial x_\alpha} + \frac{g}{c\hbar} A_\alpha(x) \right)^2 + \frac{c^2}{\hbar^2} m^2 \right] G(x, y | A_\alpha) = \delta(x - y) \quad (2)$$

Where m - mass of a scalar particle, and g - is the coupling constant of interaction. In this case, we obtain the non-relativistic limit with $(c \rightarrow \infty)$ of the loop function $\Pi(x)$. For so doing, let us restore the parameters \hbar and c in (2).

The gauge field averaging is defined as follows:

$$\left\langle \exp \left\{ i \int dx A_\alpha(x) J_\alpha(x) \right\} \right\rangle_A = \exp \left\{ - \frac{1}{2} \iint dx_1 dx_2 J_\alpha(x) D_{\alpha\beta}(x - y) J_\beta(y) \right\} \quad (3)$$

Here $J_\alpha(x)$ is a real current, and

$$D_{\alpha\beta}(x - y) = \delta_{\alpha\beta} D(x - y) + \partial_{\alpha\beta}^2 \tilde{D}(x - y) \quad (4)$$

The mass of the bound state (1) is determined as:

$$M_{system} = - \lim_{|x-y| \rightarrow \infty} \frac{\ln \Pi(x-y)}{|x-y|} \quad (5)$$

The solution of (2) can be represented in the form of the following functional integral:

$$G(x, y|A) = \int_0^\infty \frac{ds}{(4s\pi)^2} \exp\left\{-sm^2 - \frac{(x-y)^2}{4s}\right\} \int d\sigma_\beta \exp\left\{ig \int_0^1 d\xi \frac{\partial Z_\alpha(\xi)}{\partial \xi} A_\alpha(\xi)\right\} \quad (6)$$

Where we used the notations:

$$Z_\alpha(\xi) = (x-y)_\alpha \xi + J_\alpha - 2\sqrt{S} B_\alpha(\xi),$$

$$d\sigma_B = N \delta \vec{B} \exp\left(-\frac{1}{2} \int_0^1 d\xi \vec{B}^2(\xi)\right) \quad (7)$$

The conditions $B_\alpha(0) = B_\alpha(1)$ and $\int d\sigma_B = 1$. Substituting (6) in (1) and after some calculations, we get for the loop function:

$$\Pi(x) = \int_0^\infty \int_0^\infty \frac{d\mu_1 d\mu_2}{(8x\pi^2)^2} \exp\left\{-\frac{x}{2} \left(\frac{m_1^2}{\mu_1} + \mu_1\right) - \frac{x}{2} \left(\frac{m_2^2}{\mu_2} + \mu_2\right)\right\} \cdot J_\mu(\mu_1, \mu_2) \quad (8)$$

Where

$$J(\mu_1, \mu_2) = N_1 N_2 \iint \delta \vec{r}_1 \delta \vec{r}_2 \exp\left\{-\frac{1}{2} \int_0^x d\tau (\mu_1 \dot{r}_1^2(\tau) + \mu_2 \dot{r}_2^2(\tau))\right\} \cdot \exp\{-W_{i,j}\} \quad (9)$$

$$W_{ij} = \frac{g^2}{2} \int_0^x \int_0^x d\tau_1 d\tau_2 (\dot{r}_1^2(\tau_1) \cdot \dot{r}_2^2(\tau_2)) \cdot D_{\alpha\beta} Z(\beta') \quad (10)$$

The functional integral in (9) is similar to the Feynman Path integral trajectories in non-relativistic quantum mechanics (Feynman, Hibbs, 1965) for the motion of two particles with masses μ_1, μ_2 . The interaction of these particles is described by the nonlocal functional in (10), in which they contain both potential and non-potential interaction.

Taking (8) and (9) into account in the limit $|x-y| \rightarrow \infty$ from (5) for the mass of the bound state we get (for detail see (Jahanshir, 2010)

$$M_{system} = \sqrt{m_1^2 - 2\mu^2} \cdot \frac{\partial E(\mu)}{\partial \mu} + \sqrt{m_2^2 - 2\mu^2} \cdot \frac{\partial E(\mu)}{\partial \mu} + \mu \cdot \frac{\partial E(\mu)}{\partial \mu} + E(\mu) \quad (11)$$

Where the parameter μ is determined from the equation:

$$\frac{1}{\mu} = \frac{1}{\mu_1} + \frac{1}{\mu_2} = \frac{1}{\sqrt{m_1^2 - 2\mu^2} \cdot \frac{\partial E(\mu)}{\partial \mu}} + \frac{1}{\sqrt{m_2^2 - 2\mu^2} \cdot \frac{\partial E(\mu)}{\partial \mu}} \quad (12)$$

Here $E(\mu)$ is the Eigenvalue of the non-relativistic Hamiltonian which is defined by

$$\lim_{|x| \rightarrow \infty} I(\mu_1, \mu_2) = const \cdot e^{-|x|E(\mu_1, \mu_2)} \quad (13)$$

We will consider parameters μ_1, μ_2 as the components of mass of the bound state. This mass is different from the masses m_1, m_2 of free condition.

Thus, we should obtain specific expression for $W_{i,j}$ from (13). It is necessary to determine the structure of Hamiltonian for determining the mass of the bound state, which is defined in form of Functional integral from (9) and (10) (Dineykan, 2002).

According to (7), the interaction potential, we rewrite equation (10) in normal measure system:

$$W_{i,j} = \int_0^x \int_0^x d\tau_1 d\tau_2 \frac{g^2}{2} (-1)^{i+j} \left(\bar{n} + \frac{1}{c} \dot{\vec{r}}_i(\tau) \right) \left(\bar{n} + \frac{1}{c} \dot{\vec{r}}_j(\tau_2) \right) \cdot \int \frac{d\vec{q}}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{ds}{2\pi} \times \\ \times \tilde{D} \left(\vec{q}^2 + \frac{s^2}{c^2} \right) \exp \left\{ is(\tau_1 - \tau_2) + \frac{is}{c} [r_i^{(4)}(\tau_1) - r_j^{(4)}(\tau_2)] + i\vec{q} [\vec{r}_i(\tau_1) - \vec{r}_j(\tau_2)] \right\} \quad (14)$$

In the work[13], the limit $c \rightarrow \infty$ is obtained:

$$H = \frac{1}{2\mu} \vec{P}^2 + V(r) \quad (15)$$

Where $V(r)$ - is the interaction potential. For Coulomb interaction, it is equal:

$$V(r) = -\frac{Z\alpha}{r} \quad (16)$$

Therefore, we must use idea (14) to determine the potential structure of the Hamiltonian interactions, and then the Eigenvalue of the Hamiltonian and the result define the mass of bound state. For this purpose, we consider following Schrödinger equation (Dineykhon, Efimov, 1991), (Dineykhon, Efimov, 1995) and (Dineykhon, Nazmitdinov, 1999):

$$\left[\frac{1}{2\mu} \cdot \vec{P}^2 - \frac{Z\alpha}{r} \right] \Psi = E(\mu) \Psi \quad (17)$$

from this equation we find the energy spectrum of Coulomb potential:

$$E(\mu) = -\frac{Z^2 \alpha^2}{2n^2} \mu \quad (18)$$

where α - is the coupling constant of electromagnetic interaction and n - is the principal quantum number.

Let us determine the mass spectrum of atomic system with masses $m_1 = m_{nuc}$ which is the mass of nuclei, and $m_2 = m_e$ is the mass of electron. In this case, for the binder energy we have

$$E_{bin} = M_{system} - m_{nuc} \quad (19)$$

in which it is the bound state energy.

After some simplification from (10) for the mass of system, we get (Jahanshir, 2004):

$$M_{system} = m_e \cdot \left(\sqrt{y^2 + \frac{Z^2 \alpha^2}{n^2} \cdot x^2} + \sqrt{1 + \frac{Z^2 \alpha^2}{n^2} \cdot x^2} - \frac{Z^2 \alpha^2}{n^2} \cdot x \right) \quad (20)$$

And after some calculation from (11) for the constituent mass of electron and nuclei:

$$\frac{1}{\mu} = \frac{1}{\mu_e} + \frac{1}{\mu_{nuc}} \quad (21)$$

$$\mu_e = m_e \cdot \left(\sqrt{1 + \frac{Z^2 \alpha^2}{n^2} \cdot x^2} \right) \quad (22)$$

$$\mu_{nuc} = m_e \cdot \left(\sqrt{y^2 + \frac{Z^2 \alpha^2}{n^2} \cdot x^2} \right) \quad (23)$$

where $y = \frac{m_{nuc}}{m_e}$ - is the mass of nuclei in atomic system and x is a parameter that is determined from:

$$x^8(b^2 - 4a^2) + x^6(2bc - 4ay^2 - 4a) + x^4(c^2 - 2by^2 - 4y^2 + x^2(-2cy^2)) + y^4 = 0,$$

$$a = \frac{Z^2 \alpha^2}{n^2}, \quad b = 2a - a^2, \quad c = 1 - a + y^2 - ay^2$$

and for the binding energy:

$$E_{bin} = m_e \cdot \left(\sqrt{y^2 + \frac{Z^2 \alpha^2}{n^2} \cdot x^2} + \sqrt{1 + \frac{Z^2 \alpha^2}{n^2} \cdot x^2} - \frac{Z^2 \alpha^2}{n^2} \cdot x - y \right) \quad (24)$$

3. Mass spectrum and recoil effect in hydrogen atom

The present study covers Hydrogen atom and it is supposed to formulate the bound state with only Coulomb interaction (Dineykan, Nazmitdinov, 1999). In this case, the first approximation the mass of nuclei is usually defined limitless $m_{nuc}=\infty$. We calculated the mass and binding energy of hydrogen atom, after some similar calculations, which have been presented above, for the constituent mass of electron from (17) with $Z=1$ we can get (Jahanshir, 2011):

$$\frac{1}{\mu} = \frac{1}{\mu_e} \quad (26)$$

$$\mu = \sqrt{m_e^2 - 2\mu^2 \cdot \frac{\partial E(\mu)}{\partial \mu}} \quad (27)$$

Then for the bound state energy we will have:

$$E_{bin} = \sqrt{m_e^2 - 2\mu^2 \cdot \frac{\partial E(\mu)}{\partial \mu}} + \mu \cdot \frac{\partial E(\mu)}{\partial \mu} + E(\mu) \quad (28)$$

The last calculations, which have been represented above, for the bound energy and the constituent mass of electron, we will get to:

$$E_{bin} = m_e \sqrt{1 - \frac{\alpha^2}{n^2}} \quad (29)$$

$$\mu_e = m_e \cdot \left(\sqrt{1 - \frac{\alpha^2}{n^2}} \right)^{-1} \quad (30)$$

The above mentioned formulations illustrate that intersystem electron mass and energy of system in hydrogen atom depend only on coupling constant and main numerical quantum which makes it independent of other parameters. The table below (Table 1), demonstrates these variations in different orders, and it asserts that increasing return constant and higher orders of intersystem electron mass result in an increase in coupling energy system and it is $m_e=0.511$ (Me V) compared to static mass[18].

Investigating atom spectrum either heavy or light, if atom mass is determined, sounds very important (recoil effect) which has not yet been presented through perturbative and variation theories. Assuming atom mass is limited; we can calculate energy of system, and intersystem electron mass and core through (20-24). If supposedly, the atom mass is limited, the following table (Table 2) shows calculating changes of coupling energy system and electron mass and core mass in the first excitation order ($n=2$). It can be clearly observed that changes of intersystem electron mass are bigger compared to intersystem core mass and it increases as the constant index increases.

Table 1

Binding energy (E , MeV) and constituent mass (μ , MeV) of electron in limitless nuclei mass of Hydrogen atom, $m_e = 0.511MeV$.

	$\alpha=0.356$			$\alpha=0.435$			$\alpha=0.500$		
	n=1	n=2	n=3	n=1	n=2	n=3	n=1	n=2	n=3
μ	0.546	0.519	0.514	0.567	0.523	0.516	0.590	0.527	0.518
E	0.477	0.502	0.507	0.460	0.498	0.505	0.442	0.494	0.503

Table 2

Binding energy (E , MeV), constituent mass(μ_e, μ_{nuc} , MeV) and Variation of constituent mass of particles electrons ($\Delta\mu_e, \Delta\mu_{nuc}$, MeV), in Hydrogen atom with recoil effect, $m_e = 0.511MeV$, $m_p = 938.272028MeV$

	μ_e	$\Delta\mu_e$	μ_{nuc}	$\Delta\mu_{sys}$	E_{bin}
$\alpha=0.356$	0.5192	0.00830	938.272030	938.77490	0.50270
$\alpha=0.435$	0.5235	0.12520	938.272035	938.77080	0.49870
$\alpha=0.500$	0.5277	0.32750	938.272038	938.76680	0.49470

4. Conclusions

In this paper, we studied hydrogen atom on the basis of investigation of asymptotic behaviour of the loop function for the scalar particles in the external gauge field and determined the Binding energy with relativistic feature of interaction. We have been able to obtain the mass spectrum of bound state and the constituent mass of hydrogen atom system. It is shown that the mass of particles is different in bound and free states. We have found out that determining the mass of the bound state systems requires; first of all, determining the Eigenvalue of the Hamiltonian with Coulomb potential and then calculating the mass and binding energy of atom which we could achieve. This method provides us with magnificent information comparing to other theories such as perturbative and variation. The current paper has calculated energy spectrum and hydrogen atom constituents mass in limited and unlimited core mass conditions and we could conclude that constituents mass in the system is different from constituents mass in free conditions. This analysis, using complementary calculations and having a determined core mass, investigates a very important atomic system i.e. recoil effect. The method presented in this paper shows that recoil effect is well-suited for equations, and it can be easily used for all atoms which have not been calculated through perturbative and variation theories so far (for $n>2$). This method can be applied as such so as to calculate necessary parameters for exotic or hadronic atoms. Therefore, the presented equation is an appropriate method for investigating quarks, glueball and pomeron systems in which we can analyse changes in energy and mass spectrum using intended potentials.

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