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Relativistic Electron in the Field of Two Coulomb Centers

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Abstract

Ground state wave function and the energy term of the relativistic electron moving in the field of two Coulomb centers are calculated analytically by the method of linear combination of atomic orbitals. Obtained analytical formula is applied to the calculation of the critical distance between two heavy nuclei at which energy term reaches the boundary of the lower continuum.

1. Introduction

The two centre Coulomb problem (i.e., the problem of motion of an electron in the field of two fixed charges Z_1 and Z_2 separated by distance R) is a classical problem of nonrelativistic quantum mechanics and is applied in the theory of chemical binding, in the physics of μ-mesons, etc.

There is ample literature devoted to this problem, examples of which may be found in [1-8]. For the nonrelativistic equation of the H_2^+ molecular ion, Heitler and London gave the first approximate solution [2]. Exact methods were derived soon after by Teller [3] and Jaffe [5], by expanding the wave functions in terms of a suitable basis functions. The equivalence of their methods was shown in [5,6] in which were published extensive calculations on the nonrelativistic one-electron problem. The corresponding problem for Dirac equation has the following characteristic properties which complicate its solution:

1. Variables in the Dirac equation with potential $V = -\alpha\left(\frac{Z_1}{r_1} + \frac{Z_2}{r_2}\right)$ can't be separated in any system of coordinates.

2. For large Z, there is the full down to the center [15].

3. The wave function is multicomponent and for $Z\alpha \approx 1$ all components are of the same order.

Interest in the relativistic two centre problem arose after prediction in [10] of the possibility of checking quantum electrodynamics in the experiments on collisions of heavy ions. As is well known, for $Z \approx Z_{cr} = 170$, lowest energy level of the one-center Dirac equation imbedded the boundare of lower continuum and for the spontoneous production of positrons will occur. As no nucleus with charge $Z > Z_{cr}$ do exist, the experiment has to be done with two colliding heavy ions. To perform the calculation of the expected positron distribution the energy of the quasimolecular states must be known as a function of the internuclear distance R. This leads us to the wave equation for an electron in the field of two Coulomb centers. There were several works [8-10] in which the energy term and the critical distance (i.e., the distance, at which energy term reaches the boundary of lower continuum) were calculated numerically as well as analitically.

In [8] the Dirac equation for a two centre Coulomb potential was solved numerically by the method of diagonalization of Dirac Hamiltonian in a finite basis. Approximate analitical calculations of critical distance were performed in [9,10], and also gave rise to formulas which allow calculation of the energy term and critical distance for the charges obeying the condition $\frac{Z_1+Z_2-Z_{cr}}{Z_{cr}} \ll 1$ (condition of small overcriticallity) and for $R \ll 1$.

In the present work the two center Coulomb problem for Dirac equation is solved by a method analogous to the method of linear combination of atomic orbitals (LCAO), which is widely used in the quantum mechanics of molecules [6]. As is well known, method of LCAO is applied for the solution of nonrelativistic two center one- and two- electron problems and energy term of the nonrelativistic electron can be calculated analytically anological calculations for dirac electron to our knowledge has not yet been performed. As a result of such calculations, we obtain analytical formula which is true for wide range of distances between charges and resulting charges of nuclei.

In this paper we use the system of units $\hbar = c = m_e = 1, R$ is the distance between charges, $Z_1 = Z_2 = Z$.

2. Hamiltonian and wave function

The motion of a relativistic electron in the field of two Coulomb centers is described by stationary Dirac equation, written in the form

$$H\Psi = E\Psi, \tag{1}$$

where $H = \vec{\alpha}\vec{p} + \beta + V$ is the Dirac Hamiltonian, and $\vec{\alpha}$ and β are the usual Dirac matrices.

We will solve equation (1) by the method of LCAO choosing the trial wave functions in the form

$$\Psi = d_1\Psi_1 + d_2\Psi_2,$$

where Ψ_1 and Ψ_2 are the wave functions of the relativistic electron moving in the field of charges Z_1 and Z_2, respectivily.

As is well known [6], symmetry of charges $(Z_1 = Z_2)$, normalising conditions $< \Psi|\Psi >= 1$, $< \Psi_j|\Psi_j >= 1$, $(j = 1, 2)$, and that the ground state does not have nodes give rise to

$$d_1 = d_2 = d = \frac{1}{\sqrt{2(1+S)}},$$

where $S =< \Psi_1|\Psi_2 >$ is the overlap integral.

Energy can be calculated as the matrix element

$$E =< \Psi|H|\Psi > \tag{2}$$

where

$$< \Psi| = [\varphi\chi], \qquad |\Psi >= \begin{bmatrix} \varphi \\ \chi \end{bmatrix}$$

As a trial function Ψ_1 and Ψ_2 we take the ground state wave functions of a relativistic hydrogenlike atom [16] with effective charge $Q\alpha$, i.e.:

$$\begin{aligned} \varphi_j = Ar_j^{\gamma-1}e^{-Q\alpha r_j}\begin{bmatrix} 1 \\ 0 \end{bmatrix} &= Ag_j\begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ \chi_j = iABr_j^{\gamma-1}e^{-Q\alpha r_j}\begin{bmatrix} \cos\theta \\ e^{i\varphi}\sin\theta \end{bmatrix} &= iABg_j\begin{bmatrix} \cos\theta \\ e^{i\varphi}\sin\theta \end{bmatrix} \end{aligned}$$

where $g_j = r_j^{\gamma-1}e^{-Q\alpha r_j}, \quad j = 1, 2$

$$\begin{aligned} A &= \frac{(2Q\alpha)^{\frac{3}{2}}}{\sqrt{4\pi}}\sqrt{\frac{1+\gamma}{2\Gamma(1+2\gamma)}}(2Q\alpha)^{\gamma-1} \\ B &= \frac{1-\gamma}{Q\alpha}, \quad \gamma = \sqrt{1-Q^2\alpha^2}, \end{aligned}$$

3. The Energy Term and the Critical Distance

Inserting trial functions into Eqn.(2) we obtain analitical formula for the the energy term in terms of five integrals which are expressed by gamma functions:

$$\begin{aligned} E &= \frac{2\pi A^2 b R^{2\gamma}}{1+S}[Q\alpha(I_1+I_2)+\frac{a\gamma}{2Q\alpha}(I_3+I_4)-2Z\alpha(I_2+I_5)] \\ S &= 2\pi A^2 R^{2\gamma+1} b I_4 \end{aligned} \tag{3}$$

where integrals $I_1 - I_5$ are written as

$$I_1 = \frac{1}{a^{2\gamma}} 2\Gamma(2\gamma) \tag{4}$$

$$I_2 = \frac{1}{a^{2\gamma}}\left[(2-\frac{a^2}{3(2\gamma-1)})\Gamma(2\gamma,a)+(\frac{1}{3}+\frac{a}{3(2\gamma-1)})a^{2\gamma}e^{-a}\right] \tag{5}$$

$$I_3 = \frac{1}{a^{2\gamma+1}} 4\gamma\Gamma(2\gamma) \tag{6}$$

$$I_4 = \frac{1}{a^{2\gamma+1}}\left[\left(4\gamma-\frac{2a^2\gamma}{3(2\gamma-1)}\right)\Gamma(2\gamma,a)+(2+\frac{2a\gamma}{3(2\gamma-1)})a^{2\gamma}e^{-a}\right] \tag{7}$$

$$I_5 = \frac{1}{a^{2\gamma+1}}\left[(a-\gamma)\Gamma(2\gamma,2a)+(a+\gamma)\Gamma(2\gamma)-\frac{1}{2}(2a)^{2\gamma}e^{-2a}\right] \tag{8}$$

$$a = 2Q\alpha R, \quad b = \frac{2}{1+\gamma}.$$

Thus we have obtained the energy term of the relativistic electron in the field of two centers as a function of distance R, charge Z and effective charge Q. In the nonrelativistic limit i.e., for $Q\alpha \ll 1\,(\gamma \simeq 1)$ formula (3) gives us

$$E = Q^2\alpha^2 F_1(a) + Q\alpha F_2(a), \tag{9}$$

where

$$F_1(a) = \frac{1}{2}\frac{1+e^{-a}\left(1+a-\frac{a^2}{3}\right)}{1+e^{-a}\left(1+a+\frac{a^2}{3}\right)}$$

and

$$F_2(a) = -Z\alpha\frac{1+2e^{-a}(1+a)+\frac{1}{a}-\left(\frac{1}{a}+1\right)e^{-2a}}{1+e^{-a}\left(1+a+\frac{a^2}{3}\right)}.$$

This formula coincides with the well known formula for nonrelativistic hydrogen molecular ion [6].

In Q/Z is given as a function of R for nonrelativistic and relativistic Br-Br systems (with charge $Z = 35$), respectively. These functions are obtained by minimizing functions (9) and (3), respectively. In Figure 2 such graphs are given for the charge $Z = 68$.

In Figures 3 and 4 relativistic and nonrelativistic energy terms which are described by formulas (3) and (9) are given for the charges $Z = 35$ and $Z = 68$.

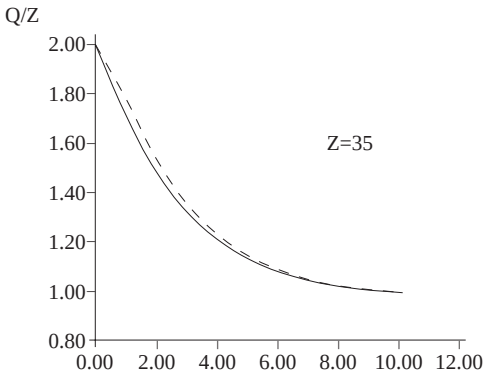

Figure 1. The ratio Q/Z as a function of distance R for $Z = 35$. Dashed line corresponds to the nonrelativistic system described by formula (9); solid line corresponds to the relativistic one describing by (3)

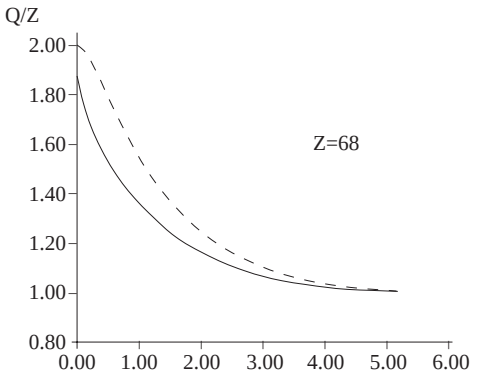

Figure 2. The ratio Q/Z as a function of distance R for $Z = 68$. Dashed line corresponds to the nonrelativistic system; solid line corresponds to the relativistic one

As seen from these Figures in the limits of $R \to 0$ and $R \to \infty$, effective charge and energy term tend to the effective charge and the energy term of the united and separated atoms, respectively, and relativistic corrections become considerable for small R.

Effective charge Q is a function of R and Z, i.e.

$$Q = Q(R, Z).$$

As is well known [6],

$$Q\,|_{R\to 0} = 2Z \tag{10}$$

$$Q\,|_{R\to \infty} = Z. \tag{11}$$

Calculating $E(R)$ in the limit $R \to 0$ from Eqn.(3) we have

$$E(R \to 0) = \sqrt{1 - 4Z^2\alpha^2};$$

i.e., for $R \to 0$ our formula goes over into the formula for the energy of relativistic hydrogenlike atom with charge $2Z$ (united atoms).

Calculation $E(R)$ for $R \to \infty$ from Eqn.(3) leads to

$$E(R \to \infty) = \sqrt{1 - Z^2\alpha^2}$$

(for separated atoms).

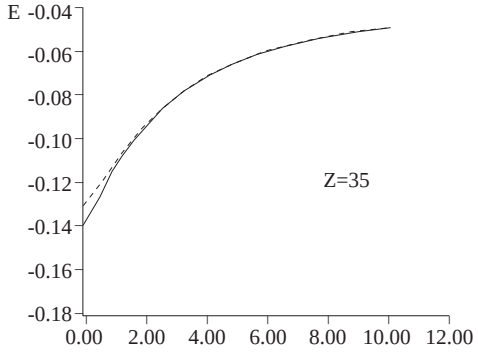

Figure 3. The energy terms of the relativistic and nonrelativistic electron moving in the field of two Coulomb centers with charge $Z = 35$. Dashed line is the energy term of nonrelativistic electron; solid line is the energy term of relativistic one

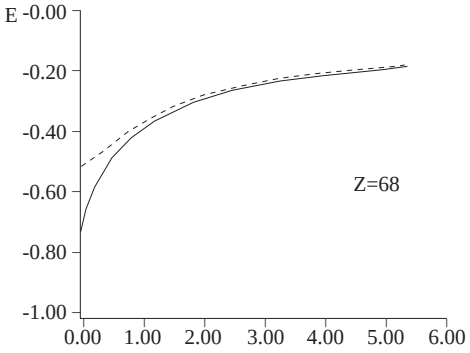

Figure 4. The energy terms of the relativistic and nonrelativistic electron moving in the field of two Coulomb centers with charge $Z = 68$. Dashed line is the energy term of nonrelativistic electron; solid line is the energy term of relativistic one

Note that in the above considered case the resulting charge of the nuclei is less than 137. In the case when $Z_1 + Z_2 > 137$, generally speaking, finite sizes of the nuclei must be taken into account. Hovewer Popov's formula for the critical distance (i.e., for the distance at which the energy term of ground state reaches the boundary of the lower continuum) which was obtained by mathcing asymptotics of wave function at the distances where finite sizes of the nuclei can be neglected can be also obtained from our formula for the energy term assuming the same conditions which were required in [13]. Indeed, taking into account that in this case $\gamma = i\sqrt{4Z^2\alpha^2 - 1}, a \ll 1$ and $Q = 2Z$ from the condition of diving of term into the lower continuum we have

$$E(R_{cr}) = -1,$$

$$\left[(1-\gamma)4^{\gamma} + 2\gamma\right] a^{2\gamma} = -4\gamma\Gamma(2\gamma + 1),$$

or

$$(2R)^{-2\gamma}\frac{4\gamma}{(1-\gamma^2)^{\gamma}((\gamma-1)4^{\gamma}-2\gamma)}\Gamma(2\gamma+1)=1\equiv e^{2\pi i}.$$

After some straightforward transformations this expression takes the form

$$R_{cr}=C\exp(-\frac{\pi}{\sqrt{4Z^2\alpha^2-1}}). \tag{12}$$

This formula coincides with known formula for R_{cr} which was derived in [13] (see also [14,17]).

4. Conclusion

We have obtained an analitical formula for the energy term of a relativistic electron moving in the field two fixed centers using method like to the nonrelativistic LCAO method. This formula is valid for wide range of the distances between centers and resulting charges Z_1+Z_2. In the case of overcritical charges this formula reproduces the well known Popov's formula for the critical distance at which the energy term, reaches the boundary of the lower continuum and production of electron- positron pairs will occur [13,14].

Finally there is the considerable interest in baryons containing two heavy quarks (QQq-baryons) [19,20]. These baryons are the analogues to the above considered system (Z_1, Z_2, e^-) in which Coulomb potential replaced with the Coulomb plus confining potential. Therefore, the method proposed in this paper can be also applied for solving the Dirac equation with two center Coulomb plus confinement potential for the calculation energy spectrum of QQq baryons. At the present time we are performing such calculations.

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