Eur. Phys. J. D **42**, 381–386 (2007)
DOI: 10.1140/epjd/e2007-00053-5

THE EUROPEAN PHYSICAL JOURNAL D

The quantum mechanical two-Coulomb-centre problem in the Dirac equation framework in 2+1 dimensions

V.V. Bondarchuk and I.M. Shvab[a]

Department of Theoretical Physics, Uzhgorod National University, Voloshina Street 54, Uzhgorod 88000, Ukraine

Received 16 August 2006 / Received in final form 18 October 2006
Published online 9 March 2007 –

Abstract. With the help of perturbation theory the asymptotic expansions (at small and large internuclear distances R) of the eigenvalues (potential curves) $E(R)$ of the two-Coulomb-centre problem in $2+1$ dimensions are obtained. We compare the results obtained with the data from similar approximation for two-Coulomb-centre problem in $3+1$ dimensions.

PACS. 31.15.Md Perturbation theory – 31.30.Jv Relativistic and quantum electrodynamic effects in atoms and molecules – 34.50.-s Scattering of atoms and molecules

1 Introduction

At the present time a severe asymmetry exists in the developments of the theories of nonrelativistic and relativistic quantum mechanical problems of two Coulomb centres (the so-called Z_1eZ_2 problem). Numerous effective asymptotic and numerical methods of solving the two-Coulomb-centre problems in Shrödinger equation theory [1] can be compared against only few examples of the same problem in Dirac equation theory within various approximations [2–7] (the Galerkin method, diagonalization, the variational method, perturbation theory, Furry-Sommerfeld-Maue approximation). This situation is a surprising example of inertia in a theoretical field in the face of the deficiency of experimental data for heavy and superheavy quasi-molecular systems due to the difficulties in construction of sources of multiply charged ions and formation of beams of rather slow particles.

Also, with the recent construction of powerful accelerators of highly charged ions in many laboratories [8,9], the need for a consistent Dirac theory of the quantum mechanical Z_1eZ_2 problems has become more and more urgent in different fields of physics. Previously, this problem was addressed, basically, in the theory of supercritical atoms for the description of effects of spontaneous and enforced creation of positrons in a supercritical field of a quasiatom formed at slow collisions of heavy ions with a total atomic number $Z_1 + Z_2 > 173$ [10].

Another application of the relativistic problem approach in the theory of collisions is more traditional, and is reduced to using the model functions of a continuous spectrum for the analysis of the scattering of relativistic electrons on heavy diatomic molecules [11,12].

Last time considerable interest challenges $(1+1)$- and $(2+1)$-dimensional versions of relativistic quantum mechanic and quantum electrodynamic [13–15]. Importance of these versions for the quantum field theory (QFT) was realized properly on the borders of 70th and 80th years, when in physics of the condense medium a number of fundamental discoveries were made, which, until now apparently warm up living interest to the models of QFT in spaces with the lowered dimension [16,17]. Not being realistically valuable for the quantum field problem, these models have presented rather effective instruments at the study of quasi one-dimensional and quasi two-dimensional medium.

Over the past years the study of systems of nonrelativistic electrons confined to a plane in an electromagnetic field background has attracted much attention in view of possible applications. This problem is of practical interest because of the technological advances in nanofabrication technology that have made the creation of low dimensional structures like quantum wells, quantum wires and quantum dots possible [18]. The relativistic extension of this problem has also turned out to be of importance in the description of quantum two-dimensional phenomena such as the quantum Hall effect and high-temperature superconductivity [19]. Different condensed matter physics phenomena point to the existence of (2+1)-dimensional with an energy spectrum determined by the Dirac equation Hamiltonian [13,14]. In particular, the degenerate planar semiconductor with low-energy electron dynamics is assumed to admit an adequate description in terms of the $(2+1)$-dimensional relativistic Dirac theory [20]. In conclusion, the study of physical effects occurring in $(2+1)$-dimensional systems of charged particles in strong external fields is an interesting problem from the theoretical point of view as well from its practical

[a] e-mail: igor_shvab@yahoo.com

applications [21–23]. In order to analyze relativistic quantum effects in the presence of strong electromagnetic fields one should be able to compute the Green function or to find exact solutions of the Dirac equation. Regrettably, the Dirac equation is exact solvable only in a very restricted family of electromagnetic configurations [24].

The purpose of the given work is the study of the discrete spectrum of the two-dimensional problem of two Coulomb centers (briefly, the problem $(Z_1eZ_2)_2$) using asymptotic methods. The difficulty in considering the problem consist in the fact that the Dirac equation whit the potential of two Coulomb centres does not permit complete separation of variables in any orthogonal system of coordinates and, thus, one has to deal with first-order partial differential equations. Unfortunately, solving this system of differential equations numerically is rather complicated and onerous task, requiring rather complicated calculations for each specific $(Z_1eZ_2)_2$ system. For solving the problem we use the scheme of perturbation theory, which does not require the separation of variables. As a result of the calculations performed, the asymptotic expression for the energy levels of the $(Z_1eZ_2)_2$ system for a case of small intercentre distance $R \to 0$ (large intercentre distance $R \to \infty$) are obtained to within terms $O(R^3)$ $(O(R^{-3}))$ respectively. The D-dimensional nonrelativistic two-Coulomb-centre problem was considered in [25].

The article is arranged as follows: in Section 2 the method of constructing the asymptotic expansions of the energy of the $(Z_1eZ_2)_2$ system at small internuclear distances R is proposed. In Section 3 the method of constructing the asymptotic expansions of the energy of the $(Z_1eZ_2)_2$ system at large internuclear distances R is proposed. Finally we discuss briefly and compare the results obtained with the data from similar approximation in case of three-dimensional two-centres problem Z_1eZ_2 and present some mathematical appendixes.

2 Asymptotic behavior of potential curves of the relativistic two-dimensional $(Z_1eZ_2)_2$ problem in the united-atom limit

When the total charge of the Coulomb centres $Z = Z_1 + Z_2$ is positive and the internuclear distance R tends to zero, it is possible to consider the relativistic $(Z_1eZ_2)_2$ problem within perturbation theory. The Dirac equation of the Z_1eZ_2 problem in $2+1$ dimensions is of the form $(\hbar = c = m_e = 1)$

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

$$\hat{H} = \sigma^1 p_2 - \sigma^2 p_1 + \sigma^3 - \frac{Z_1\alpha}{r_1} - \frac{Z_2\alpha}{r_2}, \tag{2}$$

where $r_{1,2}$ is the distance between the electron and corresponding nucleus, $Z_{1,2}$ is the charge of the Coulomb centres, $\vec{p} = (p_1, p_2) = -i\vec{\nabla}$ is the momentum operator, σ^i are the Pauli matrices $(i = 1, 2, 3)$, and $\alpha \approx 1/137$ is the fine-structure constant.

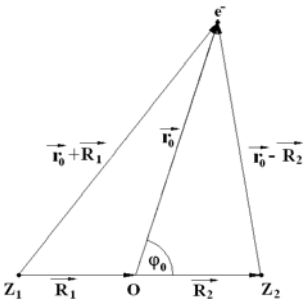

Fig. 1. The scheme of motion of an electron in case of united atom.

Let us represent the complete Hamiltonian of the two-Coulomb-centre problem, by the Hamiltonian of the zero approximation $\hat{H}^{UA}$ and a perturbation $\hat{W}$:

$$\hat{H} = \hat{H}^{UA} + \hat{W}. \tag{3}$$

The Dirac Hamiltonian of the united relativistic atom is taken as $\hat{H}^{UA}$:

$$\hat{H}^{UA} = \sigma^1 p_2 - \sigma^2 p_1 + \sigma^3 - \frac{Z\alpha}{r_0}, \tag{4}$$

where the atom is placed on the internuclear distance at the point O, which divides the internuclear distance into two segments:

$$R_1 = \frac{Z_2}{Z}R, \quad R_2 = \frac{Z_1}{Z}R. \tag{5}$$

Introduce polar coordinate system $(r_0; \varphi_0)$, as shown in a Figure 1: the origin is at the point $O(0;0)$ and the angle φ_0 is measured from the polar axis, directed from Z_1-centre to Z_2.

Now we construct the unperturbed wavefunction of a united atom. For the zero-order function we will choose the unperturbed wavefunction of a united atom with Hamiltonian (4). The eigenvalues of the operator $\hat{H}^{UA}$ are characterized by quantum numbers n, l, where n is the principal quantum number, l is the orbital angular moments(integer). For continuous approach of nuclei $R \to 0$, the solutions of the Dirac equation with the potential of two Coulomb centres should tend to the respective solution of the one Coulomb centre problem. According to this the eigenfunctions of the operator $\hat{H}^{UA}$ are represented in the form [15]

$$\Psi^{UA}_{nl}(\vec{r_0}) = \frac{1}{\sqrt{2\pi r_0}} \begin{pmatrix} F(r_0)e^{il\varphi_0} \\ G(r_0)e^{i(l+1)\varphi_0} \end{pmatrix}$$

$$\left.\begin{matrix} F \\ G \end{matrix}\right\} = \frac{\sqrt{\Gamma(2\gamma+n_r+1)}}{\Gamma(2\gamma+1)\sqrt{n_r!}} \sqrt{\frac{1 \pm \varepsilon_0}{4N(N-\kappa)}}\,(2\lambda)^{\frac{1}{2}}$$
$$\times (2\lambda r_0)^{\gamma} e^{-\lambda r_0} \left[(N-\kappa)F\left(-n_r, 2\gamma+1; 2\lambda r_0\right)\right.$$
$$\left. \mp n_r F\left(-n_r+1, 2\gamma+1; 2\lambda r_0\right)\right]. \tag{6}$$

where

$$\lambda = \sqrt{1-\varepsilon_0^2}, \quad n_r = n - |l+1/2| - \frac{1}{2},$$

$$\varepsilon_0 = \left[1 + \frac{(Z\alpha)^2}{(n_r + \sqrt{(l+1/2)^2 - (Z\alpha)^2})^2}\right]^{-\frac{1}{2}},$$

$$\kappa = -\left(l+\frac{1}{2}\right), \quad N = \frac{Z\alpha}{\lambda}, \quad \gamma = \sqrt{(l+1/2)^2 - (Z\alpha)^2}.$$

It is seen that, for $l = n_r = 0$, and ε_0 becomes zero at $Z\alpha = 1/2$, whereas in three spatial dimensions ε_0 equals zero at $Z\alpha = 1$. Thus, in two space dimensions the expression for the electron ground state energy in the Coulomb field of a point-charge $Z|e|$ no longer has a physical meaning at a much lower value of $Z\alpha = 1/2$.

The eigenvalues of the operator $\hat{H}^{UA}$ are determined by the formula:

$$\varepsilon_0 = \frac{1}{\sqrt{1 + \left(\dfrac{Z\alpha}{n_r+\gamma}\right)^2}}. \tag{7}$$

Since the spectrum of the operator $\hat{H}^{UA}$ is degenerated for l, for application of perturbation theory first of all it is necessary to construct exact functions of the zero approximation, for which the matrix of the perturbation operator $\hat{W}$ is diagonal. We can show that the matrix $\|W_{nl}^{nl'}\|$ of the perturbation operator will be diagonal for the functions of united atom. Now we determined matrix elements of the perturbation operator of the system:

$$\hat{W} = \frac{Z\alpha}{r_0} - \frac{Z_1\alpha}{|\vec{r}_0 + \vec{R}_1|} - \frac{Z_2\alpha}{|\vec{r}_0 - \vec{R}_2|}. \tag{8}$$

For these purpose we use the expansion of $\hat{W}$ in Legendre polynomials:

$$\hat{W} = \frac{Z\alpha}{r_0} - \left\{\begin{array}{ll} Z_1\alpha \sum\limits_{l=0}^{\infty}(-1)^l R_1^l r_0^{-l-1} P_l(\cos\varphi_0), & r_0 > |\vec{R}_1| \\ Z_1\alpha \sum\limits_{l=0}^{\infty}(-1)^l R_1^{-l-1} r_0^l P_l(\cos\varphi_0), & r_0 < |\vec{R}_1| \end{array}\right\} - \left\{\begin{array}{ll} Z_2\alpha \sum\limits_{l=0}^{\infty} R_2^l r_0^{-l-1} P_l(\cos\varphi_0), & r_0 > |\vec{R}_2| \\ Z_2\alpha \sum\limits_{l=0}^{\infty} R_2^{-l-1} r_0^l P_l(\cos\varphi_0), & r_0 < |\vec{R}_2| \end{array}\right\}. \tag{9}$$

The coefficient of $r_0^{-2}P_1$ for $r_0 > \max\{|\vec{R}_1|, |\vec{R}_2|\}$ is equal to $Z_2\alpha R_2 - Z_1\alpha R_1$ and, according to equation (5) this is equal to zero. The estimates of all radial and angular integrals made with functions (5), (6) show that at $R \to 0$ the matrix $\|W_{nl}^{nl'}\|$ is built from matrix elements

$$W_{nl}^{nl'} = \int \Psi_{nl}^{UA^+}(\vec{r}_0)\hat{W}\Psi_{nl'}^{UA}(\vec{r}_0)d\vec{r}_0,$$

is diagonal within members $O\left(R^3\right)$ with respect to each group of mutually degenerated states, i.e.

$$W_{nl}^{nl'} = \delta_{ll'}\left[W_{nl}^{nl'}\right]_2 + O\left(R^3\right).$$

The leading term $\left[W_{nl}^{nl'}\right]_2$ of the expansion of the diagonal matrix element of $\hat{W}$ is determined by the expansion (9) for $r_0 > \max\{|\vec{R}_1|, |\vec{R}_2|\}$, in which the integration over r_0 is carried out from the zero point:

$$\begin{aligned}\left[W_{nl}^{nl'}\right]_2 &= -\left(Z_1\alpha R_1^2 + Z_2\alpha R_2^2\right) \\ &\quad \times \int \left|\Psi_{nl}^{UA}(\vec{r}_0)\right|^2 r_0^{-3} P_2(\cos\varphi_0)d\vec{r}_0 \\ &= -\frac{Z_1Z_2\alpha^4(3\varepsilon_0\kappa(\varepsilon_0\kappa-1) - \gamma^2 + 1)(ZR)^2}{2N^3\gamma(\gamma^2-1)(4\gamma^2-1)}.\end{aligned} \tag{10}$$

The formulae (7), (10) determine the two first terms of the expansion in small R of a total energy(which includes the rest energy of an electron) of the $(Z_1eZ_2)_2$ system:

$$E_{nl}(Z_1, Z_2; R) = \varepsilon_0 + \left[W_{nl}^{nl'}\right]_2 + O(R^3). \tag{11}$$

3 Asymptotic behavior of potential curves of the relativistic two-dimensional $(Z_1eZ_2)_2$ problem in the separated-atom limit

Now we shall determine the energy $E(R)$ and the wavefunctions $\Psi(\vec{r}; R)$ of an electron in the asymptotic region when the distance R between the Coulomb centres is large. This distance should be so large that the quantum penetrability of the potential barrier separating the atomic particles is mach smaller than unity. When charges Z_1, Z_2 are different, eigenvalues $E(R)$ of the two-Coulomb-centre problem are divided into two classes in the asymptotic limit $R \to \infty$: E_I and E_{II^-} potential curves that, for $R \to \infty$, transform into the energy levels of isolated atoms 1 and 2, respectively. The criterion of applicability of the expansion given below is the requirement that the wavefunction of the Ψ_{1^-} state, for instance, of atom 1, should not be strongly perturbed by the other particle. The distortion of the dependence of this function on the coordinates should be small. This is related to he energy shift of the state induced by the interaction with perturbing particle 2. The external(Coulomb) field of the latter has to be weak compared to the typical intra-atomic fields in order for perturbation theory to be applicable.

Similarly to (3) we represent a complete Hamiltonian of the two-Coulomb-centre problem by a Hamiltonian zero-approximation $\hat{H}^{SA}$ and perturbation $\hat{V}$:

$$\hat{H} = \hat{H}^{SA} + \hat{V}. \tag{12}$$

Introduce the polar coordinate system (r_1, φ_1), as shown in a Figure 2, the origin is at the centre of the

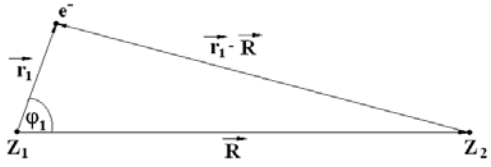

Fig. 2. The scheme of motion of an electron in case of separated atom.

hydrogen-like ion eZ_1, and the angle φ_1 is measured from the axis directed from the Z_1-center to Z_2-center. We will choose in quality $\hat{H}^{SA}$ the Hamiltonian of the separated atom with charge Z_1:

$$\hat{H}^{SA} = \sigma^1 p_2 - \sigma^2 p_1 + \sigma^3 - \frac{Z_1\alpha}{r_1}. \tag{13}$$

At large internuclear distances the operator of the interaction between the electron and the Z_2-nucleus $\hat{V} = -Z_2\alpha/|\vec{r_1} - \vec{R}|$ can be considered as a small perturbation of the Hamiltonian $\hat{H}^{SA}$.

Like to $\hat{H}^{UA}$ the eigenvalues of the operator $\hat{H}^{SA}$ are characterized by the set of quantum numbers n_1, l_1. The eigenfunctions $\Psi^{SA}_{n_1 l_1}(\vec{r}_1)$ are represented by formulae which are obtained from (6) by making the substitution $\vec{r}_0 \to \vec{r}_1$ and introducing index 1 in other formulae. The eigenvalue of the operator $\hat{H}^{SA}$ are determined by the formula:

$$\varepsilon_1 = \frac{1}{\sqrt{1 + \left(\dfrac{Z_1\alpha}{n_{r_1} + \gamma_1}\right)^2}}. \tag{14}$$

The matrix elements of the operator $\hat{V}$ can be determined from the expansion:

$$\hat{V} = -\begin{cases} Z_2\alpha \sum\limits_{s=0}^{\infty} R^s r_1^{-s-1} P_s(\cos\varphi_1), & r_1 > |\vec{R}| \\ Z_2\alpha \sum\limits_{s=0}^{\infty} R^{-s-1} r_1^s P_s(\cos\varphi_1), & r_1 < |\vec{R}| \end{cases}. \tag{15}$$

A matrix $\|V^{n_1 l_1'}_{n_1 l_1}\|$ which consist from matrix elements

$$V^{n_1 l_1'}_{n_1 l_1} = \int \Psi^{SA^+}_{n_1 l_1}(\vec{r}_1)\hat{V}\Psi^{SA}_{n_1 l_1'}(\vec{r}_1)d\vec{r}_1,$$

is not diagonal about l_1 as in the case of united atom.

For the wavefunctions of the zero-order approximation we can write

$$\Psi_0 = \sum_{l_1'} C^{l_1}_{l_1'}(R)\Psi^{SA}_{n_1 l_1'}(\vec{r}_1). \tag{16}$$

By substituting expansion (16) into the Dirac equation (1), and integrating over the electron coordinates, we find expansion coefficient given by

$$\sum_{l_1'} \left[(E_I - \varepsilon_1)\delta_{l_1 l_1'} - V^{n_1 l_1'}_{n_1 l_1}\right] C^{l_1}_{l_1'}(R) = 0, \tag{17}$$

where δ_{lm} is the Kronecker delta.

Obviously that the first term in expansion perturbation operator (17) is diagonal with respect to mutually degenerated states, the second term contain nonzero not diagonal elements:

$$V^{n_1 l_1}_{n_1 l_1} = -\frac{Z_2\alpha}{R}, \tag{18}$$

$$V^{n_1 l_1}_{n_1 l_1'} = V^{n_1 l_1'}_{n_1 l_1} = -(\delta_{l_1,0} + \delta_{l_1,-1})\sqrt{N_1^2 - \kappa_1^2}\frac{Z_2(n_{r_1} + \gamma_1)}{Z_1 R^2}. \tag{19}$$

By using matrix elements (18, 19) and solving the equation obtained from the condition that the determinant in (17) should be equal to zero, we obtain the expression for the energy terms in first-order perturbation theory:

$$E_I(R) = \varepsilon_1 - \frac{Z_2\alpha}{R} + \frac{Z_2\xi_1}{R^2} + O(R^{-3}), \tag{20}$$

$$\xi_1 = \pm\,(\delta_{l_1,0} + \delta_{l_1,-1})\sqrt{N_1^2 - \kappa_1^2}\frac{(n_{r_1} + \gamma_1)}{Z_1}. \tag{21}$$

Formula (20) gives the expansion in the multipoles of the energy of the electrostatic interaction of the atom eZ_1 with the distant point charge eZ_2.

The asymptotic expansion of the potential curve E_{II} is obtained from E_I by making the substitutions $\varepsilon_1 \to \varepsilon_2$, $Z_{1,2} \to Z_{2,1}$, $n_1, \kappa_1 \to n_2, \kappa_2$, where n_2, κ_2 is the set of quantum number of the isolated hydrogen-like atom eZ_2.

4 Conclusion

In this work we have calculated by means of perturbation theory the asymptotic expansions of the eigenvalues (potential curves) $E(R)$ of the two-dimensional two-Coulomb-centre problem in the limits of united ($R \to 0$) and separated ($R \to \infty$) atoms with the precision $O(R^3)$ and $O(R^{-3})$, respectively.

To illustrate applications of the resulting asymptotic formulas (10, 11) and (20, 21), we use them to calculate electron states of the simplest two-center systems. To estimate the contribution of the dimensionality factor in potential curves in the united atom limit, we consider the relation $Q1(Z,R) = E^{3D}_{\rm bin}/E^{2D}_{\rm bin}$ between three-dimensional and two-dimensional expression for the binding energy $E_{\rm bin} = (E^2 - 1)/2$, when $Z_1 = Z_2$. Figure 3 presents a relative contribution of the dimensionality factor of the ground state energy values for the three-dimensional $3D$ and two-dimensional $2D$ molecule ion calculated by the asymptotic formula (2.15) [26] for the three-dimensional case and formula (11). As is seen from Figure 3, the term relation $Q1(Z,R)$ does not depend on the value of charge Z, as well as should be. At increase internuclear distance R relation $Q1$ decreases.

Figure 4 presents an analogous relative contribution $Q2(Z_1,R) = E^{3D}_{\rm bin}/E^{2D}_{\rm bin}$ of the dimensionality factor of the ground state energy values for the $3D$ and $2D$ molecule ion in the separating atom limit, calculated by the asymptotic formula (2.26) [26] for the three-dimensional case and

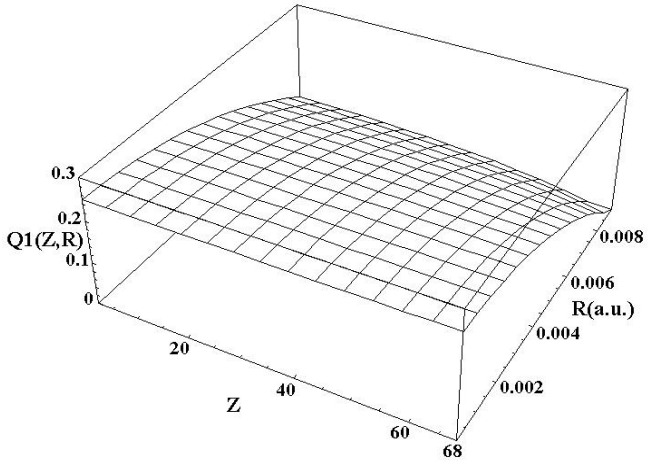

Fig. 3. The relative contribution $Q1(Z,R)$ of the ground state energy values for the $3D$ and $2D$ molecule ion in the united atom limit.

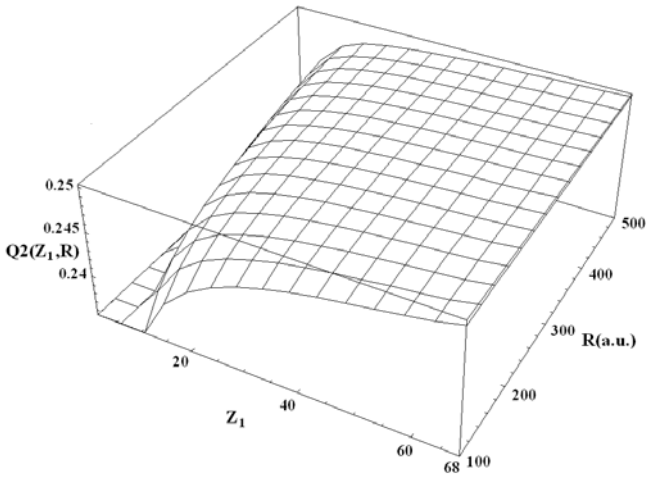

Fig. 4. The relative contribution $Q2(Z_1,R)$ of the ground state energy values for the $3D$ and $2D$ molecule ion in the separating atom limit.

formula (20). The data in this figure show that, as the Z_1 and R increase, the term relation $Q2(Z_1,R)$ increases and asymptotically tend to value 0.25.

Note that asymptotic expressions obtained here for the potential curves (11) and (20) are applicable under the condition that the quantities γ, γ_1 are purely real, which corresponds to the range of applicability of the Dirac equation solutions for the point charge.

We gratefully acknowledge O.K. Reity for many useful discussions.

Appendix A

Angular integrals are needed for the calculation matrix elements have the following form

$$\int_0^{2\pi} P_n(\cos\varphi)e^{im\varphi}d\varphi, \tag{A.1}$$

where m-integer.

For the simplest calculating it is convenient to use trigonometric representation of the Legendre polynomials [27]

$$\begin{aligned} P_n(\cos\varphi) = 2\frac{1\times 3\times 5\ldots(2n-1)}{2^n n!} \\ \times\Big[\cos n\varphi + \frac{1}{1}\frac{n}{2n-1}\cos(n-2)\varphi \\ +\frac{1\times 3}{1\times 2}\frac{n(n-1)}{(2n-1)(2n-3)}\cos(n-4)\varphi \\ +\frac{1\times 3\times 5}{1\times 2\times 3}\frac{n(n-1)(n-2)}{(2n-1)(2n-3)(2n-5)} \\ \times\cos(n-6)\varphi+\ldots\Big]. \end{aligned} \tag{A.2}$$

It is necessary here to take into account that if n odd integer, a sum is closed on a member from $\cos n\varphi$; if n even – on a member that does not depend on $\cos n\varphi$, thus this member is additionally multiply on 1/2. After the substitution of representation (A.2) in integral (A.1) they are taken to the known expression [28]:

$$\int_0^{2\pi} e^{im\varphi}\cos n\varphi d\varphi = \begin{cases} 0[m\neq n] \\ \pi[m=n\neq 0] \\ 2\pi[m=n=0] \end{cases}.$$

Appendix B

1. For a calculation radial integrals in matrix elements of perturbation operator in case small internuclear distances it is necessary to find the following integral

$$K_1 = \int_0^\infty z^{\nu-1}e^{-kz}F(-n_1,\gamma;kz)F(-n_2,\gamma;kz)dz,$$

where $F(\alpha,\beta;z)$ is confluent hypereheometric function.

The function $F(-n_2,\gamma;kz)$ can be determined in the form of contour integral:

$$\begin{aligned} F(\alpha,\beta;z) = -\frac{1}{2\pi i}\frac{\Gamma(1-\alpha)\Gamma(\beta)}{\Gamma(\beta-\alpha)} \\ \times\oint_{C'} e^{tz}(-t)^{\alpha-1}(1-t)^{\beta-\alpha-1}dt. \end{aligned} \tag{B.1}$$

After integrating over z with the help by a formula $(f.2)$ [29] will get

$$\begin{aligned} K_1 = -\frac{1}{2\pi i}\frac{\Gamma(n_2+1)\Gamma(\gamma)\Gamma(\nu)}{k^\nu\Gamma(\gamma+n_2)}\oint_{C'}(-t)^{n_1-n_2-1} \\ \times(1-t)^{\gamma+n_2-n_1-\nu-1}F(-n_1,\gamma-\nu,\gamma;\frac{1}{t})dt, \end{aligned}$$

where $F(a,b,c;z)$ is hypereheometric function.

Taking into account that at integer $a = n$ a hypereheometric function is a polynomial degrees of n, will get

$$K_1 = -\frac{1}{2\pi i}\frac{n_2!\Gamma(\gamma)\Gamma(\nu)}{\Gamma(\gamma+n_2)k^\nu}\oint_{C'}\Big\{(-t)^{n_1-n_2-1} \times(1-t)^{\gamma-\nu+n_2-n_1} + \sum_{m=0}^{n_1-1}\frac{n_1\dots(n_1-m)(\gamma-\nu)\dots(\gamma-\nu+m)}{(m+1)!\gamma(\gamma+1)\dots(\gamma+m)} \times(-t)^{n_1-n_2-s-2}(1-t)^{\gamma-\nu+n_2-n_1-1}\Big\}\,dt.$$

Now taking into account an integral representation (B.1) and properties $F(\alpha,\beta,0)=1$, will get

$$K_1 = \frac{n_2!\Gamma(\gamma)\Gamma(\nu)}{\Gamma(\gamma+n_2)k^\nu}\frac{\Gamma(\gamma-\nu+n_2-n_1)}{(n_2-n_1)!\Gamma(\gamma-\nu)} \times\left\{1+(n_2-n_1)!\sum_{m=0}^{n_1-1}\frac{n_1(n_1-1)\dots(n_1-m)}{(m+1)!(n_2-n_1+m+1)!} \times\frac{(\gamma-\nu-m-1)(\gamma-\nu-m)\dots(\gamma-\nu+m)}{\gamma(\gamma+1)\dots(\gamma+m)}\right\}.$$

2. For a calculation radial integrals in matrix elements of perturbation operator in case large internuclear distances it is necessary to find the following integral

$$K_2 = \int_0^\infty z^\gamma e^{-z}F(-n_1,\gamma;z)F(-n_2,\gamma;z)dz.$$

The function $F(-n_2,\gamma;z)$ can be determined in the form of contour integral (B.1) and integrating over z using a formula $(f.3)$ (with $n=1$) [29] will have

$$K_2 = \frac{1}{2\pi i}\frac{\Gamma^2(\gamma)\Gamma(n_2+1)}{\Gamma(\gamma+n_2)}\oint_{C'}\left(-\frac{n_1}{\gamma}\right)^{n_1-n_2-1} \times(-x)^{n_1-n_2-2}(1-x)(1+\frac{n_1}{\gamma}x)^{n_2-n_1-2}dx.$$

Replacement $t=-(n_1/\gamma)x$ was executed here. If to take into account an integral representation of hypereheometric function will have

$$K_2 = -\frac{\Gamma^2(\gamma)\Gamma(n_2+1)n_1(-\frac{n_1}{\gamma})^{n_1-n_2-1}}{\Gamma(\gamma+n_2)\Gamma(n_2-n_1+2)\Gamma(n_1-n_2+1)} \times F(n_1-n_2-1,n_1-n_2+2,n_1-n_2+1;-\frac{n_1}{\gamma}).$$

References

1. I.V. Komarov, L.I. Ponomarev, S.Yu. Slavyanov, *Spheroidal and Coulomb Spheroidal Functions* (Nauka, Moscow, 1976) (in Russian)
2. S.K. Luke, G. Hunter, R.P. McFachran, M. Cohen, J. Chem. Phys. **50**, 1644 (1969)
3. V.S. Popov, Pis. Zh. Eksp. Teor. Fiz. **11**, 254 (1970)
4. V.S. Popov, Yad. Fiz. **12**, 429 (1970)
5. V.S. Popov, Zh. Eksp. Teor. Fiz. **59**, 965 (1970)
6. V.A. Lyul'ka, Theor. Math. Phys. **28**, 212 (1976)
7. B. Muller, W. Greiner, Z. Naturf. a **31**, 1 (1976); J. Rafelski, B. Muller, Phys. Lett. B. **65**, 205 (1976)
8. H. Gould, C.T. Munger, Phys. Rev. Lett. **57**, 2927 (1986)
9. Yu.N. Pokotilovski, Part. Nucl. **24**, 5 (1993)
10. J. Reinhardt, W. Greiner, Rep. Progr. Phys. **40**, 219 (1977)
11. K.-H. Wietschorke, Phys. Rev. A **36**, 377 (1987)
12. H.K. Chauhan, P.K. Raina, J. Phys. B **29**, 5889 (1996)
13. A. Neagu, A.M.J. Schakel, Phys. Rev. D **48**, 1785 (1993)
14. A.M.J. Schakel, Phys. Rev. D **43**, 1428 (1991)
15. V.R. Khalilov, Theor. Math. Phys. **116**, 277 (1998)
16. W.P. Su, J.R. Schrieffer, A.J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979)
17. K. Von Klitzing, G. Dorda, M. Pepper, Phys. Rev. Lett. **45**, 494 (1980)
18. T. Chakraborty, Comm. Cond. Mat. Phys. **16**, 35 (1992)
19. R.E. Prange, S.M. Girvin, *The Quantum Hall Effect* (Springer Verlag, New York, 1990)
20. A.M.J. Schakel, G.W. Semenoff, Phys. Rev. Lett. **66**, 2653 (1991)
21. V.R. Khalilov, *Electrons in strong magnetic fields* (Energoatomizdat, Moscow, 1988)
22. C.M. Chiang, C.L. Ho, Phys. Rev. A **63**, 062105 (2001)
23. C.L. Ho, V.R. Khalilov, Phys. Rev. A **61**, 032104 (2000)
24. V.G. Bagrov, D.M. Gitman, *Exact solutions of relativistic wave equations* (Kluwer, Dordretch, 1990)
25. D.I. Bondar, V.Yu. Lazur, I.M. Shvab, S. Chalupka, J. Phys. Stud. **9**, 304 (2005)
26. O.K. Reity, V.Yu. Lazur, A.V. Katernoga, J. Phys. B **35**, 1 (2002)
27. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, edited by M. Abramowitz, I.A. Stegun (Wiley, New York, 1972)
28. I.S. Gradshteyn, I.M. Ryzhik, *Table of Imtegrals, Series, and Products* (Academic, New York, 1980)
29. L.D. Landau, E.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1981)