WKB-METHOD IN THE TWO-CENTER PROBLEM FOR THE DIRAC EQUATION

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Analytical quasiclassical solutions of the Dirac equation with an axially symmetrical potential, which does not permit complete separation of variables, are obtained. The two-center wave function of the Dirac electron is constructed. The first two terms of the asymptotic behavior of the exchange splitting of the potential curves are calculated. Spin-flipping effect is taken into account. The obtained results are compared with similar nonrelativistic results.

Introduction

The quantum-mechanical problem of the motion of an electron in a field of two fixed nuclei with charges Z_1 and Z_2 placed at a distance R from each other (the so-called Z_1eZ_2 problem) has been thoroughly studied in the framework of the Schröedinger equation since the late 1920s. Status of the problem and references on the subject up to 1976 can be found in [1]. The intensive studies of this problem during the last twenty years were stimulated not only by the availability of powerful computers and the successes achieved with asymptotic methods in solving ordinary differential equations, but also by the requirements of mesomolecular physics [2, 3] and the theory of ion-atom collisions [4]. New results were obtained both for the problem of the hydrogen molecular ion H_2^+ (see, for instance, [5] and references therein) and for the problem of two centers with strongly differing charges [6-8]. At the same time, perturbative estimations were made for relativistic effects in the two-center problem [9]. This problem was also considered in [10-13] for the Dirac equation within various approximations (the Galerkin method, diagonalization, variational method, etc.) due to the possibility of experimental observation of the spontaneous creation of the positron in a quasi-atomic supercritical field formed by two approaching heavy ions with a total atomic number $Z_1 + Z_2 > 173$.

It should be noted that within these problems, at many world laboratories [14, 15] equipped with heavy-ion accelerators, studies to verify the fundamental aspects of quantum electrodynamics are being carried out in superstrong fields whose sources are the nuclei of heavy colliding elements. Note also that the problem of taking relativistic effects into account arises in a number of traditional problems of the theory of ion-atom collisions. Thus, we are at the threshold of investigating phenomena induced by slow, highly charged ions. Krypton and xenon nuclei completely devoid of electrons were obtained previously in [16]. Quite recently, communications [15] appeared from a group of physicists working at the ion accelerator at the Lawrence Laboratory (Berkeley, USA), saying that they had obtained and detected H- and He-like uranium ions (U^{91+} and U^{90+}) with energies lower than 100 eV per unit charge. The still-unstudied interaction of such ions with matter should be essentially quasi-molecular and its consistent theory should be based on relativistic equations. The next step is to investigate multielectron processes and reactions with rearrangement (charge exchange, ionization, and so on) in the collisions of highly charged ions with atoms and molecules, as well as the properties of the transuranium elements by means of forming superheavy quasimolecules and processes in the electron shells of fissionable nuclei. All of this, in

essence, represents new promising fields for application of the relativistic two-center problem.

The difficulty in considerating the problem consists of the fact that the Dirac equation with the potential of two Coulomb centers does not permit a complete separation of variables in any orthogonal system of coordinates and, thus, one has to deal with partial differential equations. As a suitable method for calculating the wave functions and all other quantities required in the problem of the interaction of two heavy ions, we propose to employ the WKB approach. This approach allows us to obtain analytic solutions, but it is limited by asymptotically large internuclear distances R. These distances should be so large that the quantum penetrability of the potential barrier separating atomic particles is much smaller than unity. A great number of problems can be pointed out (see, for instance, [17-19]), whose solution depends on that region of internuclear distance. We stress, however, that analytic expressions derived for the asymptotic behavior of various splittings and shifts of the potential curves can sometimes be used in the region of internuclear distances that are smaller than those given by the formal criteria of applicability of the asymptotic expansions. Qualitatively, this can be explained by the fact that asymptotic solutions of the two-center problem retain the basic analytic properties of the exact solution [1] rather well, even the first term of the wave function expansion in powers of R^{-1}, up to sufficiently small R.

The paper is organized as follows. In the first section we solve the Dirac equation with an axially symmetrical potential by the WKB method. In the second section we construct the two-center wave function of the Dirac electron for a system of an arbitrary ion+atom (ion). Using this function, in the third section we compute the first two terms of the potential curve splitting in the relativistic two-center problem for the general nonresonance case. In the last section we discuss and compare obtained results with the data of similar nonrelativistic approximations.

Axially symmetrical problem

Let us consider an axially symmetrical problem, when two classically allowed regions are separated by a potential barrier. The examples of the application of such problem are an atom in an uniform electric field, the two-center problem, and so on. Let us find the wave function in the below-barrier region. In this case, the wave function is localized in the vicinity of the most probable tunneling way, that is the potential symmetry axis z.

For the bispinor

$$\Psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix} \tag{1}$$

the Dirac equation is of the form

$$\begin{aligned} c\vec{\sigma}\vec{p}\xi &= (E - V + c^2)\eta, \\ c\vec{\sigma}\vec{p}\eta &= (E - V - c^2)\xi, \end{aligned} \tag{2}$$

Inserting first equation of the system (2) into second one and using substitution

$$\begin{aligned} \xi &= (W^{\mp})^{1/2}\Phi, \\ W^{\pm} &= E - V \pm c^2, \end{aligned} \tag{3}$$

we obtain the second-order equation

$$\begin{aligned} &\Delta\Phi + k^2\Phi = 0, \\ &k^2 = \frac{1}{\hbar^2 c^2}\left[(E-V)^2 - c^4\right] - \\ &-\frac{\Delta V}{2W^{+}} - \frac{3}{4}\left(\frac{\vec{\nabla}V}{W^{+}}\right) + \frac{i}{W^{+}}\vec{\sigma}\left[\vec{\nabla}V, \vec{\nabla}\right] \end{aligned} \tag{4}$$

Since the potential is axially symmetrical, we seek a solution to this equation in the cylinderic system of coordinates of the form

$$\Phi = \begin{pmatrix} F_1(z,\rho)\exp\left[i\left(m - 1/2\right)\varphi\right] \\ F_2(z,\rho)\exp\left[i\left(m + 1/2\right)\varphi\right] \end{pmatrix}. \tag{5}$$

Substituting (5) into (4) gives the matrix equation

$$(\Delta+\partial)F=(\hbar^{-2}q^2+\gamma)F,\qquad F=\begin{pmatrix}F_1\\F_2\end{pmatrix},(6)$$

$$q=\frac{1}{c}\left[c^4-(E-V)^2\right]^{1/2},$$

$$\partial=\frac{1}{W^+}\left(\frac{\partial V}{\partial\rho}\frac{\partial}{\partial z}-\frac{\partial V}{\partial z}\frac{\partial}{\partial\rho}\right)\begin{pmatrix}0&-1\\1&0\end{pmatrix},$$

$$\gamma=\begin{pmatrix}a_{m-1/2}&b_{m+1/2}\\b_{m-1/2}&a_{-m-1/2}\end{pmatrix},$$

$$a_\mu(z,\rho)=\frac{\mu^2}{\rho^2}+\frac{1}{W^+}\left[\frac{\mu}{\rho}\frac{\partial V}{\partial\rho}+\frac{\Delta V}{2}+\frac{3}{4}\frac{(\vec\nabla V)^2}{W^+}\right],$$

$$b_\mu(z,\rho)=-\frac{\mu}{\rho W^+}\frac{\partial V}{\partial z}.$$

Let us represent the solution of Eq. (6) in the form

$$F=\varphi\exp(\hbar^{-1}S),\qquad \varphi=\sum_{n=0}^{\infty}\hbar^n\varphi^{(n)}. \qquad (7)$$

Inserting (7) into (6) and equating to zero the coefficient of each power of $\hbar$, we obtain the system

$$\left[(\vec\nabla S)^2-q^2\right]\varphi^{(0)}=0, \qquad (8.1)$$

$$\left[(\vec\nabla S)^2-q^2\right]\varphi^{(1)}+2\vec\nabla S\vec\nabla\varphi^{(0)}+\Delta S\varphi^{(0)}+\hat\partial S\varphi^{(0)}=0 \qquad (8.2)$$

$$\left[(\vec\nabla S)^2-q^2\right]\varphi^{(n+2)}+2\vec\nabla S\vec\nabla\varphi^{(n+1)}+\Delta S\varphi^{(n+1)}+\hat\partial S\varphi^{(n+1)}+\Delta\varphi^{(n)}+\hat\partial\varphi^{(n)}-\gamma\varphi^{(n)}=0 \qquad (8.3)$$

n=0,1,2,...

Let us find the wave function in the below-barrier region. In this case, the wave function is localized in the vicinity of the most probable tunneling way, that is the potential symmetry axis z. Therefore, we seek the solutions of system (8) in the form of the expansion over small coordinate ρ. From Eq. (8.1) we obtain

$$(\vec\nabla S)^2=q^2,$$

$$q^2(z,\rho)=q_0^2(z)+\sum_{k=1}^{\infty}Q_k(z)\rho^{2k}, \qquad (9)$$

$$q_0^2(z)=q^2(z,0),\quad Q_k=\frac{1}{(2k)!}\frac{\partial^{2k}q^2(z,0)}{\partial\rho^{2k}}.$$

Substituting the solution in the form

$$S(z,\rho)=\sum_{n=0}^{\infty}S_n(z)\rho^{2n} \qquad (10)$$

into Eq. (9) and equating to zero the coefficient of each power of ρ, we obtain a system of first-order equation. Its solutions are expressed by

$$S_0=-\int q_0dz+const, \qquad (11.1)$$

$$S_1=\frac{q_0(z)}{2}\left(\frac{1}{2}\frac{q_0'(z)}{q_0(z)}-\frac{\sigma'(z)}{\sigma(z)}\right), \qquad (11.2)$$

$$S_2=\frac{q_0^2}{2\sigma^4}\left\{\int\frac{\sigma^4}{q_0^3}\left[(S_1')^2-Q_2\right]dz+const\right\}, \qquad (11.3)$$

$$\sigma''+\left[\frac{1}{4}\left(\frac{q_0'}{q_0}\right)^2-\frac{1}{2}\frac{q_0''}{q_0}-\frac{Q_1}{q_0^2}\right]\sigma=0. \qquad (12)$$

We seek the solutions of Eq. (8.2), (8.3) of the form

$$\varphi^{(n)}(z,\rho)=\begin{pmatrix}\rho^{|m-1/2|}\sum_{k=0}^{\infty}\varphi_{1k}^{(n)}(z)\rho^{2k}\\ \rho^{|m+1/2|}\sum_{k=0}^{\infty}\varphi_{2k}^{(n)}(z)\rho^{2k}\end{pmatrix}. \qquad (13)$$

Substituting (13) into respective equations and equating to zero the coefficient of each power of ρ, we obtain the system of ordinary first-order differential equations, which are soluble. The solutions are expressed by integrals. The lower component η of Ψ is obtained from the upper one ξ by operation $\xi\xrightarrow{W^+\to W^-}\eta$.

Two-center wave function

Let us now find the wave function of the Dirac electron in the field of two fixed nuclei with charges Z_1 and Z_2 placed at a large distance R from each other. Since in the below-barrier region the electron is placed far from each nucleus, we consider that the potential is Coulomb:

$$V=-\frac{Z_1}{r_1}-\frac{Z_2}{\left|\vec R-\vec r_1\right|}. \qquad (14)$$

When atoms 1 and 2 are different, the eigenvalues (potential curves) $E(R)$ of the

two-center problem dependent on the internuclear distance R as a parameter, are divided into two classes: $E_I -$ and $E_{II} -$ potential curves that, for $R \to \infty$, transform into the energy levels of isolated atoms 1 and 2, respectively. The energy $E_I(R)$ in the first approximation of perturbation theory is equal to

$$E_I(R) = E_1 - Z_2/R + Z_2\xi_1/R^2 + \ldots, \quad (15)$$

where E_1 is the energy of a nonperturbed isolated state of atom 1. We search for solution to the Dirac equation with potential (14) under the boundary condition $\Psi_I \xrightarrow[z<<R]{} \Psi_1$, which means that when the electron approaches atom 1, the two-center function Ψ_I tends to the unperturbed atomic wave function Ψ_1.Using Eq. (14), (15), we obtain the expression for the functions

$$S_0 = -\lambda_I z - \frac{Z_I^2}{2\lambda_I^3 z} + \frac{Z_2^2 z}{2\lambda_I^3 R(R-z)} + \frac{\varepsilon_I Z_I}{\lambda_I} ln\, z - \frac{\varepsilon_I Z_2}{\lambda_I}\left(1 + \frac{Z_I - Z_2}{\varepsilon_I \lambda_I^2 R}\right) ln\left(1 - \frac{z}{R}\right), \quad (16.1)$$

$$S_I = -\frac{q_0}{2z}\left[1 + \frac{\varepsilon_I Z_2}{2\lambda_I^2}\frac{z}{(R-z)^2}\right], \qquad S_2 = \frac{\lambda_I}{8z^3}, \qquad \varepsilon_{1,I} = \frac{E_{1,I}}{c^2}, \qquad \lambda_{1,I} = c\sqrt{1-\varepsilon_{1,I}^2}, \quad (16.2)$$

$$\varphi = \frac{1}{\sigma}\begin{pmatrix} K_I^{\pm}\left(\frac{\rho\sqrt{q_0}}{\sigma}\right)^{|m_I - 1/2|}\left[1 + L_I^{\pm} * \left(\frac{\rho}{z}\right)^2 + U_I^{\pm}(z)\right] \\ K_2^{\pm}\left(\frac{\rho\sqrt{q_0}}{\sigma}\right)^{|m_I + 1/2|}\left[1 + L_2^{\pm} * \left(\frac{\rho}{z}\right)^2 + U_2^{\pm}(z)\right] \end{pmatrix}, U_{1,2}^{\pm}(z) = \frac{\alpha_{1,2}^{\pm}}{4W_0^{\pm}}\frac{z(2R-z)}{(R-z)^2} + \frac{\kappa_1(\kappa_1 \pm 1)}{2\lambda_I z}, \quad (17)$$

where $K_{1,2}^{\pm}, L_{1,2}^{\pm}, \alpha_{1,2}^{\pm}$ are defined constants, +(-) corresponds to the component $\xi(\eta)$. By the same way we obtain the wave function Ψ_{II} corresponding to the potential curves E_{II}.

Exchange splitting of adiabatic potential curves

For calculating the exchange splitting of terms we have obtained the representation through the integral over the surface S conditionally separating the domains, where the electron is in initial Ψ_I and final Ψ_{II} states [21]:

$$\Delta E = 2ic\int_S d\vec{S}(\Psi_{II}^{+}\vec{\alpha}\Psi_I). \quad (18)$$

Calculating integral (18) by the stationary phase method, we arrive at expression for the first two terms of the asymptotic behavior of $\Delta E(R)$:

$$\Delta E = \frac{2A_1A_2}{(|m|-1/2)!(\lambda_I+\lambda_2)^{|m|-1/2}} D_{j_1 j_2 m} R^{\frac{\varepsilon_1 Z_2}{\lambda_1}+\frac{\varepsilon_2 Z_2}{\lambda_2}-|m|-1/2} exp\left\{-\frac{R(\lambda_I+\lambda_2)}{2} - \frac{1}{2}\left(\frac{\varepsilon_I Z_2}{\lambda_I} + \frac{\varepsilon_2 Z_I}{\lambda_2}\right)\right\}\left[1 + \frac{I}{R}\right], \quad (19)$$

$$D_{j_1 j_2 m} = \sqrt{\frac{(j_1+|m|)!(j_2+|m|)!}{(j_1-|m|)!(j_2-|m|)!}}, \qquad m = m_1 = m_2, \qquad \kappa_{1,2} = \mp(j_{1,2} + 1/2), \quad (20)$$

$$I = \frac{1}{\lambda_I+\lambda_2}\left[\kappa_I^2 + \kappa_2^2 - (|m|-1/2)^2 - \frac{\kappa_I\kappa_2}{|m|+1/2}\right] + \frac{|m|+1/2}{2}\left(\frac{\varepsilon_I Z_2}{\lambda_I^2} + \frac{\varepsilon_2 Z_I}{\lambda_2^2}\right) + \frac{\varepsilon_I Z_2 \xi_1}{2\lambda_I} + \frac{\varepsilon_2 Z_I \xi_2}{2\lambda_2} - \frac{Z_I^2}{4\lambda_I^3} - \frac{Z_2^2}{4\lambda_2^3} \quad (21)$$

Discussion

In this work we have obtained the analytical quasi-classical solutions of the Dirac equation with an axially symmetrical potential, which does not permit a complete separation of variables. Our method allows to take into account the spin-orbit and spin-spin interactions. We have obtained the relativistic two-center wave function and calculated the exchange splitting of potential curves, which expressed through the known characteristics of disconnected atoms: charges of atomic cores Z_1 and Z_2, asymptotic coefficients A_1, A_2, binding energies $\lambda_{1,2}^2/2$ and quantum numbers of the electron in the considered states of atoms (ions). First the spin-flipping effect is taken into account. Our results and analogous nonrelativistic results of the exchange splitting show (Table 1) that the role of relativistic effects increases with increasing charges Z_1, Z_2 and the relative contribution of relativistic effects amounts to about 50%, even at $Z_1 = Z_2 = 48$.

Table 1. Results of the calculation of the exchange splitting ΔE within various approaches.

Methods	Relativistic quasi-classical approach [this work]	Non-relativistic quasi-classical approach [20]	Relativistic asymptotic approach [21]
$Z_1 = 1,\ Z_2 = 10,\ n_2 = 7$			
R_p	17.271	17.294	17.271
$\Delta E(R_p)$	1.626×10^{-2}	1.321×10^{-2}	1.525×10^{-2}
$Z_1 = 1,\ Z_2 = 20,\ n_2 = 12$			
R_p	21.319	21.375	21.319
$\Delta E(R_p)$	2.623×10^{-2}	1.917×10^{-2}	4.881×10^{-2}
$Z_1 = 1,\ Z_2 = 30,\ n_2 = 17$			
R_p	27.324	27.434	27.324
$\Delta E(R_p)$	1.053×10^{-3}	7.273×10^{-4}	5.040×10^{-3}
$Z_1 = 1,\ Z_2 = 40,\ n_2 = 22$			
R_p	33.643	33.828	33.643
$\Delta E(R_p)$	3.505×10^{-4}	2.313×10^{-4}	4.724×10^{-3}

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МЕТОД ВКБ В ЗАДАЧІ ДВОХ КУЛОНІВСЬКИХ ЦЕНТРІВ ДЛЯ РІВНЯННЯ ДІРАКА

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За допомогою методу ВКБ рівняння Дірака з аксіально симетричним потенціалом, який не допускає повного відокремлення змінних, аналітично розв'язано в підбар'єрній області в околі осі симетрії потенціалу. Цей підхід враховує спін-спінову та спін-орбітальну взаємодії. В рамках розробленої схеми побудована релятивістська двоцентрова хвильова функція. Обчислено перші два члени асимптотики (за великими між'ядерними відстанями) потенціалу обмінної взаємодії іона з атомом. При цьому вперше враховано ефект перевороту спіну.