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Boundary-Layer Method in the Problem of One-Electron Exchange Interaction between Atom and Multiply Charged Ion

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Abstract

Using the idea of the boundary-layer method the recurrent scheme of obtaining the quasiclassical solutions of the quantum mechanical two-centre problem is elaborated. By means of this scheme the two-centre wave function is constructed in the classically forbidden regions. This allows for the first time to calculate the asymptotic (at large internuclear distances) behavior of the exchange interaction potential for an ion with an atom.

Radiation and collision processes occurring in laboratory and astrophysical plasmas are determined by the interaction of plasma particles (electrons, atoms, molecules, and ions) among themselves and with photons. These so-called elementary processes include excitation, ionization, recombination due to electron-atom and ion-atom collisions, and photoprocesses. Elementary processes are of interest in many branches of atomic physics and spectroscopy, plasma physics, quantum electronics, accelerator physics, and thermonuclear fusion. Moreover, determination of the relations among the characteristics of elementary processes and radiation intensities allows one to develop reliable spectroscopic and corpuscular methods for plasma diagnostics. The properties and the role of elementary processes in laboratory and astrophysical plasmas have been considered in many review articles and books (see for example [1, 2, 3, 4, 5, 6, 7]).

During recent years, interest in the investigation of atomic processes involving heavy many-electron ions has strongly increased. This is related with the fast development of accelerator techniques and the employment of heavy ions in many applications, such as thermonuclear fusion [8], slowing down of heavy-ion beams in matter [9], particle beam diagnostics of laboratory plasmas [10], fragmentation of exotic nuclei [11], investigation of the interaction of laser-produced plasmas with a solid surface [12] and the generation of extreme states of matter [13], in astrophysics [14], in beam tumor therapy, in the design of the new types of accelerators and storage rings, etc. Investigations of heavy ions accelerated up to relativistic energies are the focus of special attention in the new international FAIR project (Facility for Antiproton and Ion Research) started in 2011 at Gesellschaft für Schwerionenforschung (GSI) in Darmstadt [15].

We consider the one-electron charge exchange

$$\mathrm{A} + \mathrm{B}^{Z+} \to \mathrm{A}^{+} + \mathrm{B}^{(Z-1)+}, \tag{1}$$

where A is a neutral atom (or ion), B^{Z+} is a highly charged ion with the charge Z.

In slow collisions of atomic particles (1) the transition of an electron from one nucleus to the other occurs at large distances between the colliding particles. The value of the energy splitting between the terms of the system, in the range of their pseudocrossing, determines the nonadiabatic transition probability. In order to find the energy splitting two-center wave function of high accuracy is to be used.

The two-centre problem was solved by means of asymptotic and numerical methods within both the nonrelativistic [16] and relativistic (see for example [17] and references therein) theory. But results obtained early do not satisfy requirements for accuracy of modern experimental facilities, and necessary to elaborate new more perfect approaches arises. This is the main aim of the present paper.

The stationary Schrödinger equation is ($m_e = |e| = \hbar = 1$):

$$\Delta\Psi(\rho, z, \phi) + 2\left(E - V(\rho, z)\right)\Psi(\rho, z, \phi) = 0, \tag{2}$$

where

$$V(\rho, z) = -\frac{Z_1}{\sqrt{z^2+\rho^2}} - \frac{Z_2}{\sqrt{(R-z)^2+\rho^2}} \tag{3}$$

is the two-centre potential, R is the internuclear distance, ρ, z, ϕ are the cylindrical coordinates.

Having substituted

$$\Psi(\rho, z, \phi) = \Phi(\rho, z)e^{im\phi} \tag{4}$$

into (2) we arrive at the equation

$$\Delta\Phi(\rho, z) + \left[2(E - V) - \frac{m^2}{\rho^2}\right]\Phi(\rho, z) = 0. \tag{5}$$

Now we shall use the idea of the boundary-layer method that the wave function is localized in the vicinity of the most probable tunnelling direction that is the internuclear axis. For this purpose we can represent its solution and all quantities in it in the form of expansions in powers of coordinate the ρ^2 like in [18]:

$$\Phi = \varphi\cdot e^{S}, \quad S = -\int q_0 dz + \sum_{n=0}^{\infty} S_n(z)\rho^{2n}, \quad \varphi = \rho^m \sum_{n=0}^{\infty}\varphi_k\rho^{2k}, \tag{6}$$

$$V\left(z, \rho\right) = \sum_{k=0}^{\infty} V_k(z)\rho^{2k}, \quad V_k = \frac{1}{k!}\frac{\partial^k V(z,0)}{\partial\rho^{2k}}, \tag{7}$$

where $q_0 = \sqrt{2(V_0 - E)}$.

By inserting (6), (7) into (5) and equating to zero the coefficients of each power of ρ^2, we obtain the recurrent system of first-order differential equations containing the Riccati equation for $S_1(z)$ which is analytically unsolvable. To solve it at large z we can use the following expansion of $S_1(z)$

$$S_1(z) = \sum_{i=0}^{\infty} S_{1i}(z), \tag{8}$$

where $S_{1i}(z) \sim z^{-(i+1)}$. By substituting (7) into the corresponding equation and equating to zero terms of common order of z, we obtain a system of ordinary first-order differential equations, which is solvable.

In the similar way we can find other corrections:

$$S_n(z) = \sum_{i=0}^{\infty} S_{ni}(z), \quad \varphi_k(z) = \sum_{i=0}^{\infty} \varphi_{ki}(z). \tag{9}$$

All arbitrary constants arisen here we can determinate by means of the boundary condition

$$\Psi \xrightarrow[z_1 \ll z \ll z_b]{} \Psi_0^{(as)}, \tag{10}$$

which means that close to an atom the wave function should be reduced to asymptotic behavior of the atomic wave function Ψ_0. Here $z_b < z_m$, z_1, z_2 are roots of equation $q_0(z) = 0$, z_m is a maximum of "potential" $V_0(z)$.

As a result, we obtain all corrections $S_{ni}(z)$ and $\varphi_{ki}(z)$ normalized, for example

$$S_{10} = -\frac{\gamma}{2z}, \quad S_{20} = \frac{\gamma}{8z^3}, \quad S_{30} = \frac{\gamma}{16z^5}, \quad \ldots \tag{11}$$

Collecting obtained formulas together we see that corrections of the same order are in both the exponent and pre-exponent, and the structure of wave function is rather complicated. To simplify it we seek a solution of (5) in the form

$$\Phi = \varphi \cdot e^S, \quad S = -\int q_0 dz + \sum_{n=1}^{\infty} S_{n0}(z)\rho^{2n}, \quad \varphi = \rho^m \sum_{n=0}^{\infty} \varphi_k \rho^{2k}, \tag{12}$$

where $S_{n0}(z)$ are determined previously (see (9)).

By inserting (10), (7) into (5) and equating to zero the coefficients of each power of ρ^2, we obtain the recurrent system ($\gamma = \sqrt{-2E}$)

$$2q_0\varphi_0' + \left(q_0' + \frac{2(m+1)\gamma}{z}\right)\varphi_0 = 4(m+1)\varphi_1 + \varphi_0'', \tag{13}$$

$$2q_0\varphi_1' + \left(q_0' + \frac{2(m+3)\gamma}{z}\right)\varphi_1 = \left[\frac{\gamma(\gamma - q_0)}{z^2} + \frac{(m+1)\gamma}{z^3} - Q_1\right]\varphi_0 + \\ + \frac{\gamma}{z^2}\varphi_0' + 8(m+2)\varphi_2 + \varphi_1'', \tag{14}$$

$$2q_0\varphi_2' + \left(q_0' + \frac{2(m+5)\gamma}{z}\right)\varphi_2 = \left[\frac{\gamma(\gamma - q_0)}{z^2} + \frac{(m+3)\gamma}{z^3} - Q_1\right]\varphi_1 + \frac{\gamma}{z^2}\varphi_1' - \\ - \frac{3\gamma}{4z^4}\varphi_0' + \left[\frac{3\gamma(q_0 - \gamma)}{4z^4} - \frac{3(m+1)\gamma}{4z^5} - Q_2\right]\varphi_0 + 12(m+3)\varphi_3 + \varphi_2'', \tag{15}$$

whose solutions we seek in the form (9). Then the corrections $\varphi_{ki}(z)$ satisfy the following system

$$\varphi_{00}' + \frac{m+1}{z}\varphi_{00} = 0, \tag{16}$$

$$\varphi_{01}' + \frac{m+1}{z}\varphi_{01} = \frac{1}{2\gamma^2}\left[-V_0'\varphi_{00} - 2V_0\varphi_{00}' + \gamma\left\{4(m+1)\varphi_{10} + \varphi_{00}''\right\}\right], \tag{17}$$

$$\varphi_{02}' + \frac{m+1}{z}\varphi_{02} = \frac{1}{2\gamma^4}\left[V_0(V_0\varphi_{00}' + V_0'\varphi_{00}) - \gamma^2(2V_0\varphi_{01}' + V_0'\varphi_{01}) + \right.$$
$$\left. +\gamma^3\left\{4(m+1)\varphi_{11} + \varphi_{01}''\right\}\right], \tag{18}$$

$$\varphi_{10}' + \frac{m+3}{z}\varphi_{10} = \frac{1}{2\gamma z^3}\left[\left\{(m+1)\gamma - zV_0 - z^3Q_1\right\}\varphi_{00} + \gamma z\varphi_{00}'\right], \tag{19}$$

$$\varphi_{11}' + \frac{m+3}{z}\varphi_{11} = \frac{1}{4\gamma^3 z^3}\left[zV_0^2\varphi_{00} - 4\gamma z^3 V_0\varphi_{10}' - 2\gamma z^3 V_0'\varphi_{10} + 2\gamma^2\left\{(m+1)\gamma - \right.\right.$$
$$\left.\left. -z^3Q_1 - zV_0\right\}\varphi_{01} + 2\gamma^2 z^3\left\{8(m+2)\varphi_{20} + \varphi_{10}''\right\} + 2\gamma^3 z\varphi_{01}'\right], \tag{20}$$

$$\varphi_{20}' + \frac{m+5}{z} = \frac{1}{8\gamma z^5}\left[\left\{3zV_0 - 3(m+1)\gamma - 4z^5Q_2\right\}\varphi_{00} + \right.$$
$$\left. +4z^2\left\{(m+3)\gamma - zV_0 - z^3Q_1\right\}\varphi_{10} + \gamma z\left\{4z^2\varphi_{10}' - 3\varphi_{00}'\right\}\right]. \tag{21}$$

Solving the system (9) and inserting them into (10) we obtain the final expression of the two-center wave function normalized:

$$\Psi = \left(\frac{2\gamma^2 ze}{Z_1}\right)^{\frac{Z_1}{\gamma}} \rho^m\left\{\varphi_{00} + \varphi_{01} + \varphi_{02} + \left[\varphi_{10} + \varphi_{11}\right]\rho^2 + \varphi_{20}\rho^4\right\} \times$$
$$\times\exp\left[-\int q_0 dz - \frac{\gamma}{2z}\rho^2 + \frac{\gamma}{8z^3}\rho^4 - \frac{\gamma}{16z^5}\rho^6 + im\varphi\right], \tag{22}$$

where

$$\varphi_{00} = \frac{1}{z^{m+1}}, \quad \varphi_{01} = \frac{1}{2\gamma^2 z^{m+1}}\left[\frac{Z_1 + l\,(l+1)\,\gamma}{z} - \frac{mZ_2 z}{R\,(R-z)} - \frac{3Z_1}{R}\right], \tag{23}$$

$$\varphi_{02} = \frac{1}{8\gamma^4 z^{m+1}}\left[\frac{5Z_1^2 + 2Z_1\gamma\,(2l\,(l+1)-1) + \gamma^2\,(l-1)\,l\,(l+1)\,(l+2)}{z^2} - \right.$$
$$- \frac{2Z_2\left[Z_1\,(5m+3) + Z_2\,(m\,(m+1)+1) + m\gamma\,(l\,(l+1)-m-1)\right]}{R\,(R-z)} +$$
$$+ \frac{Z_2\,(Z_2\,(m\,(m-3)+1) + m\gamma\,(m-1))}{(R-z)^2} -$$
$$\left. - \frac{Z_2\,(2Z_1\,(5m+3) + Z_2\,(m\,(m+5)+1)) + m\,(2l\,(l+1)-3m-1)}{R^2}\right], \tag{24}$$

$$\varphi_{10} = \frac{1}{z^{m+3}}\left[A_{10} + \frac{Z_2 z\,(2R-3z)}{4\gamma\,(R-z)^2}\right], \tag{25}$$

$$\varphi_{11} = \frac{1}{8\gamma^3 z^{m+3}}\left[\frac{Z_1Z_2\left(9R^2 - (2m+17)\,zR + (2m+5)\,z^2\right)}{R\,(R-z)^2} + \right.$$

$$+\frac{Z_2 z\gamma m}{R}\left(m+\frac{z^2}{(R-z)^2}\right)+\frac{Z_2^2 z\left(2R^2-2\left(m+2\right)zR+\left(3m+1\right)z^2\right)}{R\left(R-z\right)^2}+$$
$$+\frac{Z_2 z l\left(l+1\right)\left(\left(2m+3\right)R-\left(3m+4\right)z\right)}{\left(m+1\right)R\left(R-z\right)^2}-$$
$$-\frac{3Z_1^2\left(2m+3\right)-2l\left(l+1\right)\left(m+2\right)Z_2\gamma+Z_1\left(\left(3m-1\right)Z_2-3\gamma\left(m\left(m+3\right)+2\right)\right)}{\left(m+1\right)R}+$$
$$\frac{1}{z}\left(4Z_1^2-Z_1\gamma\left(m+4-\left(2m+1\right)\frac{l\left(l+1\right)}{m+1}\right)-\gamma^2 l\left(l+1\right)\left(m+4+\frac{l\left(l+1\right)}{m+1}\right)\right)\Big].$$

$$\varphi_{20}=\frac{1}{z^{m+5}}\Big\{\Big[Z_2 z\Big(Z_2 z\left(2R-3z\right)^2-\gamma\left(2R^2\left(2R+7z\right)\left(4A_{10}-1\right)\right.\ +$$
$$\left.+4z^2R\left(16A_{10}-5\right)+z^3\left(24A_{10}-13\right)\right)\Big)\Big]/\left(32\gamma^2\left(R-z\right)^4\right)+A_{20}\Big\}. \qquad (26)$$

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