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

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By the WKB approach and boundary-layer method the Dirac equation with an axially symmetrical potential, unpermitting a complete separation of variables, is analytically solved. In the framework of this scheme, the relativistic two-center wave function is constructed. The first two terms of the asymptotic (at large internuclear distance) behaviour of the exchange interaction potential of an ion with an atom are calculated.

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 $Z_1 + Z_2 > 173$.

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

First we consider an axially symmetrical problem, when two classically allowed regions are separated by a potential barrier. The application of the WKB method to this problem is based on reducing the Dirac equation to the second-order equation looking like the Schrödinger equation. Carrying out the expansion in powers of $\hbar$, we arrive at the system of matrix first-order partial differential equations that can be successively solved, using the relativistic version of the boundary-layer method [14,15], founded by M. A. Leontovich and V. A. Fock. It consists in following.

The cases are not infrequent, when for the solution of a quantum-mechanical problem it is enough to find a wave function not in all configurational space, and only in a vicinity of some the manifold M of smaller dimensionality, where a wave function is localized. The states described by such wave functions, are termed "localized". The example of such states is the problem of exchange interaction of atomic particles at large distances that results in splitting of potential curves in point of quasi-crossing . Exchange splitting, as is known [16], is mainly defined by the electron distribution region lying in the vicinity of the internuclear axis R (M is a straight line). Another example of localized state is the process of the tunneling ionization of a hydrogen atom in a rather weak constant electric field when in the below-barrier region the probability flux is localized in the vicinity of a symmetry axis (M is a straight line, too).

In such cases it is naturally to expand the potential in powers of the perpendicular to M coordinate. This allows us to carry out the approximate separation of variables, to find approximate analytical solutions of the obtained system of matrix partial differential equations in the vicinity of the manifold M and consider the extensive range of problems of the theory of slow atomic collisions. Our method allows to take into account the spin-orbit and spin-spin interactions.

Now let us employ the elaborated approach to the two-center problem, when internuclear distances R are large, and obtain the two-center wave function. Since in the below-barrier region the electron is placed far from each nucleus, we consider that the potential is Coulomb.

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 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 the applicability of the expansion performed below is the requirement that the wave function of the Ψ_1-state, for instance, of atom 1, not be strongly perturbed by the other particle. The distortion of the dependence of this function on the coordinates should be small. This is

connected with the energy shift of the state induced by the interaction with perturbing particle 2. The external (Coulomb) field of the latter is considered to be weak compared to the typical intra-atomic fields in order to make use of perturbation theory. The energy $E_I(R)$ in the first approximation of perturbation theory is equal to

$$E_I(R) = E_1 - Z_2/R + Z_2\xi_1/R^2 + \ldots, \quad (1)$$

We search for solution to the Dirac equation with potential of two Coulomb centers under the boundary condition

$$\Psi_I \xrightarrow[z<<R]{} \Psi_1, \quad (2)$$

which means that when the electron approaches atom 1, the two-center function Ψ_I tends to the unperturbed atomic wave function Ψ_1 [17]. Using the elaborated for axially symmetrical potential general scheme to the Dirac equation with the potential of two Coulomb centers, we obtain the relativistic two-center wave function.

For calculating the exchange splitting of the potential curves we have obtained [18] by the Green's function method the representation for ΔE through the integral over the surface S conditionally separating the domains where the electron is in the initial Ψ_I and final Ψ_{II} states,

$$\Delta E = 2ic\int_S d\vec{S}(\Psi_{II}^{+}\vec{\alpha}\Psi_I). \quad (3)$$

Here the surface element $d\vec{S}$ is directed from atom 1 to atom 2. Note that representation (3) is a relativistic analog of the well-known Firsov formula representing $\Delta E(R)$ in the non-relativistic case. As the surface S we take the midplane between the two nuclei. Calculating the integral (3) by the stationary phase method, we arrive at the following expression for the first two terms of the asymptotic behaviour of $\Delta E(R)$ 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). For the first time, the spin-flipping effect is taken into account Our results and analogous non-relativistic results of the exchange splitting show 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 $Z_1 = Z_2 = 48$.

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