

Adiabatic potential curves of $H-p$ and $He^+ - p$ ions: relativistic treatment© A. Danilov¹, A. Anikin^{1,2}, D. Glazov^{1,3}, E. Korzinin², A. Kotov¹, D. Solovyev^{1,4}¹ St. Petersburg State University,
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In the present paper, a completely relativistic approach is used to obtain adiabatic potential curves for molecular terms within the A-DKB method. Solving the two-center Dirac equation, two compounds are described: one-electron homonuclear $H - p$ and one-electron heteronuclear $He^+ - p$ (quasi-)molecular ions. In the framework of the Born-Oppenheimer approximation, the electron binding energies (ground and several first excited states) in a wide range of inter-nuclear distances have been obtained. Using the relativistic approach, energy splittings, crossings, and identification of energy terms are discussed. The results are compared with those characterized within the nonrelativistic approach, widely covered in the literature.

Keywords: Dirac equation, relativistic effects, potential curves, quasimolecules, A-DKB method.

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1. Introduction

Diatomic molecules have been the object of study since the emergence of quantum mechanics (QM) [1,2]. Interest in such systems was stimulated by the necessity to describe bound states of electrons as part of quantum theory and to develop a theory for solving the many-body problem. At the dawn of the development of quantum theory, the determination, for example, of the equilibrium internuclear distance in light molecular systems served as a test of the theory [3]. Since then, the continuous development of the theory, combined with increasing accuracy of measurements of molecular systems, has found many applications in various fields of physics and chemistry. For example, in plasma physics, the description of the process of proton scattering on atomic hydrogen is of particular interest [4–6]. In lots of astrophysical problems, light molecular ions (H_2^+ and $He^+ - p$) are studied, and collisional processes leading to the formation of atomic hydrogen in the early Universe are reviewed [7]. Recently, the molecular hydrogen ion and its isotopes have been proposed to be used as molecular optical clocks based on theoretical and experimental advances [8]. As a consequence, it has been shown that such systems can be used to accurately determine fundamental physical constants such as the electron-proton mass ratio and the proton charge radius [9].

Single-electron binuclear ions, along with the helium atom, are the simplest case of the many-body problem. The traditional way to describe such systems is to use numerical methods. One widely used method is to use a nonrelativistic approach. The Schrödinger equation is solved with the

aim of accurately calculating the electron bond energy, and then various relativistic and radiation-induced corrections are taken into account, calculated within the framework of nonrelativistic quantum electrodynamics (NRQED). The most outstanding results were obtained using the variational principle [10–15], as part of which corrections were calculated up to the orders $m\alpha^6$ and $m\alpha^6 (m/M)$ (m and M electron and nucleus masses, respectively, α fine structure constant). An alternative approach is to solve the Dirac equation with a two-center potential. A widely used method is the expansion of Dirac wave functions in partial waves. As part of this approach, the energies of low-lying states of the molecular ion H_2^+ were calculated with an accuracy of the order of 10^{-13} – 10^{-14} [16–20] and higher for the ground state [21]. The results obtained by other methods are presented in [22,23].

In this work, a different fully relativistic approach is used to study the single-electron ionic compounds hydrogen-proton ($H - p$) and singly ionized helium-proton ($He^+ - p$). As part of the Born – Oppenheimer approximation, the Dirac equation with a two-center potential is solved using the expansion of the wave function in B -splines [24]. The dual-kinetic balance (DKB) method built on B -splines was extended to the case of systems with axial symmetry (A-DKB) [25] in the work [26]. Recently, a theoretical analysis of heavy single-electron quasi-molecular compounds has been carried out using the A-DKB approach [27,28].

We apply the A-DKB method to calculate the ground and first few excited quasi-molecular terms of the light ions $H - p$ and $He^+ - p$. A detailed analysis of adiabatic

potential surfaces is carried out based on the calculation results. In particular, the behavior of the ground and excited quasi-molecular terms depending on the internuclear distance is considered and their classification is carried out as part of a strict relativistic approach. Typically, the identification of the energy states of molecules, along with correlation diagrams, is carried out in a nonrelativistic approximation, which leads to the necessity to adapt it to the relativistic case. The presence of a large number of (pseudo)intersections, as well as fine splitting, complicates the classification of adiabatic potential surfaces of a bound electron. Therefore, we will directly focus on the issue of direct relativistic definition of quasi-molecular terms.

2. Method and results

A-DKB method

In the Born –Oppenheimer approximation, the steady Dirac equation for an electron in a two-center potential has the form:

$$[\alpha\mathbf{p} + \beta + V(\mathbf{r})]\Psi_n(\mathbf{r}) = E_n\Psi_n(\mathbf{r}), \quad (1)$$

where \mathbf{r} — electron radius vector, \mathbf{p} — momentum operator, α and β are Dirac matrices. The two-center potential is given by:

$$V(\mathbf{r}) = V_1(|\mathbf{r} - \mathbf{R}_1|) + V_2(|\mathbf{r} - \mathbf{R}_2|) \\ \equiv -\frac{\alpha Z_1}{|\mathbf{r} - \mathbf{R}_1|} - \frac{\alpha Z_2}{|\mathbf{r} - \mathbf{R}_2|}, \quad (2)$$

where $V_{1,2}(\mathbf{r})$ is a Coulomb potential corresponding to nuclei with charges Z_1, Z_2 at the location of the electron, specified by the radius vector \mathbf{r} . The origin is chosen on the quasi-molecule axis z between two nuclei so that the vectors $\mathbf{R}_{1,2}$ specify the coordinates of the nuclei.

For systems with axial symmetry, the wave function can be written as

$$\Psi(r, \theta, \varphi) = \frac{1}{r} \begin{pmatrix} G_1(r, \theta) e^{i(m_j-1/2)\varphi} \\ G_2(r, \theta) e^{i(m_j+1/2)\varphi} \\ iF_1(r, \theta) e^{i(m_j-1/2)\varphi} \\ iF_2(r, \theta) e^{i(m_j+1/2)\varphi} \end{pmatrix}$$

where m_j — projection onto the axis z of the total angular momentum of the electron j . The components $G_{1,2}(r, \theta)$ and $F_{1,2}(r, \theta)$ of the Dirac function can be represented as an expansion:

$$\phi(r, \theta) \cong \sum_{u=1}^4 \sum_{i_r=1}^{N_r} \sum_{i_\theta=1}^{N_\theta} C_{i_r i_\theta}^u \Lambda B_{i_r}(r) Q_{i_\theta}(\theta) e_u. \quad (4)$$

Here the set $\{B_{i_r}(r)\}_{i_r=1}^{N_r}$ is represented by B -splines, the angle dependence θ is given by the set of Legendre polynomials $\{Q_{i_\theta}(\theta)\}_{i_\theta=1}^{N_\theta}$, $\{e_u\}_{u=1}^4$ — four-component basis

vectors. The matrix Λ imposes the DKB condition on the basis set [25]. Further calculations consist of numerical calculations, for example, in recent works [22,23] an accuracy of 27 – 32 significant figures for the main term was achieved.

To calculate the energy of a bound electron, an approach is used that is completely similar to the nonrelativistic one, i.e. numerical calculations are carried out for a specific fixed internuclear distance in the approximation of infinitely heavy nuclei. It is worth noting that the solution of the two-center Dirac equation automatically takes into account relativistic effects. Meanwhile (even if having achieved outstanding results), non-relativistic methods necessarily include the calculation of the corresponding relativistic corrections in the required order.

In the general case, the molecular energy state of an electron is characterized by the projection of the total angular momentum onto the axis of the molecule. Being a conserved quantity for systems with axial symmetry, such a description leads to degeneracy in sign m_j . For homonuclear systems in which two nuclei are identical, there is an additional quantum number g (gerade) for even states and u (ungerade) for odd states, expressing symmetry with respect to reflection in a plane perpendicular to the axis of the molecule. In addition, a specific energy state of an electron can be considered in the limit of zero internuclear distance, i.e. in the limit of a „united“ atom. Then the „coherent“ nuclear charge is given by the sum of Z_1 and Z_2 and the usual atomic notation for the energy state can be used: nl_j , where n — principal quantum number, l — orbital momentum, and j — total angular momentum of the electron. Thus, the electron molecular term can be determined by the formula $nl_j\lambda_p m_j$ [29], where λ — the projection of the orbital momentum of the electron onto the axis of the molecule, and p denotes the parity of the state when rearranging nuclei (only for homonuclear systems). Similar notation can be introduced by reviewing the limit of infinite internuclear distance, when the electron is localized on only one of the nuclei. In this work we adhere to the notation corresponding to the „united“ atom.

Homonuclear quasi-molecular ion H – p

As part of the A-DKB method, the energies of the homonuclear hydrogen-proton compound, H – p , arise as a result of the numerical solution of the two-center Dirac equation (1), with the expansion of the wave function given, for example, by expression (4). According to the A-DKB method [25,26], the entire Dirac energy spectrum (including the negative and positive continuum) is reproduced as a discrete set of states with a given angular momentum projection, the lowest of which correspond to real discrete quasi-molecular terms. In the nonrelativistic case, the state of the electron in the molecule is determined by the absolute value of the projection of its orbital angular momentum onto the axis of the molecule λ . Taking into account the electron

spin results in a fine splitting of the molecular term into two states $\lambda + 1/2$ and $\lambda - 1/2$ [30].

Further, we will review the adiabatic potential surfaces of the ground and first four excited quasi-molecular states. Since the curves for excited states can intersect each other and (or) be close in energy, states that lie higher should also be reviewed, including states with large projection values m_j . Figure 1 shows adiabatic potential curves obtained by the A-DKB method.

Determining the ground state, $1s_{1/2}\sigma_g$ ($m_j = -1/2$), does not reveal any difficulties. In particular, in the united atom limit, this adiabatic curve transitions to the ground state of an ion with a core consisting of two protons, ${}^2\text{He}^+$. For it, the energy in the nonrelativistic limit is equal to -2 atomic units (hereinafter a.u.). It should be noted that the parity of states with respect to permutation of nuclei can also be calculated within the A-DKB approach, allowing for the identification of terms. However, on the scale of Fig. 1, the curves of different fine sublevels are indistinguishable, and possible intersections or splitting of terms require separate analysis. To do this, let us review the region of small distances, where the quasi-molecular terms are degenerate in the nonrelativistic limit. For states with $n = 2$ in the atomic ion ${}^2\text{He}^+$, Fig. 2 shows the adiabatic surfaces of the first four excited levels depending on the internuclear distance in the region of several thousand Fermi (the region $R \leq 600$ fm is inserted).

According to Fig. 2, the splitting of the state with nonrelativistic energy of the united atom -0.5 a.u. starts from the internuclear distance ≈ 1000 fm. The inset in Fig. 2, corresponding to smaller internuclear distances, shows a fine level splitting. This splitting is well known and arises in the relativistic Dirac theory for a bound atomic state. Numerical calculation results for the states $2p_{1/2}\sigma_u(m_j = -1/2)$, $2s_{1/2}\sigma_g(m_j = -1/2)$,

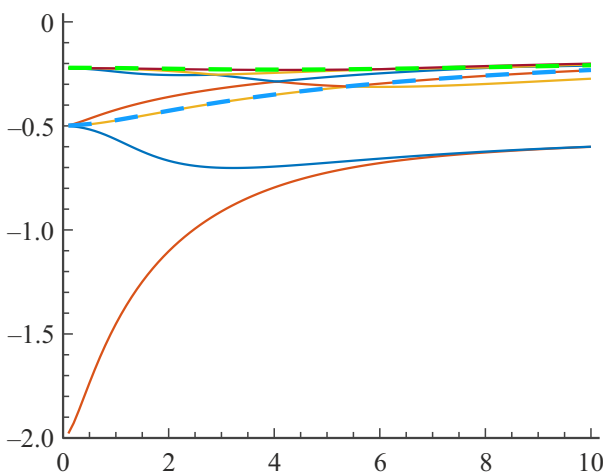


Figure 1. Adiabatic potential surfaces of the quasi-molecular ion H - p for the first seven states with $m_j = -1/2$ (solid lines) and the first two states with $m_j = -3/2$ (dashed lines). Energy is plotted along the ordinate axis, and internuclear distance is plotted along the abscissa axis. All values are given in atomic units.

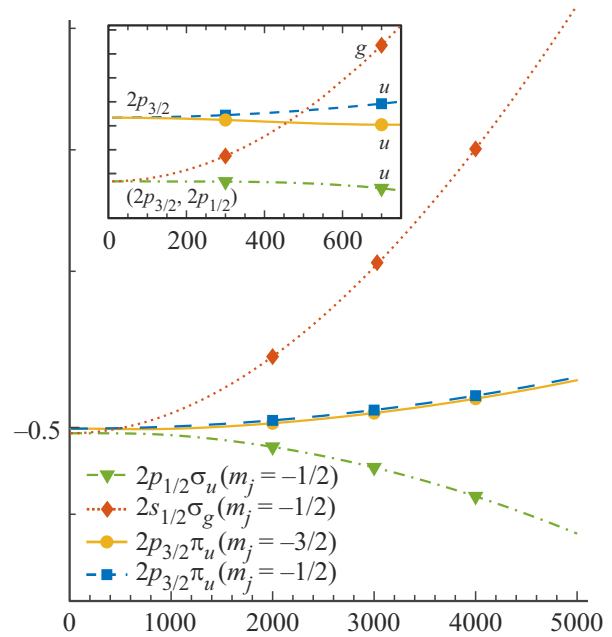


Figure 2. Adiabatic potential surfaces of the first four excited states of the H_2^+ ion in the region of small internuclear distances (fm). Energy is plotted along the ordinate axis, and internuclear distance is plotted along the abscissa axis. The energies are given in atomic units.

$2p_{3/2}\pi_u(m_j = -1/2)$ and $2p_{3/2}\pi_u(m_j = -3/2)$ are given in Table 1. Based on the obtained values and Dirac theory, the corresponding states can be unambiguously identified.

In particular, the states $2s_{1/2}$ and $2p_{1/2}$ are degenerate at $R \rightarrow 0$, their splitting in the lowest order is determined by the effects of quantum electrodynamics (Lamb shift). Then, according to Dirac theory, the upper states are separated by an interval of fine structure and correspond to the atomic level $2p_{3/2}$. The two emerging terms correspond to different projections of the total angular momentum: the upper one is $m_j = -3/2$ and the lower one is $m_j = -1/2$. Both are quasi-molecular π -terms and can therefore be defined as $2p_{3/2}\pi_u(m_j = -3/2)$ for the upper curve and $2p_{3/2}\pi_u(m_j = -1/2)$ for the lower one.

Finally, the inset in Fig. 2 clearly demonstrates the intersection of the quasi-molecular terms $2p_{3/2}\pi_u(m_j = -3/2)$ and $2p_{3/2}\pi_u(m_j = -1/2)$ with one of the terms emanating from $2s_{1/2}$, $2p_{1/2}$, in the vicinity of 450 fm. Meanwhile, it can be assumed that in a more accurate calculation, this intersection could represent a splitting of terms. According to [1.31] the intersection of adiabatic curves is possible only for terms with different symmetries. Symmetry, in particular, is determined by the rearrangement of nuclei. By calculating the corresponding parity of states, the quasi-molecular terms are defined as follows: the curve going up is $2s_{1/2}\sigma_g(m_j = -1/2)$ and the curve going down is $2p_{1/2}\sigma_u(m_j = -1/2)$. Therefore, $R \approx 450$ fm represents the intersection point. The intersections/splitting of terms in Fig. 1 are analyzed similarly for other distances. Thus,

Table 1. Bond energies of the first four excited states in the quasi-molecular ion $H - p$ at small internuclear distances. Energy values are given in a.u., distances are given in fm

State	R, fm		
	10	100	300
$2p_{1/2}\sigma_u(m_j = -1/2)$	-0.500033286	-0.500033287	-0.500033375
$2s_{1/2}\sigma_g(m_j = -1/2)$	-0.500033274	-0.500032098	-0.500022679
$2p_{3/2}\pi_u(m_j = -1/2)$	-0.500006658	-0.500006774	-0.500007638
$2p_{3/2}\pi_u(m_j = -3/2)$	-0.500006655	-0.500006538	-0.500005585

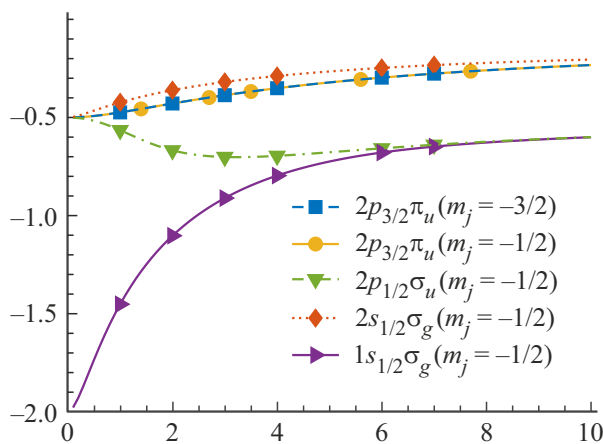


Figure 3. Adiabatic potential curves of the ground and first four excited states of the quasi-molecular ion $H - p$. Energy is plotted along the ordinate axis, and internuclear distance is plotted along the abscissa axis. All values are given in atomic units.

by reviewing the limit of small internuclear distances, it is possible to identify all quasi-molecular terms. The final picture of adiabatic potential surfaces is presented in Fig. 3.

Heteronuclear quasi-molecular ion $He^+ - p$

In this part of the work, a detailed analysis of the classification of quasi-molecular terms is carried out within the framework of a completely relativistic approach using the example of a compound of singly ionized helium with a proton $He^+ - p$. In this case, the picture becomes somewhat different due to the lack of parity of states established by the permutation symmetries of nuclei. Therefore, to determine the intersection or splitting of quasi-molecular terms, we will use the condition of continuity of adiabatic potential surfaces.

As before, the adiabatic potentials of the ground and first excited states in the compound $He^+ - p$ can initially be classified only as sets of states with different projections of the total angular momentum m_j . The diagram of quasi-molecular terms is presented in Fig. 4.

The lower curve in Fig. 4, as before, represents the ground quasi-molecular state of $1s_{1/2}\sigma(m_j = -1/2)$. In the limit of zero internuclear distance (united atom), this term goes into

the ground state of a one-electron ion with a lithium-like nucleus. The following four above curves are degenerate in the limit of zero internuclear distance and represent, in the nonrelativistic approximation, the state of a united atom with $n = 2$, etc. for subsequent states.

To classify the first four excited quasi-molecular terms, we consider the limit of small internuclear distances. The corresponding graph for the $R \in [0, 5000]$ fm distances is presented in Fig. 5, which also shows the $R \leq 600$ fm region.

The numerical values of quasi-molecular energies depending on internuclear distances for the states $2p_{1/2}\sigma(m_j = -1/2)$, $2s_{1/2}\sigma(m_j = -1/2)$, $2p_{3/2}\pi(m_j = -1/2)$ and $2p_{3/2}\pi(m_j = -3/2)$ are given in Table 2. The latter allow to identify the states of the ion in the limit of a united atom. In particular, in the limit $R \rightarrow 0$ the degenerate states $2s_{1/2}$ and $2p_{1/2}$ are visible, which form the terms $2s_{1/2}\sigma(m_j = -1/2)$ and $2p_{1/2}\sigma(m_j = -1/2)$, respectively. The two incumbent states correspond to the united atom state $2p_{3/2}$, which

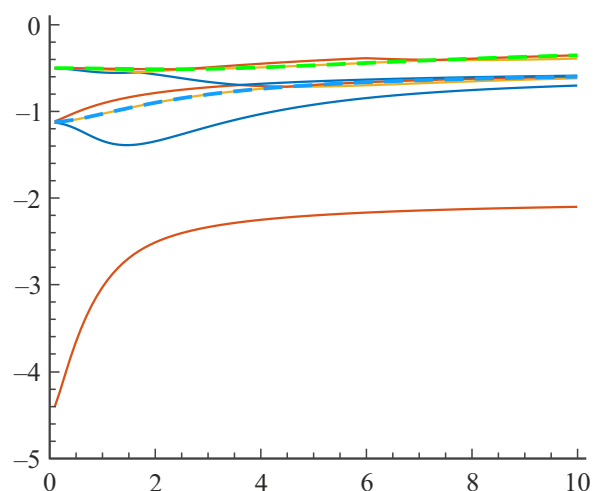
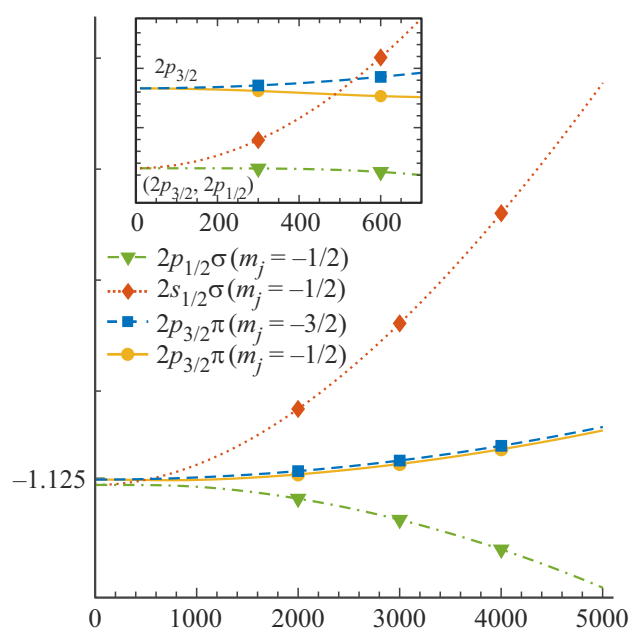


Figure 4. Adiabatic potential curves obtained by numerical calculation using the A-DKB method for the first seven states with $m_j = -1/2$ (solid lines) and the first two states with $m_j = -3/2$ (dashed lines) in the one-electron quasi-molecular ion $He^+ - p$. Energy is plotted along the ordinate axis, and internuclear distance is plotted along the abscissa axis. All values are given in atomic units.

Table 2. Bond energies of the first four excited states in the quasi-molecular ion H - p at small internuclear distances. Energy values are given in atomic units, while internuclear distances are in fm.

State	R, fm		
	10	100	300
$2p_{1/2}\sigma(m_j = -1/2)$	-1.125168533	-1.125168537	-1.125168886
$2s_{1/2}\sigma(m_j = -1/2)$	-1.125168474	-1.125163183	-1.125120996
$2p_{3/2}\pi(m_j = -1/2)$	-1.125033706	-1.125034232	-1.125038165
$2p_{3/2}\pi(m_j = -3/2)$	-1.125033695	-1.125033164	-1.125028878

**Figure 5.** Adiabatic potential surfaces for the first four excited states of the He⁺ - p ion in the region of small internuclear distances. Energy is plotted along the ordinate axis (in atomic units), and internuclear distance is plotted along the abscissa axis (in fm).

splits into two components with $m_j = -1/2$ (lower) and $m_j = -3/2$ (upper).

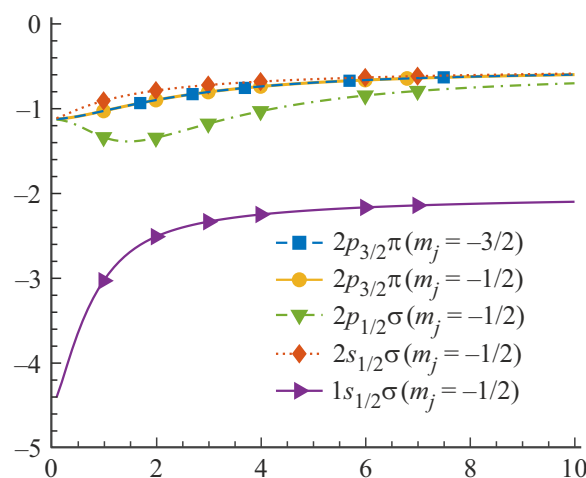
According to the inset in Fig. 5, there is a point at which it is required to determine whether the terms intersect or split. This point, as in the case reviewed in the previous section, is located in the vicinity of 450 fm. We also discovered by corresponding numerical calculations that this point is practically independent of the nuclei charge. In contrast to the case of a homonuclear quasi-molecule, identification of the intersection/splitting of terms in this case can be carried out only using the condition of continuity of adiabatic curves. Therefore, as part of the A-DKB method, tracking the potential minimum of the curve, the first derivative of the adiabatic potentials was numerically calculated. This kind of approach is valid for both hetero- and homonuclear systems, and was also used for the H-p ion. According to the continuity condition, the quasi-molecular terms emerg-

ing from the two lower degenerate states are defined as $2p_{1/2}\sigma(m_j = -1/2)$ and $2s_{1/2}\sigma(m_j = -1/2)$. These states in the united atom limit correspond to the atomic levels $2s_{1/2}$ and $2p_{1/2}$. Further, the state $2p_{3/2}$, separated from them by a fine structure interval in the limit $R \rightarrow 0$, splits into quasi-molecular terms $2p_{3/2}\pi(m_j = -1/2)$ (downward curve) and $2p_{3/2}\pi(m_j = -3/2)$ (upward curve). This kind of picture qualitatively repeats the case of the quasimolecule H - p, reviewed previously.

Carrying out a similar analysis for intersection/splitting points at large internuclear distances, Fig. 4, we obtain the final results for the adiabatic potential curves presented in Fig. 6.

3. Conclusion

In this work, a detailed analysis of adiabatic potential surfaces obtained as part of completely relativistic calculations was carried out. Using the A-DCB method, two examples were considered, the homonuclear quasi-molecular ion H - p and the heteronuclear quasi-molecular ion He⁺ - p. Using numerical calculations, adiabatic potential curves were constructed for the ground state and

**Figure 6.** The adiabatic potential surfaces of the ground and first four excited states of quasi-molecular ion He⁺ - p. Energy is plotted along the ordinate axis, and internuclear distance is plotted along the abscissa axis. All values are given in atomic units.

the first few excited states. Quasi-molecular terms of compounds $H - p$ and $He^+ - p$ are presented in Figs. 1 and 4, correspondingly [32].

Precise identification of terms is required since adiabatic potential curves have obvious intersections. Although the classification of quasi-molecular terms is well represented within the nonrelativistic approach [1,31], additional complexity arises in the fully relativistic picture. This is due to the presence of states that are non-degenerate in Dirac theory and correspond to different total angular momenta of the electron. Identification of quasi-molecular terms in the compounds $H - p$ and $He^+ - p$ was carried out as follows. First, the limit $R \rightarrow 0$ was reviewed, in which the system under study can be described as a united one-electron ion (as an alternative, the limit of infinite internuclear distance can be reviewed). As part of Dirac theory, the corresponding energy states can be unambiguously identified taking into account fine splitting. Then, introducing standard notations for molecular terms, the points of intersection/splitting of adiabatic potential curves were analyzed.

In the case of a homonuclear quasimolecule, intersection/splitting is characterized, in particular, by the parity of states determined by the rearrangement of nuclei in a plane perpendicular to the axis of the molecule. This parity of quasi-molecular terms is calculated as part of the A-DKB approach. However, for heteronuclear compounds this symmetry is absent. Thus, to interpret the intersection/splitting in this kind of systems, for example in $He^+ - p$, we applied the condition of continuity of adiabatic potential surfaces. By tracking the values of the first derivative of an adiabatic curve, it can be determined whether there is an intersection or splitting of terms by finding possible extrema or „jumps“ in the values.

The combination in this work of the analysis of adiabatic curves at small internuclear distances with the study of intersection/splitting points made it possible to determine the main and first four (as an example) excited quasi-molecular terms in both homo- and heteronuclear compounds $H - p$, $He^+ - p$. Corresponding results are shown in Figures 3 and 6. The presented analysis is not limited to one-electron light quasi-molecular ions and can obviously be applied to heavier quasi-molecular compounds.

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Conflict of interest

The authors declare that they have no conflict of interest.

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