Article

One-electron energy spectra of heavy highly charged quasimolecules

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Abstract: The generalized dual-kinetic-balance approach for axially symmetric systems is employed to solve the two-center Dirac problem. The spectra of one-electron homonuclear quasimolecules are calculated and compared with the previous calculations. The analysis of the monopole approximation with two different choices of the origin is performed. Special attention is paid to the lead and xenon dimers, Pb^{82+}–Pb^{82+}–e^- and Xe^{54+}–Xe^{54+}–e^-, where the energies of the ground and several excited σ-states are presented in the wide range of internuclear distances. The developed method provides the quasicomplete finite basis set and allows for construction of the perturbation theory, including within the bound-state QED.

Keywords: Two-center Dirac equation; Quasimolecules; Heavy-ion collisions

1. Introduction

Due to the critical phenomena of the bound-state quantum electrodynamics, such as spontaneous electron-positron pair production, quasimolecular systems emerging in ion-ion or ion-atom collisions attract much interest [1–8]. While collisions of highly charged ions with neutral atoms are presently available for experimental investigations, in particular, at the GSI Helmholtz Center for Heavy Ion Research [9–11], the upcoming experiments at the GSI/FAIR [12], NICA [13], and HIAF [14] facilities will allow observation of the heavy ion-ion (up to U^{92+}–U^{92+}) collisions. The relativistic dynamics of the heavy-ion collisions has been investigated for decades by various methods, see, e.g., Refs. [6–8,15–21] and references therein. Theoretical predictions of the quasimolecular spectra are also in demand for analysis of the experimental data in these collisions.

Within the Bohr-Oppenheimer approximation, the one-electron problem is reduced to the Dirac equation with Coulomb potential of two nuclei at a fixed internuclear distance D. This problem was investigated previously by a number of authors, see, e.g., Refs. [15,20,22–37]. Majority of these works relied on the partial-wave expansion of the two-center potential in the center-of-mass coordinate system. Alternative approaches include, e.g., usage of the Cassini coordinates [33] and the atomic Dirac-Sturm basis-set expansion [35,36]. We consider the method based on the dual-kinetic-balanced finite-basis-set expansion [38] of the electron wave function for the axially symmetric systems [39]. The results for the ground state of uranium dimers with one and two electrons were already presented in Ref. [40]. In this work, we extend the one-electron calculations to the lowest excited σ-states and present the results for the one-electron dimers, Pb^{82+}–Pb^{82+}–e^- and Xe^{54+}–Xe^{54+}–e^-. For the ground state we demonstrate the accuracy of this method for the nuclear charge numbers Z from 1 to 100 at the so-called "chemical" distances, $D = 2/Z$ a.u. We also investigate the difference between the two-center values and those obtained within the monopole approximation.

The relativistic units ($\hbar = 1$, $c = 1$, $m_e = 1$) and the Heaviside charge unit ($\alpha = e^2/(4\pi)$, $e < 0$) are used throughout the paper.

2. Method

In heavy atomic systems the parameter αZ (α is the fine-structure constant and Z is the nuclear charge), which measures the coupling of electrons with nuclei, is not small. Therefore, the calculations for these systems should be done within the fully relativistic approach, i.e., to all orders in αZ. With this in mind, we start with the Dirac equation for the two-center potential,

$$\left[\vec{\alpha} \cdot \vec{p} + \beta + V(\vec{r})\right] \Psi_n(\vec{r}) = E_n \Psi_n(\vec{r}), \tag{1}$$

$$V(\vec{r}) = V_{\text{nucl}}^{\text{A}}(|\vec{r} - \vec{R}_1|) + V_{\text{nucl}}^{\text{B}}(|\vec{r} - \vec{R}_2|). \tag{2}$$

Here $\vec{r}$ and $\vec{R}_{1,2}$ are the coordinates of the electron and nuclei, respectively, $V_{\text{nucl}}^{\text{A,B}}(r)$ is the nuclear potential at the distance r generated by nucleus with the charge $Z_{\text{A,B}}$, $\vec{\alpha}$ and β are the standard 4×4 Dirac matrices:

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \tag{3}$$

where $\vec{\sigma}$ is a vector of the Pauli matrices.

In the following we consider the identical nuclei, i.e. $Z_{\text{A}} = Z_{\text{B}}$, with the Fermi model of the nuclear charge distribution:

$$V_{\text{nucl}}(r) = -4\pi\alpha Z \int_0^\infty \frac{\rho(r')}{\max(r, r')} r'^2 \, dr', \qquad \rho(r) = \frac{\rho_0}{1 + \exp{(r - c)/a}}, \tag{4}$$

where ρ_0 is the normalization constant, a is skin thickness constant and c is the half-density radius, for more details see, e.g., Ref. [41].

The solution of Eq. (1) is obtained within the dual-kinetic-balance (DKB) approach, which allows one to solve the problem of "spurious" states. Originally, this approach was implemented for spherically symmetric systems, like atoms, [38], using the finite basis set constructed from the B-splines [42,43]. Later, authors of Ref. [39] generalized it to the case of axially symmetric systems (A-DKB) — they considered atom in the external homogeneous field. This situation was also considered within this method in Refs. [44–46] to evaluate the higher-order contributions to the Zeeman splitting in highly charged ions. In Ref. [40] we have adapted the A-DKB method to diatomic systems, which also possess axial symmetry. Below we provide a brief description of the calculation scheme.

The system under consideration is rotationally invariant with respect to the z-axis directed along the internuclear vector $\vec{D} = \vec{R}_2 - \vec{R}_1$. Therefore, the z-projection of the total angular momentum with the quantum number m_J is conserved and the electronic wave function can be written as,

$$\Psi(r, \theta, \varphi) = \frac{1}{r} \begin{pmatrix} G_1(r, \theta)e^{i(m_J - \frac{1}{2})\varphi} \\ G_2(r, \theta)e^{i(m_J + \frac{1}{2})\varphi} \\ iF_1(r, \theta)e^{i(m_J - \frac{1}{2})\varphi} \\ iF_2(r, \theta)e^{i(m_J + \frac{1}{2})\varphi} \end{pmatrix}. \tag{5}$$

The (r, θ)-components of the wave function are represented using the finite-basis-set expansion:

$$\Phi(r, \theta) = \frac{1}{r} \begin{pmatrix} G_1(r, \theta) \\ G_2(r, \theta) \\ F_1(r, \theta) \\ F_2(r, \theta) \end{pmatrix} \cong \sum_{u=1}^{4} \sum_{i_r=1}^{N_r} \sum_{i_\theta=1}^{N_\theta} C_{i_r, i_\theta}^u \Lambda B_{i_r}(r) Q_{i_\theta}(\theta) e_u, \tag{6}$$

where $\left\{B_{i_r}(r)\right\}_{i_r=1}^{N_r}$ are B-splines, $\left\{Q_{i_\theta}\right\}_{i_\theta=1}^{N_\theta}$ are Legendre polynomials of the argument $2\theta/\pi - 1$, and $\left\{e_u\right\}_{u=1}^4$ are the standard four-component basis vectors:

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{7}$$

The Λ-matrix

$$\Lambda = \begin{pmatrix} I & -\frac{1}{2}D_{m_J} \\ -\frac{1}{2}D_{m_J} & I \end{pmatrix}, \tag{8}$$

$$D_{m_J} = (\sigma_z \cos\theta + \sigma_x \sin\theta)\left(\frac{\partial}{\partial r} - \frac{1}{r}\right)$$

$$+ \frac{1}{r}(\sigma_x \cos\theta - \sigma_z \sin\theta)\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\left(im_J\sigma_y + \frac{1}{2}\sigma_x\right), \tag{9}$$

imposes the dual-kinetic-balance conditions on the basis set. With the given form of Φ and the finite basis set one can find the corresponding Hamiltonian matrix H_{ij}. The eigenvalues and eigenfunctions are found by diagonalization of H_{ij}. As a result, we obtain quasicomplete finite set of wave functions and electronic energies for the two-center Dirac equation. Ground and several lowest excited states are reproduced with high accuracy while the higher-excited states effectively represent the infinite remainder of the spectrum. The negative-energy continuum is also represented by the finite number of the negative energy eigenvalues. This quasicomplete spectrum can be used to construct the Green function, which is needed for the perturbation theory calculations.

3. Results

Relativistic calculations of the binding energies of heavy one-electron quasimolecules were presented, in particular, in Refs. [20,28,31,33,35,36], see also references therein. Ref. [36] provides nearly the most accurate up-to-date values for the very broad range of Z and taking into account the finite nuclear size. So, we use just these data for comparison, see Table 1, where the ground-state energies are presented for $Z = 1 \ldots 100$ at the so-called "chemical" distances, $D = 2/Z$ a.u. We observe that the results are in good agreement, the relative deviation varies from 2×10^{-6} for hydrogen to 5×10^{-5} for $Z = 100$. This deviation is consistent with our own estimation of the numerical uncertainty, which is evaluated by inspecting the convergence of the results with respect to the size of the basis set. In this calculation up to $N_r = 320$ B-splines and $N_\theta = 54$ Legendre polynomials are used, for heavy nuclei this number of basis functions ensures the uncertainty, which is comparable to or smaller than the uncertainty of the finite nuclear size effect at all internuclear distances from 0 to $2/Z$ a.u.

Next, we present the obtained one-electron spectra of the Pb^{82+}–Pb^{82+}–e^- and Xe^{54+}–Xe^{54+}–e^- quasimolecules in the wide range of the internuclear distances from few tens of fermi up to the "chemical" distances. In the present figures only σ-states ($m_J = \pm\frac{1}{2}$) are shown. The precise quantum numbers are m_J and parity, g (*gerade*) or u (*ungerade*). In addition, we determine the quantum numbers of the "merged atom", i.e. the state of the system with internuclear distance $D \to 0$, and put it to the left of molecular term symbol, e.g., the ground state is $1s_{1/2}\sigma_g$.

In Figure 1, the energies of the ground ($n = 1$) and first 9 ($n = 2\ldots10$) excited states of Pb^{82+}–Pb^{82+}–e^- system as the functions of the internuclear distance are shown. Here, n has no connection with atomic principal quantum number, it simply enumerates the σ-states. To visually compare the data obtained with the ones by Soff *et al.* we zoom the second plot in Fig. 1 to match the scale of the corresponding figure from Ref. [15]. Although we cannot compare the numerical results, the plots for all the states under consideration appear to be in very good agreement — all the states are

Table 1. Comparison of the ground-state energies (in a.u.) of one-electron quasimolecular systems with $Z = 1 \ldots 100$ at the internuclear distance $D = 2/Z$ a.u.

Z	This work	Dirac-Sturm [36]
1	-1.1026433	-1.102641581032
2	-4.4106607	-4.410654714140
10	-110.33722	-110.3371741499
20	-442.23969	-442.2392996469
30	-998.4194	-998.4214646525
40	-1783.5479	-1783.563450815
50	-2804.5304	-2804.571434254
60	-4070.971	-4071.036267926
70	-5595.889	-5595.926978290
80	-7397.003	-7397.028800116
90	-9498.452	-9498.588788490
92	-9957.567	-9957.775519122
100	-11935.89	-11936.41770218
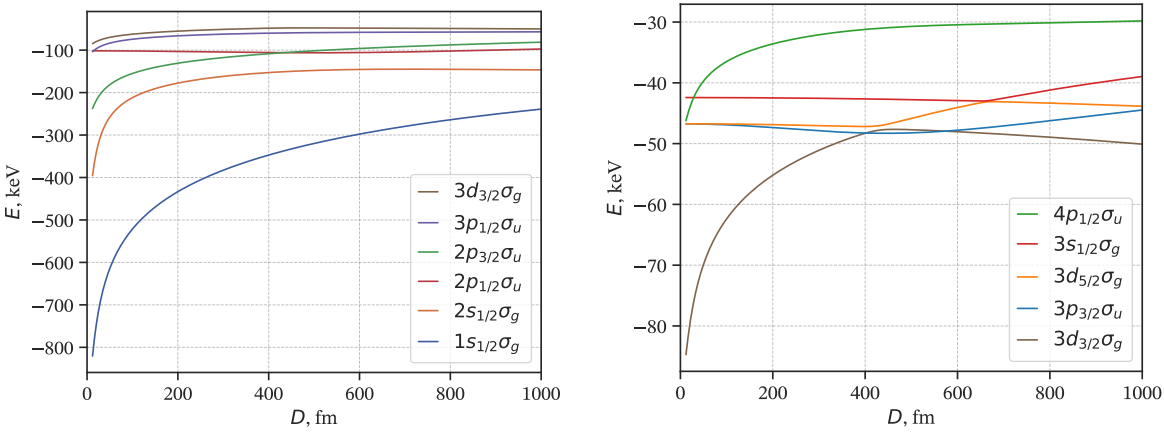
(a) Energies of states with $n = 1 \ldots 6$.

(b) Energies of states with $n = 6 \ldots 10$.

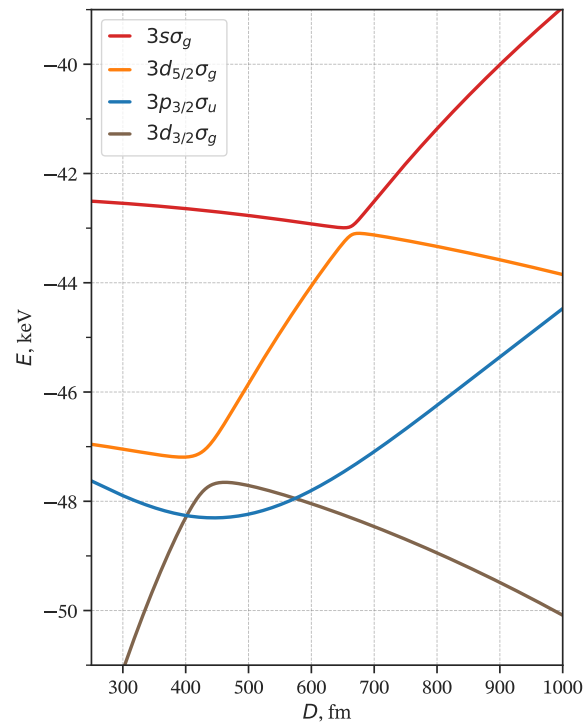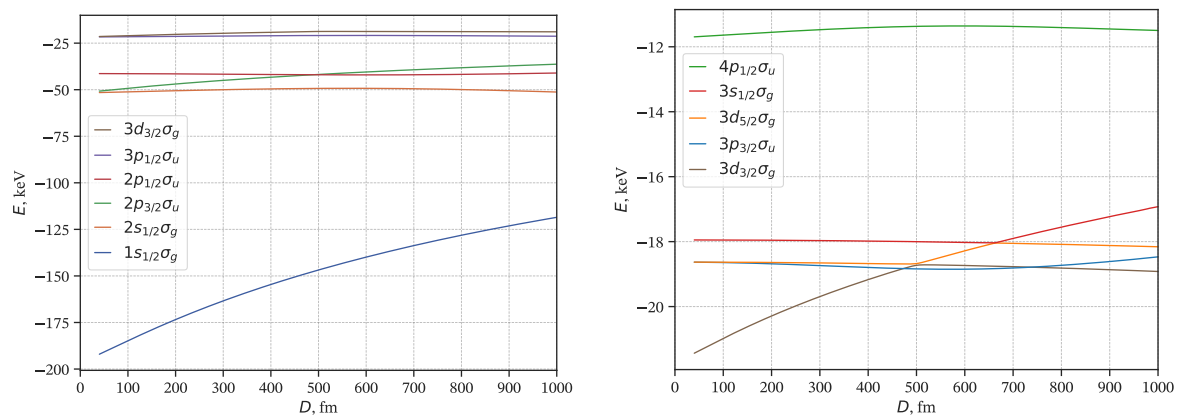**Figure 1.** Electronic terms of the one-electron Pb^{82+}–Pb^{82+} quasimolecule.

Figure 2. Electronic terms of the one-electron Pb^{82+}–Pb^{82+} quasimolecule. Energies of states with $n = 6 \ldots 9$ (scaled).

identified correctly, all the crossings and avoided crossings appear at the same internuclear distances. The similar results for xenon, i.e., the energies of the ground ($n = 1$) and first 9 ($n = 2 \ldots 10$) excited states of Xe^{54+}–Xe^{54+}–e^- system are shown in Figure 3.

Also, in Tables 2 and 3, we compare the ground-state binding energies obtained within our approach for the two-center (TC) potential with those for the widely used monopole approximation (MA), where only the spherically symmetric part of the two-center potential is considered. Within MA the potential and all the results depend on where to place the origin of the coordinate system (c.s.). At the same time, for the TC potential the results should be identical within the numerical error bars. We compare two different placements of the c.s. origin: (1) at the center of mass of the nuclei, (2) at the center of one of the nuclei, see Figure 4. The agreement between TC(1) and TC(2) within the anticipated numerical uncertainty serves as a non-trivial self-test of the method, since the basis-set expansion (6)

(a) Energies of states with $n = 1 \ldots 6$.   **(b)** Energies of states with $n = 6 \ldots 10$.
Figure 3. Electronic terms of the one-electron Xe^{54+}–Xe^{54+} quasimolecule.
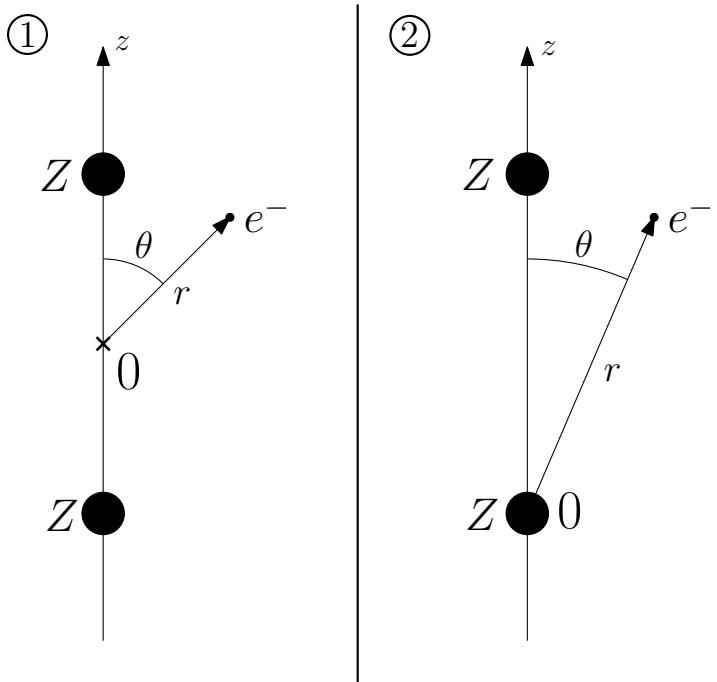
Figure 4. Two different coordinate systems considered. Left: (1) origin is at the center-of-mass of the system, right: (2) origin is at the center of one of the nuclei.

is essentially different for the two cases. In fact, due to the lower symmetry of the second c.s., the uncertainty of the TC(2) values is much larger and completely determines the difference between TC(1) and TC(2). The differences between the TC(1) and MA(1) results are presented in the second-to-last column, they can be interpreted as inaccuracy of the MA. In the last column, the differences between the MA(1) and MA(2) results are given, a kind of "inherent inconsistency" of the MA. As one can see from these data, except for the regions where MA(1) − MA(2) is anomaly small due to the sign change, it is comparable to TC(1) − MA(1). This observation can be used to quantify the inaccuracy of the MA for the contributions, which are not yet available for the TC calculations, e.g., the two-photon-exchange and QED corrections [40].

Table 2. Ground-state binding energy $E_{1\sigma_g}$ (in eV) of the Pb^{82+}–Pb^{82+}–e^- quasimolecule for the two-center potential (TC) and for the monopole-approximation potential (MA), with coordinate system origin at the center of mass of the nuclei (1) and at the one of the nuclear centers (2).

D, fm	TC(1)	TC(2)	MA(1)	MA(2)	TC(1) − MA(1)	MA(1) − MA(2)
40	−646254	−646254	−637032	−598564	−9222	−38468
50	−614504	−614504	−604643	−568188	−9861	−36455
80	−550575	−550575	−539861	−506742	−10714	−33119
100	−521373	−521373	−510350	−478423	−11023	−31927
200	−433348	−433347	−421146	−392345	−12202	−28801
250	−405450	−405450	−392687	−365185	−12763	−27502
500	−319773	−319769	−304337	−283510	−15436	−20827
$1/Z$ [a.u.] $\simeq$ 645	−289068	−289067	−272212	−255389	−16856	−16823
700	−279462	−279464	−262095	−246756	−17367	−15339
1000	−238887	−238873	−218905	−211937	−19982	−6968
$2/Z$ [a.u.] $\simeq$ 1291	−212020	−212003	−189652	−190174	−22368	522

Table 3. Ground-state binding energy $E_{1\sigma_g}$ (in eV) of the Xe^{54+}–Xe^{54+}–e^- quasimolecule. The notations are the same as in Table 2.

D, fm	TC(1)	TC(2)	MA(1)	MA(2)	TC(1) $-$ MA(1)	MA(1) $-$ MA(2)
40	-192031	-192031	-191860	-190033	-171	-1827
50	-190845	-190845	-190607	-188314	-238	-2293
80	-187217	-187216	-186775	-183199	-442	-3576
100	-184805	-184805	-184228	-179895	-577	-4333
200	-173425	-173425	-172190	-165031	-1235	-7159
250	-168242	-168242	-166695	-158621	-1547	-8074
500	-146803	-146802	-143860	-133919	-2943	-9941
700	-133710	-133710	-129828	-120118	-3882	-9710
$1/Z$ [a.u.] $\simeq 980$	-119414	-119413	-114421	-105971	-4993	-8450
1000	-118529	-118528	-113464	-105233	-5065	-8231
$2/Z$ [a.u.] $\simeq 1960$	-89269	-89276	-81433	-79488	-7836	-1945

4. Discussion

In this work, the two-center Dirac equation is solved within the dual-kinetic-balance method [38, 39]. The energies of the ground and several excited σ-states in such heavy diatomic systems as Pb^{82+}–Pb^{82+}–e^- and Xe^{54+}–Xe^{54+}–e^- are plotted as a function of the internuclear distance D. The ground-state energies at the "chemical" distances ($D = 2/Z$ a.u.) are presented for one-electron dimers with $Z = 1 \ldots 100$. Obtained data are compared with the available previous calculations and a good agreement is observed. The comparison of the results for different origin placement of the coordinate system is used as a self-test of the method. The values obtained within the monopole approximation are also presented. It is shown that their dependence on the origin placement can serve to estimate the deviation from the two-center results.

The developed method, in addition to the energies and wave functions of the ground and lowest excited states, provides the quasicomplete finite spectrum. The Green function computed on the basis of this spectrum gives an access, in particular, to evaluation of the Feynman diagrams within the bound-state QED.

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

QED   Quantum Electrodynamics
PT   Perturbation Theory

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