A coupled channel study on a binding mechanism of positronic alkali atoms

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Abstract. In order to investigate the binding mechanism of weakly bound states of positronic alkali atoms, we calculate the energies and wavefunctions using the Gaussian expansion method (GEM) where a positronium (Ps)–alkali ion channel and a positron–alkali atom channel are explicitly introduced. The energies of the bound states are updated using a model potential that reproduces well the observed energy levels of alkali atoms. The binding mechanism of the positronic alkali atom is analyzed by the wavefunctions obtained. The structure of the positronic alkali atom has been regarded as a Ps cluster orbiting the alkali ion, which is described by the Ps–alkali ion channel. We point out that the fraction having the positron–alkali atom configuration is small but plays an indispensable role for the weakly bound system.

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1. Introduction

A positron ($e^+$) is the antiparticle of an electron ($e^-$), having the same mass as the electron and equal but opposite charge. A positron and an electron form a positronium (Ps) which is a hydrogen-like bound state. In matter, a positron touches atoms and annihilates with one of the electrons mainly emitting two $\gamma$-rays in opposite directions. The features of these $\gamma$-rays have been used for analysing the various properties of the material and positron emission tomography (PET). Recently, it has been pointed out that a temporal binding of a positron to a molecule may influence the resolution of positron spectroscopy \[1\]. A similar effect was predicted in the profile of the $\gamma$-ray which depended on the electronic states of the atom \[2\]. It has been found that some atoms can bind a positron and those bound states are located just below the Ps threshold \[3\]. The first calculations demonstrated the stability of a positronic lithium atom ($e^+\text{Li}$) \[4, 5\]. Subsequently, it was predicted that a positronic sodium atom ($e^+\text{Na}$) also had a bound state, but no bound state was found in positronic potassium and rubidium atoms \[6–8\]. Since the positronic alkali atom is relatively simple, calculations based on few-body theories have been performed for the systems with various methods: a stochastic variational method (SVM) by Ryzhikh and Mitroy \[4\], a fixed-core stochastic variational method (FCSVM) by Mitroy and Ryzhikh \[9\], hyper-spherical close-coupling (HSCC) by Le et al \[10\] and a finite element method (FEM) by Shertzer and Ward \[11\]. Since ionization potentials (IP) of alkali atoms (A) are smaller than the Ps(1s) binding energy (6.8 eV), the valence electrons are transferred to the positron, forming a Ps cluster. It has been believed that the residual ion core (A$^+$) binds the Ps by a polarization of the Ps. The positronic alkali atom evolves into an A$^+$–Ps configuration as a decrease of IP and binding energies of the positronic alkali atom positively correlates with the IP \[8\]. Thus, the inter-particle correlation between the ion core and positron and that between the ion core and valence electron are key points for the investigation of the binding mechanism of the positronic atom. Since a three-body model consisting of a positron, a valence electron and a residual ion core is a good approximation for the positronic alkali atom \[7\], the mechanism can be investigated in detail by a high-precision three-body calculation. In addition, the positronic alkali atom is suited for studying the correlation, because the effective charge of the ion core is the same as the positron charge and the ratio of the interaction between the electron and positron to that between the electron and ion core is relatively larger than other positronic atoms. In the present paper, we perform a coupled channel calculation for positronic alkali atoms using a model potential that reproduces well the observed energy levels of the alkali atoms, and we discuss the binding mechanism of the positronic alkali atom from a view of the correlation. Atomic units (au; $m_e = \hbar = e = 1$) are used throughout this paper except where mentioned otherwise.

2. Theory

We employ a Gaussian expansion method (GEM) which has been applied to a variety of few-body systems (see \[12\] and references therein). In the following, we briefly review the GEM by applying it to the three-body system. In order to directly take the inter-particle correlations into account, we introduce two sets of coordinates ($r_{ep}, R$) and ($r_e, r_p$) of rearrangement channels ($c = 1$ and 2) illustrated in figure 1. The first channel ($c = 1$) is suited to describing the configuration of A$^+$–Ps (Ps channel). The second channel ($c = 2$) is suited to describing the configuration of A–e$^+$ (alkali atom channel). Here, we consider the positronic alkali atom to
be in the S-state. A total three-body wavefunction $\Psi_0$ is described as a sum of the channel wavefunctions of the two arrangement channels

$$\Psi_0 = \Phi_0^1(r_{cp}, R) + \Phi_0^2(r_e, r_p).$$

(1)

Each channel wavefunction is expanded in terms of Gaussian basis functions,

$$\Phi_0^c(x_c, y_c) = \sum_{n_c,N_l} A_{n_c,N_l}^c x_c^{l_c} y_c^{l_c} \exp(-\mu_{n_c} x_c^2 - \nu_{N_l} y_c^2) P_l(\cos \hat{x}_c \cdot \hat{y}_c),$$

(2)

where $(x_1, y_1) = (r_{ep}, R)$ and $(x_2, y_2) = (r_e, r_p)$. The Gauss range parameters $\mu_{n_c}$ and $\nu_{N_l}$ are given according to a geometrical progression to describe both short-range correlation and long-range tail behavior. Internal angular momentum $l_c$ is restricted to $0 \leq l_c \leq l_{max}$. Eigenenergies and coefficients $A_{n_c,N_l}^c$ are determined by the Rayleigh–Ritz variational principle. Correlation functions are calculated to discuss the binding mechanism, and are given by

$$C_{ep}(r) = \int \Psi_0^* \delta(r - r_{ep}) \Psi_0 d\hat{r} dr_{ep} dR,$$

(3)

$$C_e(r) = \int \Psi_0^* \delta(r - r_e) \Psi_0 d\hat{r} dr_e dr_p,$$

(4)

and

$$C_p(r) = \int \Psi_0^* \delta(r - r_p) \Psi_0 d\hat{r} dr_p dr_e.$$  

(5)

Probabilities of finding the $nl$ state of the Ps and alkali atom in the three-body wavefunction are given by

$$P_{nl}^{(Ps)} = \int |\langle \Psi_0 | \phi_{nl}^{Ps}(r_{ep}) \rangle_{r_{ep}}|^2 dR$$

(6)

and

$$P_{nl}^{(A)} = \int |\langle \Psi_0 | \phi_{nl}^{A}(r_e) \rangle_{r_e}|^2 dr_p,$$

(7)

where $\phi_{nl}^{Ps}(r_{ep})$ and $\phi_{nl}^{A}(r_e)$ are two-body wavefunctions of the $nl$ state of the Ps and alkali atom, respectively.

The three-body Hamiltonian is given as

$$H = -\frac{1}{2} \nabla_r^2 - \frac{1}{2} \nabla_{r_p}^2 + V_e(r_e) + V_p(r_p) - \frac{1}{r_{ep}} + V_{2pol}(r_e, r_p) + \lambda \sum_i |\phi_i^{core}\rangle \langle \phi_i^{core}|.$$

(8)
where \( V_e \) is a model potential between the ion core and valence electron, \( V_p \) a model potential between the ion core and positron, and \( V_{2\text{pol}} \) a two-body correction to the polarization potentials for the electron and positron. The last term of the Hamiltonian is an orthogonalizing pseudo-potential. By introducing the two-body polarization potential and the orthogonalizing pseudo-potential, the three-body approximation was ensured in the positronic lithium atom system \[7\].

The model potential between the ion core and valence electron is written as
\[
V_e(r_e) = V_{st}(r_e) + V_{\text{exc}}(r_e) + V_{\text{pol}}(r_e),
\]
where \( V_{st}(r_e) \) is a static potential given by a standard Hartree potential \[13, 14\], \( V_{\text{exc}}(r_e) \) a local exchange potential and \( V_{\text{pol}}(r_e) \) a polarization potential. The polarization potential \( V_{\text{pol}}(r_e) \) is written as
\[
V_{\text{pol}}(r_e) = -\frac{\alpha_d}{2r_e^4} \left[ 1 - \exp \left\{ -\left(\frac{r_e}{r_c}\right)^6 \right\} \right],
\]
where \( \alpha_d \) and \( r_c \) are a dipole polarizability and a cut-off radius, respectively. In the present calculation, we adopt a model potential produced by Albright \textit{et al} \[15\]. The exchange potential is given by Furness and McCarthy \[16\] and is written as
\[
V_{\text{exc}}(r_e) = -\frac{1}{2} \left\{ [(E - V_{st}(r_e))^2 + 4\pi\rho_e(r_e)]^{1/2} - (E - V_{st}(r_e)) \right\},
\]
where \( \rho_e(r_e) \) is the electron density in the core, and the energy \( E = 0 \) is chosen to ensure orthogonal orbitals. Here, the dipole polarizability and cut-off radius are determined to reproduce the observed energy levels of alkali atoms. Using a computer program \[17\] for the model potential \[15\], we optimize the parameters for a Li atom; \( \alpha_d = 0.531 \text{ au} \), \( r_c = 1.645 \text{ au} \) and those for an Na atom; \( \alpha_d = 1.369 \text{ au} \), \( r_c = 1.941 \text{ au} \). The model potentials used in the literature calculations \[7, 9–11\] also consisted of these three potentials appearing in equation (9). However, simple analytical functions with adjustable parameters were used for the exchange potential in \[7, 9, 10\], and were used for the static and exchange potential in \[11\]. The adjustable parameters and the cut-off radius were determined to reproduce the observed energy levels of the alkali atoms. The calculated energy levels of the alkali atoms are listed in table 1 together with other calculations and experimental values. The model potential \[15\] reproduces the experimental value better than other potentials which were used for calculations of the positronic alkali atoms \[9–11\].

According to the literature calculations \[7, 9, 10\], the model potential between the ion core and positron is given by
\[
V_p(r_p) = -V_{st}(r_p) + V_{\text{pol}}(r_p).
\]
Generally, the polarization parameters concerning the positron are not always the same as those for the electron. Uncertainty of the polarization parameters concerning the positron hardly affects the binding energies of the positronic alkali atom as will be discussed later.

The two-body polarization potential \( V_{2\text{pol}}(r_e, r_p) \) \[19\] corrects a net polarization of the ion core, and is given by
\[
V_{2\text{pol}}(r_e, r_p) = 2\hat{r}_e \cdot \hat{r}_p \sqrt{V_{\text{pol}}(r_e)V_{\text{pol}}(r_p)}.
\]
Table 1. Energy levels of Li and Na atoms calculated with various model potentials. The experimental values are taken from the NIST Atomic Spectra Database [18].

| System | State | Present | Ryzhikh *et al* | Peach *et al* | Experiment |
|--------|-------|---------|-----------------|--------------|------------|
| Li     | 2s    | −0.198 136 | −0.198 121 | −0.197 952 | −0.198 140 |
|        | 3s    | −0.074 173 | −0.074 166 | −0.074 181 |            |
|        | 4s    | −0.038 613 |            | −0.038 614 |            |
|        | 5s    | −0.023 636 |            | −0.023 636 |            |
|        | 6s    | −0.015 945 |            | −0.015 944 |            |
| Na     | 3s    | −0.188 859 | −0.188 401 | −0.188 857 |            |
|        | 4s    | −0.071 586 | −0.071 456 | −0.071 578 |            |
|        | 5s    | −0.037 588 |            | −0.037 585 |            |
|        | 6s    | −0.023 134 |            | −0.023 132 |            |
|        | 7s    | −0.015 664 |            | −0.015 663 |            |

The net polarization is weakened when the positron and electron are on the same side of the core. The net polarization has an asymptotic form

$$V_{\text{net-pol}}(r_e, r_p) = V_{\text{pol}}(r_e) + V_{\text{pol}}(r_p) + V_{2\text{pol}}(r_e, r_p)$$

$$\sim -\frac{\alpha_d}{2} \left( \frac{\hat{r}_e}{r_e^2} - \frac{\hat{r}_p}{r_p^2} \right)^2$$

(14)

for $r_e$ and $r_p$ both large. This is consistent with the result obtained from a simple classical argument.

In order to avoid pseudo-states where the valence electron occupies core orbitals, the last term is added to the Hamiltonian. Here, the sum runs over all core orbitals, and the parameter $\lambda$ is a large and positive constant. With an increase in $\lambda$, energies of the pseudo-states become large and out of consideration for sufficiently large values of $\lambda$ [20]. In the present calculation, pseudo-states disappear when $\lambda$ is larger than $10^3$. The binding energies are stable from $\lambda = 10^3$ to $10^5$.

3. Results and discussion

We optimize the Gaussian range parameters, and examine convergence of the energies against the number of Gaussian basis functions and the $l_{\text{max}}$. The convergence against the number of basis functions is shown in figure 2, and we have obtained a seven-digit accuracy. As for the $l_{\text{max}}$, energies rapidly converged. Within this accuracy, the converged energies do not change for both $l_{\text{max}} = 3$ and 4.

Energies, expectation values of inter-particle distance and $2\gamma$ annihilation rate for positronic alkali atoms are shown in table 2 together with recent calculations. The bound states are located just below the $\text{Ps}(1s) + \text{A}^+$ threshold energy ($-0.25$ au). The model potential of Ryzhikh *et al* [7] was used in the calculations of the FCSVM [9] and HSCC [10], and the model potential of Peach *et al* [21] was used in the calculation of the FEM [11]. By subtracting the threshold energy, there are large discrepancies between the present results and others.
Figure 2. Convergence of the energies of bound states as a function of the number of basis functions for (a) \(e^+\text{Li}\) and (b) \(e^+\text{Na}\).

Table 2. Energies, expectation value of inter-particle distance \(\langle r_p \rangle\), \(\langle r_e \rangle\), \(\langle r_{ep} \rangle\) and \(2\gamma\) annihilation rate \(\Gamma\) for the bound state of positronic alkali atoms. Values with an asterisk are the present calculation (GEM) with the Peach model potential \([21]\). \(\Gamma\) is given in units of \(10^9\) s\(^{-1}\).

| System   | Method               | Energy  | \(\langle r_p \rangle\) | \(\langle r_e \rangle\) | \(\langle r_{ep} \rangle\) | \(\Gamma\) |
|----------|----------------------|---------|--------------------------|------------------------|--------------------------|----------|
| \(e^+\text{Li}\) | The present GEM       | -0.252615 | 9.824                     | 8.950                  | 3.404                    | 1.747    |
|          | FCSVM [9]            | -0.252477 | 9.966                     | 9.108                  | 3.397                    | 1.749    |
|          | HSCC [10]            | -0.25247 |                           |                        |                          |          |
|          | FEM [11]             | -0.252371 | 9.87(10)                  | 9.01(10)               | 3.40(5)                  |          |
|          | The present GEM      | -0.252391* | 10.744*                  | 9.226*                 | 3.391*                   |          |
| \(e^+\text{Na}\) | The present GEM       | -0.250401 | 18.25                     | 17.87                  | 3.152                    | 1.914    |
|          | FCSVM [9]            | -0.250473 | 17.25                     | 16.82                  | 3.162                    | 1.896    |
|          | HSCC [10]            | -0.250453 |                           |                        |                          |          |

other hand, our calculated value with the Peach model potential is quite close to that of the FEM. Since our calculation is based on the variational principle and the value is slightly lower than that of the FEM, our result is more accurate than that of the FEM. Therefore, discrepancies in binding energies are ascribed to the choice of model potentials.

Expectation values \(\langle r_e \rangle\) and \(\langle r_p \rangle\) of \(e^+\text{Na}\) are about two times larger than those of \(e^+\text{Li}\), but \(\langle r_{ep} \rangle\) of \(e^+\text{Na}\) is 7.4\% smaller than that of \(e^+\text{Li}\). The \(\langle r_{ep} \rangle\)s are much smaller than \(\langle r_e \rangle\) and \(\langle r_p \rangle\), and are somewhat larger than that of the 1s state of Ps, where \(\langle \phi^\text{Ps}_{1s}(r)|r|\phi^\text{Ps}_{1s}(r) \rangle = 3\) au. The \(\langle r_{ep} \rangle\) and \(2\gamma\) annihilation rate \(\Gamma\) are close to those of other calculations, but the \(\langle r_p \rangle\) and \(\langle r_e \rangle\) are different from other calculations. Since the bonding between the Ps cluster and ion core is very weak and the potential is long-range, the \(\langle r_p \rangle\) and \(\langle r_e \rangle\) widely change with the binding energy. Using a model potential calculated by the same computer program \([17]\), both \(e^+\text{K}\) and \(e^+\text{Rb}\) do not have a bound state. Geometries of the bound states suggest that a Ps cluster forms far from the ion core. Therefore, the first channel (Ps channel) is enough to describe the wavefunction of the bound state in equation (1), but we cannot reproduce the bound state without the second channel even if we use the maximum angular momentum \(l_{\text{max}} = 8\).
Figure 3. Correlation functions $C_{ep}(r)$ for the bound state of (a) $e^+\text{Li}$ and (b) $e^+\text{Na}$. Full curves are $C_{ep}(r)$ and broken curves the squared wavefunction of the Ps(1s) scaled with the probability $P_{1s}^{(Ps)}$ given in table 3.

Table 3. Probability of finding the ground and excited states of the Ps and alkali atom in the three-body wavefunction.

| System | $P_{1s}^{(Ps)}$ | $P_{2p}^{(Ps)}$ | $P_{2s}^{(A)}$ | $P_{2p}^{(A)}$ | $P_{3s}^{(A)}$ | $P_{3p}^{(A)}$ |
|--------|----------------|----------------|----------------|----------------|----------------|----------------|
| $e^+\text{Li}$ | 0.871         | 0.098          | 0.138          | 0.091          |                |                |
| $e^+\text{Na}$ | 0.953         | 0.038          | 0.138          | 0.091          | 0.040          | 0.037          |

(We have obtained good convergence with $l_{\text{max}} = 4$ mentioned above.) Thus, the second channel (alkali atom channel) which describes the configuration of $A-e^+$ is also necessary for the weakly bound state. Moreover, the geometries of the three-body system suggest that the net polarization potential would effectively cancel each other for the Ps cluster. Therefore, the uncertainty of the polarization parameters concerned with the positron would not affect the binding energy. If we change the cut-off parameter by 10% for example (to reproduce the energy levels of the alkali atom, the polarizability parameter is changed simultaneously), the change in the binding energy is less than 0.00001 au.

In figure 3, correlation functions $C_{ep}(r)$ for the $e^+\text{Li}$ and $e^+\text{Na}$ are shown. The correlation functions are in proportion to the squared wavefunction of the 1s state of Ps, but deviate from the squared wavefunction for a large value of $r$ because of a polarization of the Ps. Probabilities $P_{nl}^{(Ps)}$ are listed in table 3. The 1s state of Ps is dominant in the correlation function, and its amplitude is given by the probability $P_{1s}^{(Ps)}$. The probability $P_{2p}^{(Ps)}$ contributes to the polarization, which is the main mechanism of the positron binding. However, in the case of the positronic hydrogen atom where no bound state exists below the lowest threshold energy ($-0.5 \text{ au}$), interactions are almost the same as those of positronium alkali atoms when the inter-particle distances are equal to the expectation value. The S-wave elastic scattering reveals no resonance state below the Ps(1s) + H$^+$ threshold energy [22]–[27]. The polarization potential induced by the singly charged ions H$^+$ and A$^+$ cannot support the light particle of Ps, because of a large zero point energy. The doubly charged ion, i.e. He$^{2+}$, can barely support the Ps [28]–[31]. Thus, an additional mechanism having a different configuration from the Ps-ion core is necessary for the binding of the $e^+\text{Li}$ and $e^+\text{Na}$.
Correlation functions \( C_e(r) \) and \( C_p(r) \) for the bound state of (a) \( e^+\)Li and (b) \( e^+\)Na. Blue curves are \( C_e(r) \), green curves \( C_p(r) \), broken curves the squared wavefunction of the valence electron in the alkali atom scaled with the probability given in table 3 and dotted curves the squared asymptotic wavefunction of the free Ps and ion core normalized at \( r = 20 \). The inset shows an enlarged view near the ion core.

In figure 4, correlation functions \( C_e(r) \) and \( C_p(r) \) are shown. When \( r > 15 \), the correlation functions are in proportion to \( \exp(-2\kappa r)/r^2 \) which is the squared asymptotic wavefunction of the free Ps and ion core with a negative energy of \( E_{gs} - \epsilon_{Ps} = -\kappa^2/4 \). Here, \( E_{gs} \) and \( \epsilon_{Ps} \) are ground-state energies of the positronic alkali atom and Ps, respectively. The calculated profile of the tail shows the accuracy of the present calculation for the weakly bound state. Near the ion core, the \( C_e(r) \) has a large amplitude, while the \( C_p(r) \) decreases rapidly because of the strong repulsive static potential between them. Shapes of the \( C_e(r) \) near the core resemble the squared wavefunction of the valence electron of the alkali atom. However, the nodes of the valence electron wavefunction produce nonzero dips in \( C_e(r) \), rather than zero minima, because \( C_e(r) \) near the core is contributed to not only by the ground state but also by excited states. The probabilities are given in table 3, and the short-range behavior of the \( C_e(r) \) can be described with the probabilities. The alkali atom cluster would be polarized and attractively interact with the positron. When \( 5 < r < 15 \), on the other hand, the \( C_p(r) \) is larger than \( C_e(r) \). The excess of the \( C_p(r) \) would be ascribed to a positron component binding to the polarized alkali atom. If the excess is ascribed to the polarization of the Ps cluster, \( C_e(r) \) must be larger than \( C_p(r) \) because of the positive ion core. The bound state is naturally considered to be dominantly composed of the weakly coupled Ps(1s)–A\(^+\) configuration, because the bound states are located close to the Ps(1s) + A\(^+\) threshold. Similarly, the A–e\(^+\) configuration is likely to contribute to the wavefunction because the bound states are located slightly below the A + e\(^+\) threshold (0.054 475 au for Li(2s) and 0.061 544 au for Na(3s); cf the threshold energies –0.198 140 au for Li and –0.188 857 au for Na), and the alkali atom is polarized by the positron. Since the threshold energy decreases with an increase of the atomic number of alkali atoms, namely when the energy gap between the Ps(1s) + A\(^+\) and A + e\(^+\) thresholds becomes large, the probability
associated with the A−e+ channel decreases for heavier alkali atoms. The effect of the additional binding mechanism must be determined by both the polarization and the probability. Although K, Rb and H (n = 2) atoms have a large polarizability, the probability should be small because of the large energy gap. This interpretation is consistent with the result where Mitroy et al [8] found a correlation between the IP of the alkali atom and the binding energy of the positronic alkali atom.

4. Summary

In order to investigate a binding mechanism of weakly bound states of positronic alkali atoms, a precise coupled channel calculation is performed for the three-body system consisting of an electron, a positron and an ion core of the alkali atom. Employing the GEM, where the Ps channel (A+–Ps) and alkali atom channel (A−e+) are explicitly introduced, we calculate the energies and wavefunctions of the bound states of positronic alkali atoms. The model potential, which includes both the polarization of the ion core and electron exchange, is adopted for the interaction between the electron and ion core. The model potential used in the present calculation reproduces the observed energy levels of the Li and Na atoms better than other model potentials used in recent calculations. The potential between the positron and ion core is produced by refining the model potential for the alkali atoms. The energies, geometries and 2γ annihilation rates of the bound states are updated. We have shown that the two sets of the coordinates of rearrangement channels effectively describe the weakly bound state. The structure of the positronic alkali atoms has been regarded as a polarized Ps cluster orbiting the ion core A+–Ps*, which is a major mechanism of positron binding. However, we point out that a fraction of the polarized alkali atom and positron A+–e+ is also included in the three-body wavefunction. The fractions of the alkali atom are small, but cause an attractive polarization potential to the positron. This minor but indispensable mechanism assists in the positron binding.

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References

[1] Pichl L, Tachikawa M, Buenker R J, Kimura M and Rost J-M 2005 IEEE Trans. Nucl. Sci. 52 2810
[2] Ryzhikh G G and Mitroy J 1999 J. Phys. B: At. Mol. Opt. Phys. 32 4051
[3] Mitroy J, Bromley M W J and Ryzhikh G G 2002 J. Phys. B: At. Mol. Opt. Phys. 35 R81
[4] Ryzhikh G G and Mitroy J 1997 Phys. Rev. Lett. 79 4124
[5] Strasburger K and Chojnacki H 1998 J. Chem. Phys. 108 3218
[6] Yuan J, Esry B D, Morishita T and Lin C D 1998 Phys. Rev. A 58 R4
[7] Ryzhikh G G, Mitroy J and Varga K 1998 J. Phys. B: At. Mol. Opt. Phys. 31 3965
[8] Mitroy J, Bromley M W J and Ryzhikh G G 1999 J. Phys. B: At. Mol. Opt. Phys. 32 2203
[9] Mitroy J and Ryzhikh G G 1999 J. Phys. B: At. Mol. Opt. Phys. 32 L621
[10] Le A T, Bromley M W J and Lin C D 2005 Phys. Rev. A 71 032713
[11] Shertzer J and Ward S J 2006 Phys. Rev. A 73 022504
[12] Hiyama E, Kino Y and Kamimura M 2003 Prog. Part. Nucl. Phys. 51 223
[13] Hartree D R 1928 Proc. Camb. Phil. Soc. 24 111
[14] Mitroy J 1983 PhD Thesis University of Melbourne
[15] Albright B J, Bartschat K and Flicek P R 1993 J. Phys. B: At. Mol. Opt. Phys. 26 337
[16] Furness J B and McCarthy I E 1973 J. Phys. B: At. Mol. Phys. 6 2280
[17] Bartschat K 1996 Computational Atomic Physics (Berlin: Springer) chapter 2
[18] NIST Atomic Spectra Database Version 3 http://physics.nist.gov/PhysRefData/ASD/index.html
[19] Norcross D W and Seaton M J 1976 J. Phys. B: At. Mol. Phys. 9 2983
[20] Krasnopolsky V M and Kukuline V I 1974 Sov. J. Nucl. Phys. 20 883
[21] Peach G, Saraph H E and Seaton M J 1988 J. Phys. B: At. Mol. Opt. Phys. 21 3669
[22] Yamanaka N and Kino Y 2003 Phys. Rev. A 68 052715
[23] Kernohan A A, Robinson D J R, McAlinden M T and Walters H R J 1996 J. Phys. B: At. Mol. Opt. Phys. 29 2089
[24] Higgins K and Burke P G 1993 J. Phys. B: At. Mol. Opt. Phys. 26 4269
[25] Winick J R and Reinhardt W P 1978 Phys. Rev. A 18 910
[26] Humberston J W 1984 J. Phys. B: At. Mol. Phys. 17 2353
[27] Kuang Y R and Gien T T 1997 Phys. Rev. A 55 256
[28] Igarashi A and Shimamura I 1997 Phys. Rev. A 56 4733
[29] Ho Y K and Yan Z-C 2002 Phys. Rev. A 66 062705
[30] Toya Y, Kino Y and Kudo H 2004 Mater. Sci. Forum 445/446 446
[31] Igarashi A and Shimamura I 2004 Phys. Rev. A 70 012706

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