# Quantal Two-Centre Coulomb Problem treated by means of the Phase-Integral Method III. Quantization Conditions in the General Case expressed in Terms of Complete Elliptic Integrals. Numerical Illustration

N. Athavan,[1,*] N. Fröman,[2] and M. Lakshmanan[1]

[1] *Centre for Nonlinear Dynamics, Department of Physics, Bharathidasan University, Tiruchirapalli 620 024,India*

[2] *Department of Theoretical Physics, University of Uppsala, Box 803, S-751 05 Uppsala, Sweden*

In this paper we take up the quantal two-centre problem where the Coulomb centres have arbitrary positive charges. In analogy with the symmetric case, treated in the second paper of this series of papers, we use the knowledge on the quasiclassical dynamics to express the contour integrals in the first- and third-order approximations of the phase-integral quantization conditions, given in the first paper of this series of papers, in terms of complete elliptic integrals. For various values of the distance between these charges the accuracy of the formulas obtained is illustrated by comparison with available numerically exact results.

PACS numbers: PACS Numbers: 03.65.Sq, 31.15.-p, 31.15.Gy

## 1. INTRODUCTION

In this third paper in a series of papers concerning the two-centre Coulomb problem we take up the general case in which the positive charge numbers $Z_1$ and $Z_2$ of the two Coulomb centres are arbitrary. The study of such general systems is of considerable importance in the field of molecular physics and elementary particle physics. For example, the calculation of eigenvalues and electronic wave functions for one-electron diatomic molecules with fixed internuclear separation is the starting point for an accurate description of molecular vibrations and rotations and of ion-atom scattering [1, 2, 3, 4]. Also the calculation of radiative transition probabilities for a $\pi^-$ meson moving in the Coulomb field of two fixed nuclei [5] is a good example of the two-centre Coulomb problem dealt with in elementary particle physics. Such calculations are of physical interest in connection with experimental [6, 7, 8] and theoretical[9] research on the absorption of $\pi^-$ mesons stopped in substances containing hydrogen.

In the second paper in this series [10] the symmetric case, $Z_1 = Z_2$, was considered. Using for the two-centre Coulomb problem the general phase-integral quantization conditions derived in the first paper [11], the relevant contour integrals for the first- and third-order approximations were expressed in terms of complete elliptic integrals so that numerical evaluation of energy eigenvalues and separation constants can easily be carried out. The evaluation of the various contour integrals was facilitated through suitable transformations of the $\xi$- and $\eta$-variables, which can be related to the quasiclassical motion of a particle. In the symmetric case, $Z_1 = Z_2$, the square of the base function $Q^2(\eta)$ has a symmetry, as discussed in [10]. As a result of this, the evaluation of the quantities $\alpha = \beta$, $L$, $L'$ and $\bar{K}$ pertaining to the $\eta$-quantization conditions were performed with the use of particular transformations in a rather simple way, while for the quantity $\tilde{L}$ in the $\xi$-quantization condition rather general transformations are necessary. However, in the general case, where $Z_1$ may be different from $Z_2$, no such symmetric structure exists for $Q^2(\eta)$, and both $Q^2(\eta)$ and $\tilde{Q}^2(\xi)$, given by eqs.(3.2a,b) in [11], can have, besides the poles, the following structure of the zeros:

1. Case $\Lambda = |m| \neq 0$:
   (a) Four real zeros
   (b) Two real and two complex conjugate zeros
2. Case $\Lambda = 0$:
   (a) Two real zeros
   (b) Two complex conjugate zeros

*Present address: Department of Physics, Government Arts College, Ariyalur - 621 713, India.

As a consequence, the evaluation of the contour integrals in the cases of the $\xi$-equation and the $\eta$-equation are analogous, except that certain coefficients change in the different subcases. This allows one to use the "universal" functions $H^{(2n+1)}$ and $\bar{H}^{(2n+1)}$, $n = 0$ or 1, valid for the $(2n+1)$th-order approximation, which were defined in sec. 3.1.2 and sec. 3.2.2 of [10]. These functions depend on five parameters $\nu_1, \nu_2, \nu_3, g$ and $k$, which are expressed in terms of the zeros of either $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$, and on the parameter $C$ and $\tilde{C}$ in the base function $\tilde{Q}(\xi)$ or $Q(\eta)$, respectively; see eqs. (3.2a,b) in [11]. Different choices of these parameters allow one to express the relevant quantities $\alpha, \beta$ (which may now be different from $\alpha$), $L, L', \bar{K}$ and $\tilde{L}$ in the first- and third-order phase integral approximation (apart possibly from a sign or a constant factor) as the appropriate "universal" function or its real or imaginary part with the appropriate parameters inserted. When the contour integrals are evaluated, one can solve the quantization conditions to obtain the energy levels accurately.

In principle one can specialize the results of the general case when $Z_1$ may be different from $Z_2$ to the particular case when $Z_1 = Z_2$ in order to obtain the results of [10], but in practice this is cumbersome due to the different transformation formulas used for the $\eta$-part of the quantization conditions in [10]. For the $\xi$-part such a specialization implies only that $Z_1 + Z_2$ is replaced by $2Z_1$ but no essential simplification.

The plan of the present paper is as follows. In sec. 2 we express $\alpha, \beta, L, L', \bar{K}$ and $\tilde{L}$ in terms of the "universal" functions appropriate for the subbarrier case with $\Lambda = |m| \neq 0$. Then a similar treatment is given for the superbarrier case. In sec. 3 an analogous procedure is applied to the case $\Lambda = 0$. Finally, in sec. 4 a detailed numerical analysis of the phase-integral quantization conditions is carried out for $Z_1 = 1$ and different values of $Z_2$ (=2, 5 and 8), and comparision is made with existing numerically exact results for the energy and the reduced separation constant.

## 2. CASE $\Lambda = |m| \neq 0$

In this section we utilize for the case of four zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$ the "universal" functions $H^{(2n+1)}$, $n = 0$ or 1, introduced in [10] and related to the $(2n+1)$th-order contribution, and the "universal" functions $\bar{H}^{(2n+1)}$, $n = 0$ or 1, which will be introduced in sec. 3.2.2. In the different cases one finds, as explained in the introduction, that the forms of the evaluated contour integrals are similar, except for changes of the parameters. One obtains the expressions for the "universal" functions $H^{(1)}, H^{(3)}, \bar{H}^{(1)}$ and $\bar{H}^{(3)}$ by integrating one specific integral in each case explicitly and then modifying the definition of the parameters in these functions to obtain the other required quantities.

### 2.1. Four real zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$

#### *2.1.1. The quantities $\alpha$, $\beta$ and $\bar{K}$ pertaining to the $\eta$-equation: Subbarrier case [Fig. 3(a) in Ref. 11]*

Denoting the zeros $\eta_1, \eta_2, \eta_3$ and $\eta_4$ by $a, b, c$ and $d$, we write the base function for this case as

$$Q(\eta) = p\frac{[(\eta - a)(b - \eta)(c - \eta)(d - \eta)]^{\frac{1}{2}}}{1 - \eta^2}. \tag{2.1}$$

Using the transformation on p. 103 in [12], we obtain

$$\eta = \frac{a - d\nu_1^2 sn^2 u}{1 - \nu_1^2 sn^2 u}, \tag{2.2}$$

the parameter $\nu_1^2$ being defined in (2.4) below. Noting that the loop $a \to b \to a$, that is $\eta_1 \to \eta_2 \to \eta_1$ in the $\eta$-plane, denoted by $\Gamma_{a,b}$, which represents the contour $\Lambda_\alpha$ in Fig. 3(a) of [11], corresponds to $0 \to K \to 2K$ in the $u$-plane, one finds that the first-order contribution to $\alpha$ is

$$\begin{aligned}
\alpha^{(1)} &= \frac{1}{2}\int_{\Lambda_\alpha} Q(\eta)d\eta \\
&= \frac{1}{2}\int_{\Gamma_{a,b}} Q(\eta)d\eta \\
&= \frac{p}{2g}\int_0^{2K}\left(\frac{d\eta}{du}\right)^2 \frac{du}{1-\eta^2} \\
&= \frac{2p(a-d)^2\nu_1^4}{g(1-a^2)}\int_0^{2K} \frac{sn^2u(1-sn^2u)(1-k^2sn^2u)du}{(1-\nu_1^2sn^2u)^2(1-\nu_2^2sn^2u)(1-\nu_3^2sn^2u)},
\end{aligned} \tag{2.3}$$

where

$$\nu_1^2 = \frac{a-b}{d-b}, \quad \nu_2^2 = \frac{1+d}{1+a}\nu_1^2, \quad \nu_3^2 = \frac{1-d}{1-a}\nu_1^2, \tag{2.4}$$

$$g = \frac{2}{[(d-b)(c-a)]^{\frac{1}{2}}}, \quad k^2 = \frac{(d-c)(b-a)}{(d-b)(c-a)}. \tag{2.5}$$

Decomposing the integrand in (2.3) into partial fractions and evaluating the integrals by means of recurrence formulas in [12], we obtain

$$\alpha^{(1)} = H^{(1)}(\nu_1, \nu_2, \nu_3, g, k, C), \tag{2.6}$$

where $H^{(1)}$ is the "universal" function defined in eqs.(3.16a,b), (3.17a-c) and (3.18) of [10] but with $\tilde{C}$ replaced by $C$ and the parameters $\nu_i$, $i = 1, 2, 3$, given by (2.4), and $g$ and $k^2$ given by (2.5). The evaluation of the quantity $\alpha^{(1)}$ in the present case is thus similar to the evaluation of the quantity $\tilde{L}^{(1)}$ in sec. 3.1.2 of [10].

Proceeding in a similar way, the third-order contribution to $\alpha$ is found to be

$$\begin{aligned} \alpha^{(3)} &= \frac{1}{2}\int_{\Lambda_\alpha}\left(-C + \frac{1}{1-\eta^2}\right)\frac{d\eta}{2Q(\eta)(1-\eta^2)} - \frac{1}{16}\int_{\Lambda_\alpha} Q^{-3}(\eta)\left(\frac{dQ}{d\eta}\right)^2 d\eta \\ &= H^{(3)}(\nu_1, \nu_2, \nu_3, g, k, C), \end{aligned} \tag{2.7}$$

where $H^{(3)}$ is the "universal" function given in eqs.(3.16c,d), (3.19a-d) and (3.20a-d) of [10] but with $\tilde{C}$ replaced by $-C$ and the parameters $\nu_i$, $i = 1, 2, 3$, given by (2.4), and $g$ and $k^2$ given by (2.5).

In a similar manner as above we proceed for the calculation of the first- and third-order contributions to $\beta$. The loop $d \to c \to d$, that is $\eta_4 \to \eta_3 \to \eta_4$ in the $\eta$-plane, denoted by $\Gamma_{d,c}$ and represented by the contour $\Lambda_\beta$ in Fig. 3(a) of [11], corresponds to $0 \to K \to 2K$ in the $u$-plane, and hence the first- and third-order contributions to $\beta$ are

$$\begin{aligned} \beta^{(1)} &= \frac{1}{2}\int_{\Lambda_\beta} Q(\eta)d\eta \\ &= \frac{1}{2}\int_{\Gamma_{d,c}} Q(\eta)d\eta \\ &= H^{(1)}(\nu_1, \nu_2, \nu_3, g, k, C), \end{aligned} \tag{2.8a}$$

and

$$\beta^{(3)} = H^{(3)}(\nu_1, \nu_2, \nu_3, g, k, C), \tag{2.8b}$$

where now

$$\nu_1^2 = \frac{d-c}{d-b}, \quad \nu_2^2 = \frac{1+b}{1+c}\nu_1^2, \quad \nu_3^2 = \frac{1-b}{1-c}\nu_1^2, \tag{2.9}$$

and $g$ and $k^2$ are given by (2.5).

Similarly one obtains

$$\pi\bar{K}_0 = H^{(1)}(\nu_1, \nu_2, \nu_3, g, k, C), \tag{2.10a}$$

$$\pi\bar{K}_2 = H^{(3)}(\nu_1, \nu_2, \nu_3, g, k, C), \tag{2.10b}$$

where now

$$\nu_1^2 = \frac{c-b}{d-b}, \quad \nu_2^2 = \frac{1+d}{1+c}\nu_1^2, \quad \nu_3^2 = \frac{1-d}{1-c}\nu_1^2, \tag{2.11}$$

and $g$ is the same as given in (2.5) and $k^2$ is now given by

$$k^2 = \frac{(c-b)(d-a)}{(d-b)(c-a)}. \tag{2.12}$$

According to eq. (3.18a) in [11] the integrals $\alpha'$ and $\beta'$ for the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 3(a) in [11] are obtained from the formulas $\alpha' = \alpha + \frac{\Lambda\pi}{2}$ and $\beta' = \beta + \frac{\Lambda\pi}{2}$.

#### 2.1.2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the $\xi$-equation [Fig. 1 in Ref. 11]

The formulas for the first- and third-order contributions to $\tilde{L}$ and $\tilde{L}'$ are derived and presented in subsection 3.1.2 of [10], and they remain unchanged in the present case.

### 2.2. Two real and two complex conjugate zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$

When there are two real and two complex conjugate zeros of $Q^2(\eta)$, the situation of either Fig. 4(a) or Fig. 2 in [11] may occur. The latter situation has, however, so far not appeared in our applications, and therefore we disregard it in our treatment below of the $\eta$-equation.

#### 2.2.1. The quantities $\alpha, \beta$, $\bar{K}$, $L$ and $L'$ pertaining to the $\eta$-equation: Superbarrier case [Fig. 4(a) or Fig. 2 in Ref. 11]

Denoting the real zeros of $Q^2(\eta)$ by $\eta_1 = a$ and $\eta_4 = d$ and the complex conjugate zeros $\eta_2$ and $\eta_3$ by $c$ and $c^*$, we have the base function

$$Q(\eta) = p\frac{[(a-\eta)(\eta-d)(\eta-c)(\eta-c^*)]^{\frac{1}{2}}}{1-\eta^2}. \tag{2.13}$$

Defining

$$c = b_1 - ia_1, \quad c^* = b_1 + ia_1, \tag{2.14}$$

$$A = [(a-b_1)^2 + a_1^2]^{\frac{1}{2}}, \tag{2.15a}$$

$$B = [(d-b_1)^2 + a_1^2]^{\frac{1}{2}}, \tag{2.15b}$$

and using the transformation on p. 133 in [12], we get

$$\eta = \frac{aB + dA + (dA - aB)cnu}{A + B + (A - B)cnu}. \tag{2.16}$$

Here we exploit the fact that the Jacobian elliptic functions are doubly periodic, one of the periods being complex. Thus the loop $d \to a_1 + ib_1 \to d$, that is $\eta_4 \to \eta_3 \to \eta_4$ in the $\eta$-plane, denoted by $\Gamma_{d,c^*}$, for the contour $\Lambda_\beta$ in Fig. 4(a) of [11], corresponds in the $u$-plane to the path $0 \to K + iK' \to 2K + 2iK'$, where $K$ and $K'$ are complete elliptic integrals of the modulus $k$, given in (2.18e) below, and of the complementary modulus $k' = \sqrt{1-k^2}$, respectively. Making use of the transformation (2.16), we obtain for the integral in the first-order expression for $\beta$

$$\begin{aligned}\frac{1}{2}\int_{\Lambda_\beta} Q(\eta)d\eta &= \frac{1}{2}\int_{\Gamma_{d,c^*}} Q(\eta)d\eta \\ &= -\frac{p(\nu_1-\nu_2)(\nu_1-\nu_3)}{2g}\int_0^{2K+2iK'} \frac{sn^2udn^2udu}{(1+\nu_1 cnu)^2(1+\nu_2 cnu)(1+\nu_3 cnu)},\end{aligned} \tag{2.17}$$

where

$$\nu_1 = \frac{A-B}{A+B}, \tag{2.18a}$$

$$\nu_2 = \frac{(1+d)A - (1+a)B}{(1+d)A + (1+a)B}, \tag{2.18b}$$

$$\nu_3 = \frac{(1-d)A-(1-a)B}{(1-d)A+(1-a)B}, \tag{2.18c}$$

$$g = \frac{1}{\sqrt{AB}}, \tag{2.18d}$$

$$k^2 = \frac{(a-d)^2-(A-B)^2}{4AB}. \tag{2.18e}$$

Similarly one can treat the corresponding integrals in the first-order expressions for $\alpha, K$ and $\tilde{L}$. When one then evaluates the integrals containing the elliptic functions [cf. (2.17)], one finds that all these integrals can be expressed in terms of a "universal" function $\bar{H}^{(1)}$ that is given by

$$\begin{aligned}\bar{H}^{(1)}(\nu_1,\nu_2,\nu_3,g,k,C) \;=\; & -\frac{p}{g}\left\{\frac{1}{\nu_1^2}\left[\left(2k^2+\frac{\nu_1^2}{1-\nu_1^2}\right)\Pi\left(\frac{\nu_1^2}{\nu_1^2-1},k\right)+(\nu_1^2-2k^2)K(k)\right.\right.\\ & -2\nu_1^2E(k)+\nu_1k(2j+1)\pi-\frac{\nu_1^2(1-2k^2)+2k^2}{[(1-\nu_1^2)(k^2+\nu_1^2k'^2)]^{\frac{1}{2}}}\frac{\nu_1}{2}j\pi\left.\right]+\sum_{i=1}^{3}\bar{C}_i\bar{S}_i\\ & \left.+i\left[\left(2k^2+\frac{\nu_1^2}{1-\nu_1^2}\right)\Pi\left(\frac{1}{1-\nu_1^2},k'\right)-2k^2K(k')+2E(k')\right]\right\},\end{aligned} \tag{2.19}$$

where $\bar{C}_1, \bar{C}_2$ and $\bar{C}_3$ are given by eqs. (3.37a-c) in [10], that is,

$$\bar{C}_1 = \frac{\nu_1^2(2\nu_3\nu_2-\nu_1\nu_3-\nu_1\nu_2)}{(\nu_1-\nu_2)(\nu_1-\nu_3)}, \tag{2.20a}$$

$$\bar{C}_2 = \frac{(\nu_1-\nu_3)\nu_2^3}{(\nu_1-\nu_2)(\nu_2-\nu_3)}, \tag{2.20b}$$

$$\bar{C}_3 = \frac{(\nu_1-\nu_2)\nu_3^3}{(\nu_1-\nu_3)(\nu_3-\nu_2)}, \tag{2.20c}$$

and

$$\begin{aligned}\bar{S}_i \;=\; & \frac{1}{\nu_i^4}\left[k^2(1-\nu_i^2)K(k)+\nu_i^2E(k)-(k^2+\nu_i^2k'^2)\Pi\left(\frac{\nu_i^2}{\nu_i^2-1},k\right)\right]\\ & +\frac{1}{2k\nu_i^3}\left[\left(k^2(\nu_i^2-1)-\frac{\nu_i^2}{2}\right)(2j+1)\pi+k[(1-\nu_i^2)(k^2+k'^2\nu_i^2)]^{\frac{1}{2}}j\pi\right]\\ & +\frac{i}{\nu_i^2}\left\{-(k^2+\nu_i^2k'^2)\left[\Pi\left(\frac{1}{1-\nu_i^2},k'\right)-K(k')\right]-E(k')\right\}, i=1,2,3,\end{aligned} \tag{2.21}$$

$j$ being an integer $-1, 0$ or $+1$, depending upon whether the quantity $\beta^{(1)}$, $L^{(1)}$ or $\alpha^{(1)}$, respectively, is evaluated, and originating from terms $tan^{-1}(sdu)$ and $cos^{-1}(dnu)$ while applying the limits of integration. Note that the quantity $\tilde{L}^{(1)}$ given by eq.(3.36a) in [10], is just $-2Re\bar{H}^{(1)}$ with $j=0$. For $K$, which is expressed in terms of the imaginary part of $\bar{H}^{(1)}$, the value of $j$, which appears only in the real part of $\bar{H}^{(1)}$, does not matter.

Similarly we also introduce the "universal" function $\bar{H}^{(3)}$ given by

$$\begin{aligned}\bar{H}^{(3)}(\nu_1,\nu_2,\nu_3,g,k,C) \;=\; & \frac{g}{16p}\left[\left(-4C+\frac{\nu_1^2(\nu_2-\nu_3)^2}{\nu_2\nu_3(\nu_1-\nu_3)(\nu_2-\nu_1)}\right)K(k)\right.\\ & \left.+\frac{1}{(\nu_1-\nu_3)(\nu_1-\nu_2)}\left(XK(k)+YE(k)+\frac{2Zj}{k}\pi\right)\right]\\ & +i\frac{g}{16p}\left[\left(-4C+\frac{\nu_1^2(\nu_2-\nu_3)^2}{\nu_2\nu_3(\nu_1-\nu_3)(\nu_2-\nu_1)}\right)K(k')\right.\\ & \left.+\frac{1}{(\nu_1-\nu_3)(\nu_1-\nu_2)}\left\{XK(k')+Y[K(k')-E(k')]\right\}\right],\end{aligned} \tag{2.22}$$

where $C$ is the parameter in the square of the base function $Q(\eta)$ in eq. (3.2b) of [11], and

$$\begin{aligned} X &= -\frac{1+4k^2}{3}+\frac{3+4k'^2}{3}(\nu_1^2+2\nu_1\nu_2+2\nu_1\nu_3+\nu_2\nu_3)-\frac{k'^2}{3k^2}(17-4k^2)\nu_1^2\nu_2\nu_3 \\ &\quad -2\nu_1(\nu_1+\nu_2+\nu_3)+2\nu_2\nu_3+\nu_1^2\left(\frac{\nu_2}{\nu_3}+\frac{\nu_3}{\nu_2}\right), \end{aligned} \tag{2.23a}$$

$$\begin{aligned} Y &= \frac{1}{3k'^2}(1+8k^2-8k^4)+\frac{4}{3}(2k^2-1)(\nu_1^2+2\nu_1\nu_2+2\nu_1\nu_3+\nu_2\nu_3) \\ &\quad +\frac{\nu_1^2\nu_2\nu_3}{3k^2}(17-8k^2+8k^4), \end{aligned} \tag{2.23b}$$

$$Z = 2\nu_1(\nu_1\nu_2+\nu_1\nu_3+4\nu_2\nu_3), \tag{2.23c}$$

where the parameters $\nu_1, \nu_2, \nu_3, g$ and $k^2$ are defined in (2.18a-e).

Then the first- and third-order contributions to the quantities $\alpha, \beta$ and $K$ $(= \pi\bar{K})$ are

$$\alpha^{(1)} = \mathrm{Re}\bar{H}^{(1)} \quad with\ \ j = 1, \tag{2.24}$$

$$\beta^{(1)} = \mathrm{Re}\bar{H}^{(1)} \quad with\ \ j = -1, \tag{2.25}$$

$$\pi\bar{K}_0 = -2\mathrm{Im}\bar{H}^{(1)}, \tag{2.26}$$

$$\alpha^{(3)} = \mathrm{Re}\bar{H}^{(3)} \quad with\ \ j = 1, \tag{2.27}$$

$$\beta^{(3)} = \mathrm{Re}\bar{H}^{(3)} \quad with\ \ j = -1, \tag{2.28}$$

$$\pi\bar{K}_2 = -2\mathrm{Im}\bar{H}^{(3)}, \tag{2.29}$$

where $\nu_1$, $\nu_2$, $\nu_3$, $g$ and $k^2$ are still defined by (2.18a-e). Since $j$ appears only in the real part of $\bar{H}^{(2n+1)}$, we need not specify a value of $j$ in (2.26) and (2.29).

The integrals $\alpha'$ and $\beta'$ associated with the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 4(a) in [11] are obtained from $\alpha$ and $\beta$ by means of the relations (3.18a) in [11], that is, $\alpha' = \alpha + \frac{\Lambda\pi}{2}$ and $\beta' = \beta + \frac{\Lambda\pi}{2}$. The integrals $L$ and $L'$ associated with the contours $\Lambda_L$ and $\Lambda_{L'}$ in Fig. 4(a) in [11] can be obtained from $\alpha$ and $\beta$ by means of the formulas $L = \alpha + \beta$ and $L' = L + |m|$.

#### *2.2.2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the $\xi$-equation [Fig. 1(a) in Ref. 11]*

The formulas for the first- and third-order contributions to $\tilde{L}$ and $\tilde{L}'$ remain the same as the ones presented in subsection 3.2.2 of [10].

## 3. CASE $\Lambda = 0$

### 3.1. Two real zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$

One should be able to obtain the formulas pertaining to the case $\Lambda = 0$ by considering the limits of the "universal" functions $H^{(1)}$ and $H^{(3)}$ when $a \to -1$ and $d \to +1$ in the case of the $\eta$-equation. These specialization procedures are, however, much more cumbersome than the direct calculation of the quantities in question, and so we do not carry them out here. Instead we shall evaluate these quantities directly, and therefore no "universal" functions will appear in subsection 3.1.

*3.1.1. The quantities $\alpha$, $\beta$ and $\bar{K}$ pertaining to the $\eta$-equation: Subbarrier case [Fig. 3(b) in Ref. 11]*

We denote the two real zeros of $Q^2(\eta)$ by $\eta_2 = b$ and $\eta_3 = c$ and use transformations on p. 103, p. 120 and p. 112 in [12] for calculating the first- and third-order contributions to $\alpha$, $\beta$ and $K$, respectively. Here the base function reads as

$$Q(\eta) = p\left[\frac{(\eta-b)(c-\eta)}{1-\eta^2}\right]^{\frac{1}{2}}. \tag{3.1}$$

The first- and third-order contributions to $\alpha$ are

$$\alpha^{(1)} = \frac{2p}{g\nu^2}[\nu^2 E(k) - (k^2+\nu^2)K(k) + (k^2-\nu^4)\Pi(\nu^2,k)], \tag{3.2a}$$

and

$$\begin{aligned}\alpha^{(3)} &= -\frac{gCK(k)}{p} + \frac{g}{4p\nu^2}\left[\left(1-2\nu^2+\frac{\nu^4}{k^2}\right)K(k) - \left(1+\frac{\nu^4}{k^2}\right)E(k)\right] \\ &-\frac{g}{32p\nu^2}\left\{\frac{1}{3k'^2}\left[\frac{1}{k^2}(4\nu^4-6\nu^2)+5\nu^4+4\nu^2+8-k^2(4+3\nu^4)-\frac{6\nu^4}{k^4}\right]K(k)\right. \\ &\left.+\frac{1}{3k'^4}\left[-8k^4+(2+8\nu^2+4\nu^4)k^2-8+2\nu^4+\nu^2-\frac{1}{k^2}(2\nu^4+12\nu^2)+\frac{12\nu^4}{k^4}\right]E(k)\right\},\end{aligned} \tag{3.2b}$$

where

$$\nu^2 = \frac{c+1}{c-1}, \quad k^2 = \frac{(1-b)(1+c)}{(1+b)(1-c)}, \quad g = \frac{2}{[(1-c)(1+b)]^{\frac{1}{2}}}. \tag{3.3}$$

Similarly the first- and third-order contributions to $\beta$ are

$$\beta^{(1)} = \frac{2p}{g\nu^2}[\nu^2 E(k) + (k^2-\nu^2)K(k) + (\nu^4-k^2)\Pi(\nu^2,k)], \tag{3.4a}$$

and

$$\begin{aligned}\beta^{(3)} &= -\frac{gCK(k)}{2p} + \frac{g}{4p\nu^2(1-c)}\left\{\left(1-\frac{\nu^4}{k^2}\right)K(k) + \left[k^2(2k^2-1-2\nu^2)+\nu^4\right]\frac{E(k)}{k^2k'^2}\right\} \\ &-\frac{g}{16(1-c)p\nu^2}\left\{\frac{4}{3k^2}\left[(2+\nu^4+2\nu^2)k^2-3k^4-2\nu^4\right]K(k)\right. \\ &\left.+\frac{8}{3k'^2}\left(-(\nu^4+\nu^2-1)+k^2(\nu^4-\nu^2+2)+\frac{\nu^4}{k^2}\right)E(k)\right\}\end{aligned} \tag{3.4b}$$

with

$$\nu^2 = \frac{1-b}{1-c}, \tag{3.5}$$

and $k^2$ and $g$ defined in (3.3).

The first- and third-order contributions to $K(=\pi\bar{K})$ are

$$\pi\bar{K}_0 = \frac{2p}{gk^2}[(k^2-\nu^2)K(k) - \nu^2 E(k) - (\nu^4-2\nu^2+k^2)\Pi(\nu^2,k)], \tag{3.6a}$$

and

$$\begin{aligned}\pi\bar{K}_2 &= -\frac{CgK(k)}{2p} + \frac{g}{2(c^2-1)p}\left[\frac{2\nu^2}{k^4}(k^2-\nu^2)K(k) + \frac{1}{k^4k'^2}\{k^2(k^2-\nu^4-2\nu^2)+2\nu^4\}E(k)\right] \\ &-\frac{g}{24\nu^4p(c-1)}\left\{(-2+k^2+\nu^2-\nu^4)K(k)\right. \\ &\left.+2[k^4-(1+\nu^2+\nu^4)k^2-\nu^2+2\nu^4+1]E(k)\right\},\end{aligned} \tag{3.6b}$$

with

$$\nu^2 = \frac{b-c}{b+1}, \quad k^2 = \frac{2(b-c)}{(1+b)(1-c)}, \tag{3.7}$$

and $g$ defined in (3.3).

#### *3.1.2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the $\xi$-equation [Fig. 1 in Ref. 11]*

The formulas for the first- and third-order contributions to $\tilde{L}$ and $\tilde{L}'$ are the same as those derived and presented in subsection 4.1.2 of [10].

### 3.2. Two complex conjugate zeros of $Q^2(\eta)$

The situation of two complex conjugate transition zeros can occur only for $Q^2(\eta)$ but not for $\tilde{Q}^2(\xi)$.

#### *3.2.1. The quantities $\alpha, \beta$ and $\bar{K}$ pertaining to the $\eta$ equation: Superbarrier case [Fig. 4(b) in Ref. 11]*

Specializing the general formulas (2.19) and (2.22) by putting $a = -1, d = +1$, we obtain

$$\begin{aligned}\bar{H}^{(1)} \;=\; & \frac{p}{g}\left\{E(k) - K(k) + \frac{1}{1-\nu^2}\left[\Pi\left(\frac{\nu^2}{\nu^2-1}, k\right) - \left(\frac{\nu^2(1-\nu^2)}{k^2+(1-k^2)\nu^2}\right)^{\frac{1}{2}}(2j+1)\pi\right]\right\} \\ & + i\frac{p}{g}\left[K(k') - E(k') + \frac{\nu^2}{1-\nu^2}\Pi\left(\frac{1}{1-\nu^2}, k'\right)\right],\end{aligned} \tag{3.8a}$$

and

$$\begin{aligned}\bar{H}^{(3)} \;=\; & \frac{g}{16p}\left\{\left(-4C + \frac{4\nu^2}{\nu^2-1}\right)K(k) + \frac{1}{\nu^2-1}\left(\bar{X}K(k) + \bar{Y}E(k) - \frac{16\nu j}{k}\pi\right)\right. \\ & \left. + i\left[\left(-4C + \frac{4\nu^2}{\nu^2-1}\right)K(k') + \frac{1}{\nu^2-1}\left(\bar{X}K(k') + \bar{Y}[K(k') - E(k')]\right)\right]\right\},\end{aligned} \tag{3.8b}$$

where

$$\nu = \frac{A-B}{A+B}, \quad g = \frac{1}{\sqrt{AB}}, \quad k^2 = \frac{4-(A-B)^2}{4AB} \tag{3.9}$$

with

$$A = [(1-b_1)^2 + a_1^2]^{\frac{1}{2}}, \quad B = [(1+b_1)^2 + a_1^2)]^{\frac{1}{2}} \tag{3.10}$$

and

$$\bar{X} = -\frac{1}{3k^2}[k^2(14+9\nu^2) + 17\nu^2], \tag{3.11a}$$

$$\bar{Y} = \frac{1}{3k^2k'^2}[-4k^4(1+\nu^2) + k^2(5+21\nu^2) - 17\nu^2]. \tag{3.11b}$$

We now have

$$\alpha^{(1)} = \mathrm{Re}\bar{H}^{(1)} \text{ with } j = 1, \tag{3.12a}$$

$$\alpha^{(3)} = \mathrm{Re}\bar{H}^{(3)} \text{ with } j = 1, \tag{3.12b}$$

$$\beta^{(1)} = \mathrm{Re}\bar{H}^{(1)} \text{ with } j = -1, \tag{3.13a}$$

$$\beta^{(3)} = \mathrm{Re}\bar{H}^{(3)} \text{ with } j = -1, \tag{3.13b}$$

$$\pi\bar{K}_0 = -2\mathrm{Im}\bar{H}^{(1)}, \tag{3.14a}$$

$$\pi\bar{K}_2 = -2\mathrm{Im}\bar{H}^{(3)}. \tag{3.14b}$$

The integral $L'$ associated with the contour $\Lambda_{L'}$ in Fig. 4(b) in [11] is obtained from the formula $L' = \alpha + \beta$.

## 4. NUMERICAL ILLUSTRATION OF THE ACCURACY OF THE QUANTIZATION CONDITIONS

For the numerical illustration of the asymmetric case we have chosen $Z_1 = 1$ and considered three different values of $Z_2$, *viz.* $Z_2 = 2,\ 5$ and 8. The corresponding physical systems are the ions $peHe^{2+}$, $peB^{5+}$ and $peO^{8+}$, respectively, where p is a proton and e is an electron. For each one of these systems we have calculated the eigenvalue $p$ and the reduced separation constant $A'$ for two different $\sigma$-states and various values of $r_{12}$.

For the ion $peHe^{2+}$ we have calculated the eigenvalue $p$ and the reduced separation constant $A'$ for the $1s\sigma$ and $2p\sigma$ states and various values of $r_{12}$, with appropriate quantization conditions and parameters. The quantization conditions in [11] for the $1s\sigma$ state are (3.5a) with $\tilde{s} = 0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s = m = 0$ [Fig. 4(b) in Ref. 11] when $r_{12}$ is sufficiently small, but (3.5b) with $\tilde{s} = m = 0$ [Fig. 1(b) in Ref. 11] and (3.25b) with $s_\beta = m = 0$ [Fig. 3(b) in Ref. 11] when $r_{12}$ is sufficiently large. The quantization conditions in [11] for the $2p\sigma$ state are (3.5a) with $\tilde{s} = 0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s = 1$ and $m = 0$ [Fig. 4(b) in Ref. 11] when $r_{12}$ is sufficiently small, but (3.5b) with $\tilde{s} = m = 0$ [Fig. 1(b) in Ref. 11] and (3.25a) with $s_\alpha = m = 0$ [Fig. 3(b) in Ref. 11] when $r_{12}$ is sufficiently large.

For the ion $peB^{5+}$ we have computed the eigenvalue $p$ and the reduced separation constant $A'$ for the $1s\sigma$ and the $3s\sigma$ states and various values of $r_{12}$, with appropriate quantization conditions and parameters. The quantization conditions in [11] for the $1s\sigma$ state are (3.5a) with $\tilde{s} = 0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s = m = 0$ [Fig. 4(b) in Ref. 11] when $r_{12}$ is sufficiently small, but (3.5b) with $\tilde{s} = m = 0$ [Fig. 1(b) in Ref. 11] and (3.25b) with $s_\beta = m = 0$ [Fig. 3(b) in Ref. 11] when $r_{12}$ is sufficiently large. The quantization conditions in [11] for the $3s\sigma$ state are (3.5a) with $\tilde{s} = 2$ [Fig. 1(a) in Ref. 11] and (3.9) with $s = m = 0$ [Fig. 4(b) in Ref. 11] when $r_{12}$ is sufficiently small, but (3.5b) with $\tilde{s} = m = 0$ [Fig. 1(b) in Ref. 11] and (3.25b) with $s_\beta = m = 0$ [Fig. 3(b) in Ref. 11] when $r_{12}$ is sufficiently large.

For the ion $peO^{8+}$ we have calculated the eigenvalue $p$ and the reduced separation constant $A'$ for the $1s\sigma$ and the $4d\sigma$ states and various values of $r_{12}$, with appropriate quantization conditions and parameters. The quantization conditions in [11] for the $1s\sigma$ state are (3.5a) with $\tilde{s} = 0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s = m = 0$ [Fig. 4(b) in Ref. 11] when $r_{12}$ is sufficiently small, but (3.5b) with $\tilde{s} = m = 0$ [Fig. 1(b) in Ref. 11] and (3.25b) with $s_\beta = m = 0$ [Fig. 3(b) in Ref. 11] when $r_{12}$ is sufficiently large. The quantization conditions in [11] for the $4d\sigma$ state are (3.5a) with $\tilde{s} = 1$ [Fig. 1(a) in Ref. 11] and (3.9) with $s = 2$ and $m = 0$ [Fig. 4(b) in Ref. 11] when $r_{12}$ is sufficiently small, but (3.5b) with $\tilde{s} = m = 0$ [Fig. 1(b) in Ref. 11] and (3.25b) with $s_\beta = 2$ and $m = 0$ [Fig. 3(b) in Ref. 11] when $r_{12}$ is sufficiently large.

In the calculations for the above mentioned three ions we used the quantization conditions expressed in terms of complete elliptic integrals, obtained in the present paper, that correspond to the above mentioned quantization conditions in [11]. In subsection 4.1 we use the same procedure as in subsection 5.1 of [10] for optimizing the accuracy of the results obtainable in the first- and third-order approximations. Thus we determine $C$ and $\tilde{C}$ as functions of $r_{12}$ such that the first- and third-order quantization conditions give the same results, and with these values of $C$ and $\tilde{C}$ we calculate $p$ and $A'$. In subsection 4.2 we determine $C$ and $\tilde{C}$ such that the phase-integral quantization conditions give the numerically exact values of $p$ and $A'$ obtained by Winter *et al.* [4] for the ion $peHe^{2+}$ and by Ponomarev and Puzynina[13] for the ions $peB^{5+}$ and $peO^{8+}$. It is seen that the values of $C$ and $\tilde{C}$ obtained in subsection 4.1 are in qualitative agreement with those obtained in subsection 4.2.

### 4.1. Determination of $C(r_{12})$ and $\tilde{C}(r_{12})$ such that the first- and third-order quantization conditions give the same values of $p$ and $A'$

We have determined the values of $C$ and $\tilde{C}$ for several values of $r_{12}$ such that the first- and third-order quantization conditions give the same value of $p$ as well as of $A'$ . These values are tabulated and compared with the numerically exact results obtained by Winter *et al.* [4] for the ion $peHe^{2+}$ and by Ponomarev and Puzynina[13] for the ions $peB^{5+}$ and $peO^{8+}$. In Table I and Table II we give the results for the system $peHe^{2+}$. Table III and Table IV present the results for the ion $peB^{5+}$. For the ion $peO^{8+}$ the results are tabulated in Table V and Table VI. The results in Tables I - VI are presented graphically in Figs. 1 - 6.

### 4.2. Determination of $C(r_{12})$ and $\tilde{C}(r_{12})$ such that the phase-integral quantization conditions reproduce numerically exact values of $p$ and $A'$

By determining $C$ and $\tilde{C}$ for each value of $r_{12}$ such that the first-order quantization conditions reproduce the numerically exact values of $p$ and $A'$ obtained by Winter *et al.* [4] for the $1s\sigma$ and $2p\sigma$ states of the ion $peHe^{2+}$ and by Ponomarev and Puzynina[13] for the previously mentioned two states of the ion $peB^{5+}$ and two states of the ion $peO^{8+}$ we have obtained the values of $C$ and $\tilde{C}$ presented in Tables VII - XII. The numerical results in these tables are presented graphically in Figs. 7 - 12.

### Acknowledgments

We are much indebted to Professor T. G. Winter for placing the unpublished numerical material mentioned on p. 288-289 in [4] at our disposal. Also the authors are extremely grateful to Professor Per Olof Fröman for very critical reading of the manuscript and making numerous comments which resulted in a much improved presentation. The work of M.L. forms part of a Department of Science and Technology, Government of India, research project. Support from the Swedish Natural Science Research Council for M. Lakshmanan's visits to Uppsala is gratefully acknowledged.

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TABLE I: For the state $1s\sigma$ of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for $p$ as well as for $A'$. With the use of these values of $C$ and $\tilde{C}$ the values of $p$ and $A'$ have then been obtained from the quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large. The numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan and Lane [4], and obtained as private communication from Professor Winter (see p. 288-289 in [4]), are given in the columns called $p_{WDL}$ and $A'_{WDL}$.

| $r_{12}$ | $C$ | $\tilde{C}$ | $p$ | $p_{WDL}$ | $p - p_{WDL}$ | $A'$ | $A'_{WDL}$ | $A' - A'_{WDL}$ |
|---|---|---|---|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | | | | | |
| 0.2 | 0.4296362900 | 0.4986159300 | 0.2913835957 | 0.2909534228 | 0.000430173 | -0.0401742480 | -0.0495531186 | 0.00937887 |
| 0.4 | 0.4938610210 | 0.4991342047 | 0.5546735631 | 0.5544040477 | 0.000269516 | -0.16745905 | -0.1752443935 | 0.007785348 |
| 0.6 | 0.5014529650 | 0.5021936418 | 0.7949730256 | 0.7945061056 | 0.00046692 | -0.3404297821 | -0.3475381522 | 0.00710837 |
| 0.8 | 0.5023672195 | 0.5045291831 | 1.018520819 | 1.018366017 | -0.000154802 | -0.54176553 | -0.5473748938 | 0.00560936 |
| 1.0 | 0.5032793418 | 0.5061539132 | 1.231430173 | 1.231534107 | -0.000103934 | -0.75725945 | -0.7624147481 | 0.0051553 |
| 2.0 | 0.5059145550 | 0.5083606740 | 2.241478757 | 2.241514227 | -0.00003547 | -1.870558067 | -1.866548007 | -0.00401006 |
| Sufficiently large $r_{12}$ | | | | | | | | |
| 3.0 | 0.4951651150 | 0.5099904870 | 3.241389959 | 3.241868168 | -0.000478209 | -2.918225629 | -2.914992386 | -0.003233243 |
| 4.0 | 0.4904409110 | 0.5094308280 | 4.243060447 | 4.243211413 | -0.000150966 | -3.938607817 | -3.937060587 | -0.00154723 |
| 5.0 | 0.4878197130 | 0.5085272790 | 5.244268024 | 5.244326655 | -0.000058631 | -4.950729976 | -4.949835242 | -0.000894734 |
| 6.0 | 0.4861586190 | 0.5076632010 | 6.245131490 | 6.245159553 | -0.000028063 | -5.958842182 | -5.958257005 | -0.000585177 |
| 7.0 | 0.4850145200 | 0.5069119800 | 7.245774185 | 7.245789653 | -0.000015468 | -6.964658345 | -6.964245417 | -0.000412928 |
| 8.0 | 0.4841801400 | 0.5062737200 | 8.246269561 | 8.246278979 | -0.000009418 | -7.969033663 | -7.968726708 | -0.000306955 |
| 9.0 | 0.4835456720 | 0.5057325250 | 9.246662366 | 9.246668544 | -0.000006178 | -8.972444904 | -8.972207821 | -0.000237083 |
| 10.0 | 0.4830475910 | 0.5052712520 | 10.24698113 | 10.24698542 | -0.00000429 | -9.975179205 | -9.974990618 | -0.000188587 |
| 11.0 | 0.4826466130 | 0.5048751070 | 11.24724480 | 11.24724792 | -0.00000312 | -10.97741991 | -10.97726635 | -0.00015356 |
| 12.0 | 0.4823171600 | 0.5045321160 | 12.24746643 | 12.24746878 | -0.00000235 | -11.97928963 | -11.97916218 | -0.00012745 |
| 13.0 | 0.4820418880 | 0.5042327580 | 13.24765526 | 13.24765709 | -0.00000183 | -12.98087344 | -12.98076598 | -0.00010746 |
| 14.0 | 0.4818086000 | 0.5039695200 | 14.24781804 | 14.24781949 | -0.00000145 | -13.98223227 | -13.98214045 | -0.00009182 |
| 15.0 | 0.4818086000 | 0.5037364370 | 15.24795978 | 15.24796097 | -0.00000119 | -14.98341087 | -14.983331513 | -0.00007936 |

TABLE II: For the state $2p\sigma$ of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for $p$ as well as for $A'$. With the use of these values of $C$ and $\tilde{C}$ the values of $p$ and $A'$ have then been obtained from the quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large. The numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan and Lane [4], and obtained as private communication from Professor Winter (see p. 288-289 in [4]), are given in the columns called $p_{WDL}$ and $A'_{WDL}$.

| $r_{12}$ | $C$ | $\tilde{C}$ | $p$ | $p_{WDL}$ | $p - p_{WDL}$ | $A'$ | $A'_{WDL}$ | $A' - A'_{WDL}$ |
|---|---|---|---|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | | | | | |
| 0.2 | 0.5294831952 | 0.5029173619 | 0.1517930283 | 0.1507994078 | 0.000993621 | -2.009318372 | -2.013114367 | 0.003795995 |
| 0.4 | 0.5481736492 | 0.5102837463 | 0.3028910382 | 0.3062680406 | -0.003377002 | -2.049183021 | -2.053824124 | 0.004641103 |
| 0.6 | 0.5928374081 | 0.5279102827 | 0.468491904 | 0.4698372597 | -0.001345355 | -2.120325324 | -2.125935288 | 0.0056099640 |
| 0.8 | 0.6493296518 | 0.5380281837 | 0.642918371 | 0.6416038747 | 0.001314497 | -2.226301818 | -2.234147173 | 0.007845355 |
| 1.0 | 0.6918276523 | 0.5400183926 | 0.819207383 | 0.8180287700 | 0.001178613 | -2.382017327 | -2.381560387 | -0.00045694 |
| 2.0 | 0.7291847142 | 0.5410643929 | 1.641039285 | 1.640235157 | 0.000804128 | -3.839201840 | -3.846791567 | 0.007589727 |
| Sufficiently large $r_{12}$ | | | | | | | | |
| 3.0 | 0.7931298547 | 0.5426329856 | 2.304295844 | 2.303194434 | 0.00110141 | -5.443294571 | -5.444185235 | 0.000890664 |
| 4.0 | 0.8368432961 | 0.5429173921 | 2.869430632 | 2.872046343 | -0.002615711 | -7.447320938 | -7.448941809 | 0.001620871 |
| 5.0 | 0.9439467950 | 0.5427393690 | 3.398416434 | 3.395848335 | 0.002568099 | -9.524254856 | -9.526950457 | 0.002695601 |
| 6.0 | 0.7710812780 | 0.5422035320 | 3.913851362 | 3.901954918 | 0.011896444 | -11.58670782 | -11.61569923 | 0.02899141 |
| 7.0 | 0.7080781570 | 0.5407494330 | 4.425841569 | 4.404864367 | 0.020977202 | -13.63385383 | -13.68696569 | 0.05311186 |
| 8.0 | 0.6709709560 | 0.5389585440 | 4.933037475 | 4.909225930 | 0.023811545 | -15.67683067 | -15.73665989 | 0.05982922 |
| 9.0 | 0.6449125300 | 0.5370377600 | 5.438128294 | 5.414760984 | 0.02336731 | -17.71314008 | -17.77106869 | 0.05792861 |
| 10.0 | 0.6252417660 | 0.5351150510 | 5.942311467 | 5.920460066 | 0.021851401 | -19.74285483 | -19.79629610 | 0.05344127 |
| 11.0 | 0.6098017850 | 0.5332640160 | 6.445985745 | 6.425795942 | 0.020189803 | -21.76715693 | -21.81592389 | 0.04876696 |
| 12.0 | 0.5973476560 | 0.5315208600 | 6.949277104 | 6.930614764 | 0.01866234 | -23.78726983 | -23.83184680 | 0.04457697 |
| 13.0 | 0.5870841030 | 0.5298992780 | 7.452239113 | 7.434919206 | 0.017319907 | -25.80416211 | -25.84512132 | 0.04095921 |
| 14.0 | 0.5784759070 | 0.5284005350 | 7.954909402 | 7.938760040 | 0.016149362 | -27.81854786 | -27.85639810 | 0.03785024 |
| 15.0 | 0.5711495800 | 0.5270195800 | 8.457321437 | 8.442196146 | 0.015125291 | -29.83094919 | -29.86611405 | 0.03516486 |

TABLE III: For the state $1s\sigma$ of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for $p$ as well as for $A'$. With the use of these values of $C$ and $\tilde{C}$ the values of $p$ and $A'$ have then been obtained from the quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina [13] are given in the columns called $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $C$ | $\tilde{C}$ | $p$ | $p_{PP}$ | $p - p_{PP}$ | $A'$ | $A'_{PP}$ | $A' - A'_{PP}$ |
|---|---|---|---|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | | | | | |
| 0.2 | 0.51832 | 0.48329 | 0.576736 | 0.57180 | 0.004936 | -0.102639 | -0.106339 | 0.003694 |
| 0.4 | 0.51568 | 0.48937 | 1.093781 | 1.09319 | 0.000591 | -0.318422 | -0.312917 | 0.005505 |
| 0.6 | 0.51379 | 0.49583 | 1.597092 | 1.59754 | -0.000448 | -0.539704 | -0.533666 | -0.006038 |
| 0.8 | 0.51057 | 0.49961 | 2.097826 | 2.09827 | -0.000444 | -0.753875 | -0.749331 | -0.004544 |
| 1.0 | 0.50847 | 0.50137 | 2.598201 | 2.59847 | -0.000269 | -0.962648 | -0.959583 | -0.003065 |
| 2.0 | 0.50456 | 0.50273 | 5.099079 | 5.09906 | +0.000019 | -1.980607 | -1.97997 | -0.000637 |
| Sufficiently large $r_{12}$ | | | | | | | | |
| 3.0 | 0.50320 | 0.50231 | 7.599399 | 7.59936 | +0.000039 | -2.986865 | -2.98666 | -0.000205 |
| 4.0 | 0.50230 | 0.50192 | 10.099513 | 10.0995 | +0.000013 | -3.990163 | -3.99000 | -0.000163 |
| 5.0 | 0.50081 | 0.50164 | 12.599680 | 12.5996 | +0.000080 | -4.991936 | -4.99200 | +0.000064 |
| 6.0 | 0.50090 | 0.50141 | 15.099774 | 15.0997 | +0.000074 | -5.993175 | -5.99333 | +0.000155 |
| 7.0 | 0.50082 | 0.50124 | 17.599832 | 17.5997 | +0.000132 | -6.994086 | -6.99428 | +0.000194 |
| 8.0 | 0.50081 | 0.50111 | 20.099870 | 20.0998 | +0.000070 | -7.994774 | -7.99500 | +0.000226 |
| 9.0 | 0.50080 | 0.50100 | 22.599897 | 22.5998 | +0.000097 | -8.995344 | -8.99556 | +0.000026 |
| 10.0 | 0.50080 | 0.50090 | 25.099916 | 25.0998 | +0.000116 | -9.995783 | -9.99563 | -0.000153 |
| 11.0 | 0.50070 | 0.50083 | 27.599930 | 27.5998 | +0.000130 | -10.996136 | -10.9960 | -0.000136 |
| 12.0 | 0.50070 | 0.50080 | 30.099941 | 30.0998 | +0.000140 | -11.996448 | -11.9964 | -0.000048 |
| 13.0 | 0.50060 | 0.50067 | 32.599950 | 32.5998 | +0.000150 | -12.996740 | -12.9966 | -0.000140 |
| 14.0 | 0.50070 | 0.50060 | 35.099957 | 35.0998 | +0.000157 | -13.996981 | -13.9969 | -0.000081 |
| 15.0 | 0.50060 | 0.50060 | 37.599962 | 37.5999 | +0.000062 | -14.997142 | -14.9971 | -0.000042 |

TABLE IV: For the state $3s\sigma$ of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for $p$ as well as for $A'$. With the use of these values of $C$ and $\tilde{C}$ the values of $p$ and $A'$ have then been obtained from the quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina [13] are given in the columns called $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $C$ | $\tilde{C}$ | $p$ | $p_{PP}$ | $p - p_{PP}$ | $A'$ | $A'_{PP}$ | $A' - A'_{PP}$ |
|---|---|---|---|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | | | | | |
| 0.2 | 0.46900 | 0.44400 | 0.197728 | 0.196723 | +0.001005 | 0.118904 | 0.077870 | +0.041034 |
| 0.4 | 0.43100 | 0.42600 | 0.386620 | 0.386538 | +0.000082 | 0.277525 | 0.286919 | -0.009394 |
| 0.6 | 0.42620 | 0.42280 | 0.572037 | 0.572068 | -0.000031 | 0.570774 | 0.579790 | -0.009016 |
| 0.8 | 0.42800 | 0.42280 | 0.754729 | 0.754721 | +0.000008 | 0.916385 | 0.921649 | -0.005264 |
| 1.0 | 0.43110 | 0.42460 | 0.935242 | 0.935213 | +0.000029 | 1.290323 | 1.29312 | -0.002797 |
| 2.0 | 0.44550 | 0.43680 | 1.817203 | 1.81720 | +0.000003 | 3.347775 | 3.34845 | -0.000675 |
| Sufficiently large $r_{12}$ | | | | | | | | |
| 3.0 | 0.45680 | 0.44762 | 2.680126 | 2.68008 | +0.000046 | 5.536925 | 5.53664 | +0.000285 |
| 4.0 | 0.46400 | 0.45600 | 3.533310 | 3.53328 | +0.000030 | 7.777719 | 7.77753 | +0.000189 |
| 5.0 | 0.46870 | 0.46235 | 4.380874 | 4.38088 | -0.000006 | 10.045943 | 10.0461 | -0.000157 |
| 6.0 | 0.47320 | 0.46730 | 5.224967 | 5.22494 | +0.000027 | 12.331720 | 12.3314 | +0.000320 |
| 7.0 | 0.47608 | 0.47119 | 6.066647 | 6.06662 | +0.000027 | 14.627793 | 14.6276 | +0.000193 |
| 8.0 | 0.47820 | 0.47430 | 6.906648 | 6.90665 | -0.000002 | 16.931213 | 16.9313 | -0.000087 |
| 9.0 | 0.48042 | 0.47685 | 7.745476 | 7.74546 | +0.000016 | 19.240602 | 19.2405 | +0.000102 |
| 10.0 | 0.48202 | 0.47898 | 8.583369 | 8.58335 | +0.000019 | 21.553777 | 21.5537 | +0.000077 |
| 11.0 | 0.48337 | 0.48077 | 9.420559 | 9.42055 | +0.000009 | 23.870068 | 23.8700 | +0.000068 |
| 12.0 | 0.48460 | 0.48230 | 10.257201 | 10.2572 | +0.000001 | 26.188828 | 26.1888 | +0.000028 |
| 13.0 | 0.48553 | 0.48356 | 11.093399 | 11.0934 | -0.000001 | 28.509499 | 28.5095 | -0.000001 |
| 14.0 | 0.48661 | 0.48471 | 11.929252 | 11.9292 | +0.000052 | 30.831947 | 30.8318 | +0.000147 |
| 15.0 | 0.48720 | 0.48570 | 12.764781 | 12.7648 | -0.000019 | 33.155366 | 33.1554 | -0.000034 |

TABLE V: For the state $1s\sigma$ of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for $p$ as well as for $A'$. With the use of these values of $C$ and $\tilde{C}$ the values of $p$ and $A'$ have then been obtained from the quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina [13] are given in the columns called $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $C$ | $\tilde{C}$ | $p$ | $p_{PP}$ | $p - p_{PP}$ | $A'$ | $A'_{PP}$ | $A' - A'_{PP}$ |
|---|---|---|---|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | | | | | |
| 0.2 | 0.5019300 | 0.4809100 | 0.857612 | 0.855323 | +0.002289 | -0.137649 | -0.142128 | +0.004479 |
| 0.4 | 0.5039400 | 0.4943700 | 1.661131 | 1.66144 | +0.000087 | -0.366556 | -0.361348 | -0.005208 |
| 0.6 | 0.5038000 | 0.4989000 | 2.461700 | 2.46187 | -0.000170 | -0.576667 | -0.573808 | -0.002859 |
| 0.8 | 0.5033500 | 0.5004300 | 3.261920 | 3.26197 | -0.000050 | -0.782022 | -0.780407 | -0.001615 |
| 1.0 | 0.5028000 | 0.5010000 | 4.062060 | 4.06206 | 0.00000 | -0.985331 | -0.984350 | -0.000981 |
| 2.0 | 0.5017000 | 0.5012000 | 8.062283 | 8.06226 | +0.000023 | -1.992407 | -1.99219 | -0.000217 |
| Sufficiently large $r_{12}$ | | | | | | | | |
| 3.0 | 0.5013000 | 0.5010000 | 12.062372 | 12.0623 | +0.000072 | -2.994818 | -2.99479 | -0.000028 |
| 4.0 | 0.5008300 | 0.5007800 | 16.062383 | 16.0624 | -0.000017 | -3.996148 | -3.99609 | -0.000058 |
| 5.0 | 0.5005000 | 0.5007000 | 20.062566 | 20.0624 | +0.000166 | -4.996555 | -4.99687 | +0.000315 |
| 6.0 | 0.5004300 | 0.5005300 | 24.062567 | 24.0624 | +0.000167 | -5.997131 | -5.99724 | +0.000109 |
| 7.0 | 0.5005000 | 0.5005000 | 28.062564 | 28.0624 | +0.000164 | -6.997498 | -6.99764 | +0.000140 |
| 8.0 | 0.5004000 | 0.5004000 | 32.062561 | 32.0624 | +0.000161 | -7.997818 | -7.99793 | +0.000112 |
| 9.0 | 0.5005000 | 0.5004000 | 36.062557 | 36.0624 | +0.000157 | -8.998017 | -8.99816 | +0.000145 |
| 10.0 | 0.5000000 | 0.5004000 | 40.062432 | 40.0624 | +0.000032 | -9.998458 | -9.99834 | -0.000118 |
| 11.0 | 0.5004000 | 0.5003000 | 44.062551 | 44.0624 | +0.000151 | -10.998401 | -10.9985 | +0.000099 |
| 12.0 | 0.5000000 | 0.5003000 | 48.062446 | 48.0624 | +0.000046 | -11.998716 | -11.9986 | -0.000116 |
| 13.0 | 0.5000000 | 0.5003000 | 52.062451 | 52.0625 | -0.000049 | -12.998804 | -12.9987 | -0.000104 |
| 14.0 | 0.5001000 | 0.5003000 | 56.062455 | 56.0625 | -0.000045 | -13.998861 | -13.9988 | -0.000061 |
| 15.0 | 0.4999900 | 0.5002100 | 60.062459 | 60.0625 | -0.000041 | -14.998981 | -14.9989 | -0.000081 |

TABLE VI: For the state $4d\sigma$ of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for $p$ as well as for $A'$. With the use of these values of $C$ and $\tilde{C}$ the values of $p$ and $A'$ have then been obtained from the quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina [13] are given in the columns called $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $C$ | $\tilde{C}$ | $p$ | $p_{PP}$ | $p - p_{PP}$ | $A'$ | $A'_{PP}$ | $A' - A'_{PP}$ |
|---|---|---|---|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | | | | | |
| 0.5 | 0.6421800 | 0.5329500 | 0.567784 | 0.569166 | -0.001382 | -6.45764 | -6.466968 | +0.009328 |
| 1.0 | 0.6301800 | 0.5281010 | 1.597590 | 1.16192 | -0.002161 | -7.813621 | -7.82220 | +0.008579 |
| 2.0 | 0.6223000 | 0.5179000 | 2.248680 | 2.24564 | +0.003040 | -11.571664 | -11.5899 | +0.018236 |
| Sufficiently large $r_{12}$ | | | | | | | | |
| 3.0 | 0.5563400 | 0.5069600 | 3.260659 | 3.26096 | -0.000301 | -15.145897 | -15.1384 | -0.007497 |
| 4.0 | 0.5434000 | 0.5090000 | 4.265089 | 4.26518 | -0.000091 | -18.414485 | -18.4123 | -0.002185 |
| 5.0 | 0.5357000 | 0.5114000 | 5.265926 | 5.26597 | -0.000044 | -21.567077 | -21.5660 | -0.001077 |
| 6.0 | 0.5303000 | 0.5127000 | 6.265543 | 6.26552 | +0.000023 | -24.662029 | -24.6617 | -0.000329 |
| 7.0 | 0.5262000 | 0.5131400 | 7.264703 | 7.26468 | +0.000023 | -27.725910 | -27.7257 | -0.000210 |
| 8.0 | 0.5226000 | 0.5131000 | 8.263735 | 8.26374 | -0.000005 | -30.771316 | -30.7710 | -0.000316 |
| 9.0 | 0.5204500 | 0.5127600 | 9.262851 | 9.26283 | +0.000021 | -33.804409 | -33.8043 | -0.000109 |
| 10.0 | 0.5186100 | 0.5123000 | 10.261986 | 10.2620 | -0.000014 | -36.829957 | -36.8297 | -0.000257 |
| 11.0 | 0.5170000 | 0.5118000 | 11.261223 | 11.2612 | +0.000023 | -39.849843 | -39.8497 | -0.000143 |
| 12.0 | 0.5152000 | 0.5113000 | 12.260537 | 12.2605 | +0.000037 | -42.865768 | -42.8656 | -0.000168 |
| 13.0 | 0.5142000 | 0.5107500 | 13.259930 | 13.2599 | +0.000030 | -45.878744 | -45.8787 | -0.000044 |
| 14.0 | 0.5131800 | 0.5102700 | 14.259369 | 14.2594 | -0.000031 | -48.889604 | -48.8896 | -0.000004 |
| 15.0 | 0.5122100 | 0.5098200 | 15.258859 | 15.2589 | -0.000051 | -51.898778 | -51.8987 | -0.000078 |

TABLE VII: For the state $1s\sigma$ of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first-order phase-integral results, obtained from quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large, coincide for $p$ as well as for $A'$ with the numerically exact results (accurate to all digits quoted) calculated by Winter, Duncan and Lane [4], and obtained as private communication from Professor Winter (see p. 288 - 289 in [4]), and quoted in this table as $p_{WDL}$ and $A'_{WDL}$.

| $r_{12}$ | $p_{WDL}$ | $A'_{WDL}$ | $C$ | $\tilde{C}$ |
|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | |
| 0.2 | 0.2909534228 | -0.0495531186 | 0.51829036 | 0.509271872 |
| 0.4 | 0.5544040477 | -0.1752443935 | 0.532092811 | 0.512039821 |
| 0.6 | 0.7945061056 | -0.3475381522 | 0.552948218 | 0.516402819 |
| 0.8 | 1.018366017 | -0.5473748938 | 0.562018492 | 0.515629306 |
| 1.0 | 1.231534107 | -0.7624147481 | 0.5529481616 | 0.513927361 |
| 2.0 | 2.24151 | -1.86655 | 0.5406495155 | 0.5122852272 |
| Sufficiently large $r_{12}$ | | | | |
| 3.0 | 3.241868168 | -2.914992386 | 0.5148124860 | 0.5120384660 |
| 4.0 | 4.243211413 | -3.937060587 | 0.5060386160 | 0.5106252670 |
| 5.0 | 5.244326655 | -4.949835242 | 0.5018822190 | 0.5092751320 |
| 6.0 | 6.245159553 | -5.958257005 | 0.4994075600 | 0.5081813590 |
| 7.0 | 7.245789653 | -6.964245417 | 0.4977688690 | 0.5072953460 |
| 8.0 | 8.246278979 | -7.968726708 | 0.4965834380 | 0.5065545680 |
| 9.0 | 9.246668544 | -8.972207821 | 0.4957006460 | 0.5059509020 |
| 10.0 | 10.24698542 | -9.974990618 | 0.4950401840 | 0.5054199100 |
| 11.0 | 11.24724792 | -10.97726635 | 0.4943322500 | 0.5050906930 |
| 12.0 | 12.24746878 | -11.97916218 | 0.4940316000 | 0.5045504220 |
| 13.0 | 13.24765709 | -12.98076598 | 0.4934859900 | 0.5044230599 |
| 14.0 | 14.24781949 | -13.98214045 | 0.4933158850 | 0.5041397900 |
| 15.0 | 15.24796097 | -14.983331513 | 0.4931492940 | 0.5037628620 |

TABLE VIII: For the state $2p\sigma$ of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first-order phase-integral results, obtained from quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large, coincide for $p$ as well as for $A'$ with the numerically exact results (accurate to all digits quoted) calculated by Winter, Duncan and Lane [4], and obtained as private communication from Professor Winter (see p. 288 - 289 in [4]), and quoted in this table as $p_{WDL}$ and $A'_{WDL}$.

| $r_{12}$ | $p_{WDL}$ | $A'_{WDL}$ | $C$ | $\tilde{C}$ |
|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | |
| 0.2 | 0.1507994078 | -2.013114367 | 0.5419280238 | 0.50829181 |
| 0.4 | 0.3062680406 | -2.053824124 | 0.552930182 | 0.50920298 |
| 0.6 | 0.4698372597 | -2.125935288 | 0.572019821 | 0.51028392 |
| 0.8 | 0.6416038747 | -2.234147173 | 0.592038261 | 0.52978182 |
| 1.0 | 0.8180287700 | -2.381560387 | 0.619273017 | 0.542910422 |
| 2.0 | 1.640235157 | -3.846791567 | 0.632937162 | 0.569271625 |
| Sufficiently large $r_{12}$ | | | | |
| 3.0 | 2.303194434 | -5.444185235 | 0.65293027 | 0.551927319 |
| 4.0 | 2.872046343 | -7.448941809 | 0.6829729310 | 0.549321938 |
| 5.0 | 3.395848335 | -9.526950457 | 0.7689678921 | 0.5473760702 |
| 6.0 | 3.901954918 | -11.61569923 | 0.6760630853 | 0.5461458940 |
| 7.0 | 4.404864367 | -13.68696569 | 0.6153175050 | 0.5440702840 |
| 8.0 | 4.909225930 | -15.73665989 | 0.5787297600 | 0.5416277770 |
| 9.0 | 5.414760984 | -17.77106869 | 0.5582392230 | 0.5391808520 |
| 10.0 | 5.920460066 | -19.79629610 | 0.5461971300 | 0.5368472710 |
| 11.0 | 6.425795942 | -21.81592389 | 0.5382876680 | 0.5347039250 |
| 12.0 | 6.930614764 | -23.83184680 | 0.5325850510 | 0.5327246020 |
| 13.0 | 7.434919206 | -25.84512132 | 0.5281541630 | 0.5308665610 |
| 14.0 | 7.938760040 | -27.85639810 | 0.5245807700 | 0.5291925630 |
| 15.0 | 8.442196146 | -29.86611405 | 0.5216764050 | 0.5276965330 |

TABLE IX: For the state $1s\sigma$ of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first-order phase-integral results, obtained from quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large, coincide for $p$ as well as for $A'$ with the numerically exact results obtained by Ponomarev and Puzynina [13] and quoted in this table as $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $p_{PP}$ | $A'_{PP}$ | $C$ | $\tilde{C}$ |
|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | |
| 0.2 | 0.57180 | -0.106339 | 0.525368 | 0.501193 |
| 0.4 | 1.09319 | -0.312917 | 0.523294 | 0.500928 |
| 0.6 | 1.59754 | -0.533666 | 0.521226 | 0.500636 |
| 0.8 | 2.09827 | -0.749331 | 0.516453 | 0.503010 |
| 1.0 | 2.59847 | -0.959583 | 0.512521 | 0.503770 |
| 2.0 | 5.09906 | -1.97997 | 0.505470 | 0.503400 |
| Sufficiently large $r_{12}$ | | | | |
| 3.0 | 7.59936 | -2.98666 | 0.503530 | 0.502600 |
| 4.0 | 10.0995 | -3.99000 | 0.502580 | 0.502110 |
| 5.0 | 12.5996 | -4.99200 | 0.502040 | 0.501740 |
| 6.0 | 15.0997 | -5.99333 | 0.501760 | 0.501410 |
| 7.0 | 17.5997 | -6.99428 | 0.501420 | 0.501320 |
| 8.0 | 20.0998 | -7.99500 | 0.501350 | 0.501030 |
| 9.0 | 22.5998 | -8.99556 | 0.501140 | 0.501000 |
| 10.0 | 25.0998 | -9.99563 | 0.501400 | 0.501300 |
| 11.0 | 27.5998 | -10.9960 | 0.501220 | 0.501230 |
| 12.0 | 30.0998 | -11.9964 | 0.501010 | 0.501100 |
| 13.0 | 32.5998 | -12.9966 | 0.501000 | 0.501110 |
| 14.0 | 35.0998 | -13.9969 | 0.500810 | 0.501000 |
| 15.0 | 37.5999 | -14.9971 | 0.501000 | 0.500800 |

TABLE X: For the state $3s\sigma$ of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first-order phase-integral results, obtained from quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large, coincide for $p$ as well as for $A'$ with the numerically exact results obtained by Ponomarev and Puzynina [13] and quoted in this table as $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $p_{PP}$ | $A'_{PP}$ | $C$ | $\tilde{C}$ |
|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | |
| 0.2 | 0.196723 | 0.077870 | 0.428610 | 0.440763 |
| 0.4 | 0.386538 | 0.286919 | 0.440847 | 0.437841 |
| 0.6 | 0.572068 | 0.579790 | 0.436194 | 0.431006 |
| 0.8 | 0.754721 | 0.921649 | 0.434223 | 0.428242 |
| 1.0 | 0.935213 | 1.29132 | 0.433012 | 0.426215 |
| 2.0 | 1.81720 | 3.34845 | 0.446970 | 0.437520 |
| Sufficiently large $r_{12}$ | | | | |
| 3.0 | 2.68008 | 5.53664 | 0.457260 | 0.448050 |
| 4.0 | 3.53328 | 7.77753 | 0.464410 | 0.456250 |
| 5.0 | 4.38088 | 10.0461 | 0.469530 | 0.462430 |
| 6.0 | 5.22494 | 12.3314 | 0.473400 | 0.467340 |
| 7.0 | 6.06662 | 14.6276 | 0.476400 | 0.471350 |
| 8.0 | 6.90665 | 16.9313 | 0.478790 | 0.474360 |
| 9.0 | 7.74546 | 19.2405 | 0.480780 | 0.476950 |
| 10.0 | 8.58335 | 21.5537 | 0.482370 | 0.479130 |
| 11.0 | 9.42055 | 23.8700 | 0.483710 | 0.480810 |
| 12.0 | 10.2572 | 26.1888 | 0.484920 | 0.482270 |
| 13.0 | 11.0934 | 28.5095 | 0.485910 | 0.483550 |
| 14.0 | 11.9292 | 30.8318 | 0.486720 | 0.485160 |
| 15.0 | 12.7648 | 33.1554 | 0.487600 | 0.485520 |

TABLE XI: For the state $1s\sigma$ of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first-order phase-integral results, obtained from quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large, coincide for $p$ as well as for $A'$ with the numerically exact results obtained by Ponomarev and Puzynina [13] and quoted in this table as $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $p_{PP}$ | $A'_{PP}$ | $C$ | $\tilde{C}$ |
|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | |
| 0.2 | 0.855323 | -0.142128 | 0.494838 | 0.483907 |
| 0.4 | 1.66144 | -0.361348 | 0.509680 | 0.498740 |
| 0.6 | 2.46187 | -0.573808 | 0.506980 | 0.501340 |
| 0.8 | 3.26197 | -0.780407 | 0.505080 | 0.501930 |
| 1.0 | 4.06206 | -0.984350 | 0.504010 | 0.501980 |
| 2.0 | 8.06226 | -1.99219 | 0.501950 | 0.501460 |
| Sufficiently large $r_{12}$ | | | | |
| 3.0 | 12.0623 | -2.99479 | 0.501220 | 0.501160 |
| 4.0 | 16.0624 | -3.99609 | 0.501010 | 0.500800 |
| 5.0 | 20.0624 | -4.99687 | 0.500800 | 0.500700 |
| 6.0 | 24.0624 | -5.99724 | 0.500800 | 0.500800 |
| 7.0 | 28.0624 | -6.99764 | 0.500600 | 0.500700 |
| 8.0 | 32.0624 | -7.99793 | 0.500500 | 0.500620 |
| 9.0 | 36.0624 | -8.99816 | 0.500410 | 0.500600 |
| 10.0 | 40.0624 | -9.99834 | 0.500400 | 0.500600 |
| 11.0 | 44.0624 | -10.9985 | 0.500300 | 0.500500 |
| 12.0 | 48.0624 | -11.9986 | 0.500300 | 0.500500 |
| 13.0 | 52.0625 | -12.9987 | 0.500500 | 0.500300 |
| 14.0 | 56.0625 | -13.9988 | 0.500400 | 0.500300 |
| 15.0 | 60.0625 | -14.9989 | 0.500400 | 0.500200 |

TABLE XII: For the state $4d\sigma$ of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) the values of $C$ and $\tilde{C}$ have been obtained from the requirement that the first-order phase-integral results, obtained from quantization conditions that are appropriate depending on whether $r_{12}$ is sufficiently small or sufficiently large, coincide for $p$ as well as for $A'$ with the numerically exact results obtained by Ponomarev and Puzynina [13] and quoted in this table as $p_{PP}$ and $A'_{PP}$.

| $r_{12}$ | $p_{PP}$ | $A'_{PP}$ | $C$ | $\tilde{C}$ |
|---|---|---|---|---|
| Sufficiently small $r_{12}$ | | | | |
| 0.5 | 0.569166 | -6.466968 | 0.639180 | 0.552970 |
| 1.0 | 1.16192 | -7.82220 | 0.628280 | 0.547102 |
| 2.0 | 2.24564 | -11.5899 | 0.594960 | 0.535600 |
| Sufficiently large $r_{12}$ | | | | |
| 3.0 | 3.26096 | -15.1384 | 0.565392 | 0.511310 |
| 4.0 | 4.26518 | -18.4123 | 0.546141 | 0.510320 |
| 5.0 | 5.26597 | -21.5660 | 0.537100 | 0.512080 |
| 6.0 | 6.26552 | -24.6617 | 0.531130 | 0.513220 |
| 7.0 | 7.26468 | -27.7257 | 0.526900 | 0.513530 |
| 8.0 | 8.26374 | -30.7710 | 0.523520 | 0.513370 |
| 9.0 | 9.26283 | -33.8043 | 0.520970 | 0.513030 |
| 10.0 | 10.2620 | -36.8297 | 0.519020 | 0.512460 |
| 11.0 | 11.2612 | -39.8497 | 0.516950 | 0.512100 |
| 12.0 | 12.2605 | -42.8656 | 0.515510 | 0.511710 |
| 13.0 | 13.2599 | -45.8787 | 0.514440 | 0.511010 |
| 14.0 | 14.2594 | -48.8896 | 0.513870 | 0.510060 |
| 15.0 | 15.2589 | -51.8987 | 0.513060 | 0.509620 |

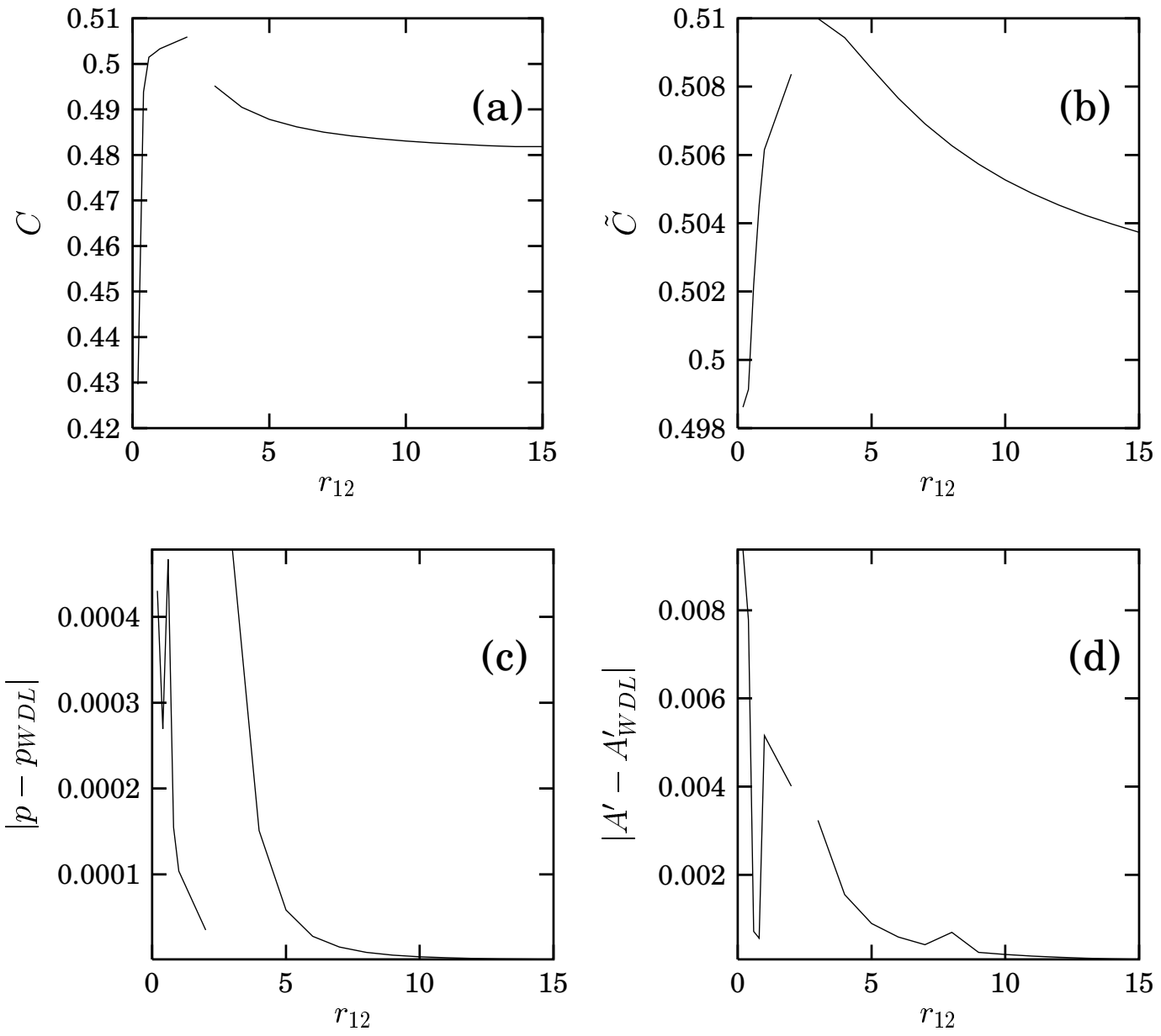


FIG. 1: Plots for the $1s\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) $C$ versus $r_{12}$, (b) $\tilde{C}$ versus $r_{12}$, (c) $|p - p_{WDL}|$ versus $r_{12}$ and (d) $|A' - A'_{WDL}|$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order and the third-order phase-integral results for $p$ as well as for $A'$ coincide. Here $p$ and $A'$ are the phase-integral values obtained in Table I, while $p_{WDL}$ and $A'_{WDL}$ are the corresponding numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan and Lane [4] (see p. 288-289 in [4]), and quoted in Table I. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

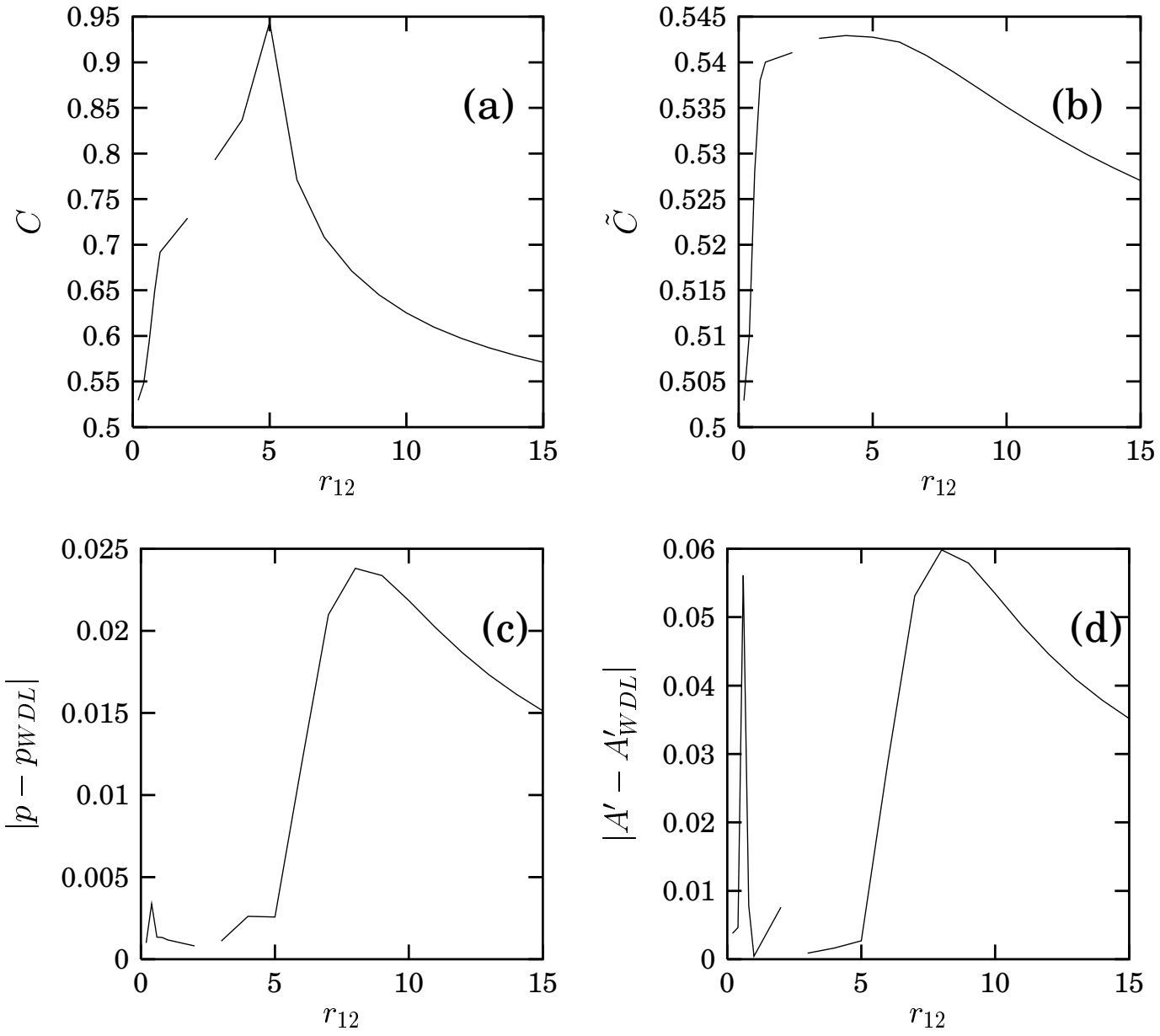


FIG. 2: Plots for the $2p\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) $C$ versus $r_{12}$, (b) $\tilde{C}$ versus $r_{12}$, (c) $|p - p_{WDL}|$ versus $r_{12}$ and (d) $|A' - A'_{WDL}|$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order and the third-order phase-integral results for $p$ as well as for $A'$ coincide. Here $p$ and $A'$ are the phase-integral values obtained in Table II, while $p_{WDL}$ and $A'_{WDL}$ are the corresponding numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan and Lane [4] (see p. 288-289 in [4]), and quoted in Table II. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

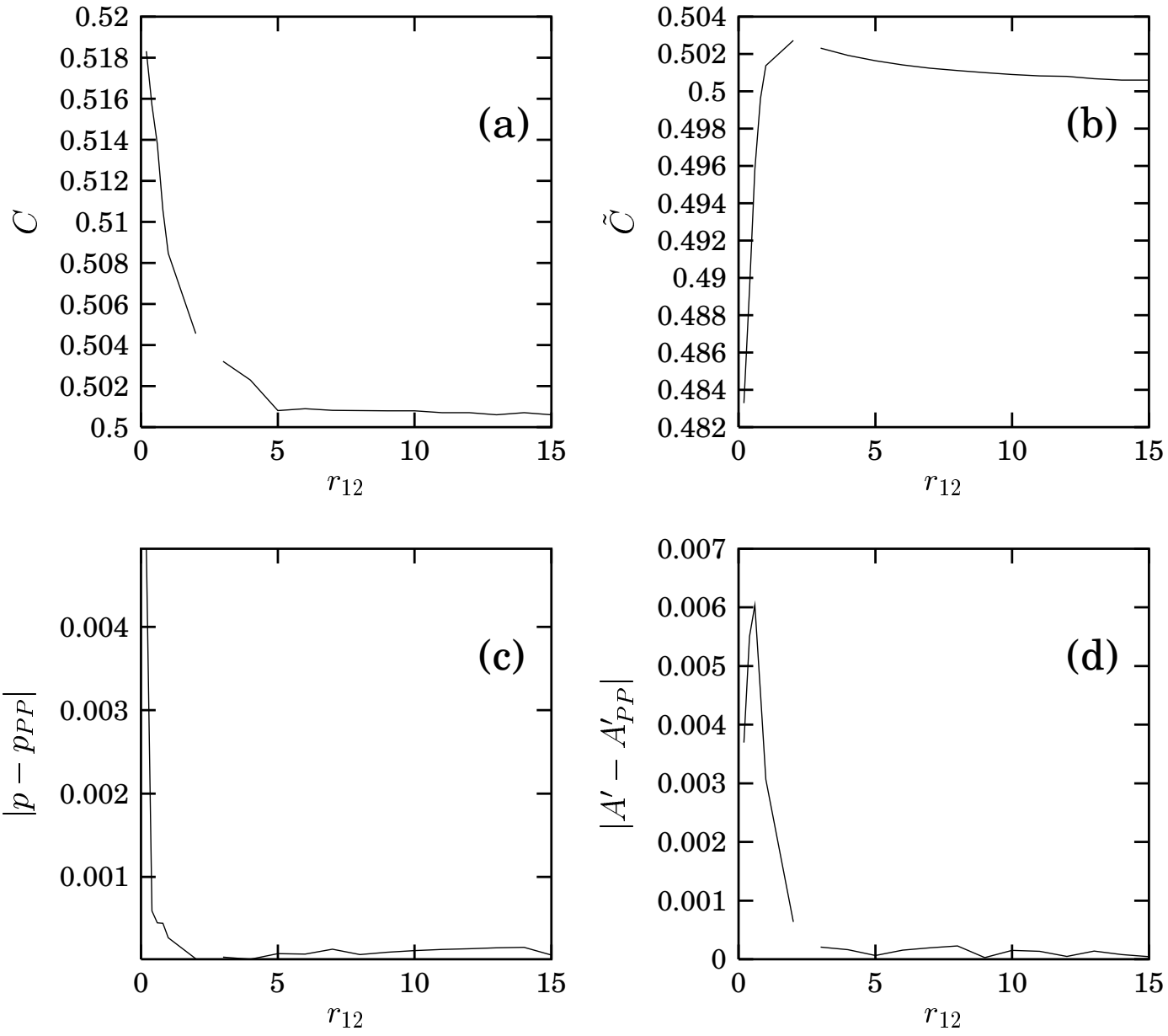


FIG. 3: Plots for the $1s\sigma$ state of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) of (a) $C$ versus $r_{12}$, (b) $\tilde{C}$ versus $r_{12}$, (c) $|p - p_{PP}|$ versus $r_{12}$ and (d) $|A' - A'_{PP}|$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order and the third-order phase-integral results for $p$ as well as for $A'$ coincide. Here $p$ and $A'$ are the phase-integral values obtained in Table III, while $p_{PP}$ and $A'_{PP}$ are the corresponding numerically exact values obtained by Ponomarev and Puzynina [13] and quoted Table III. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

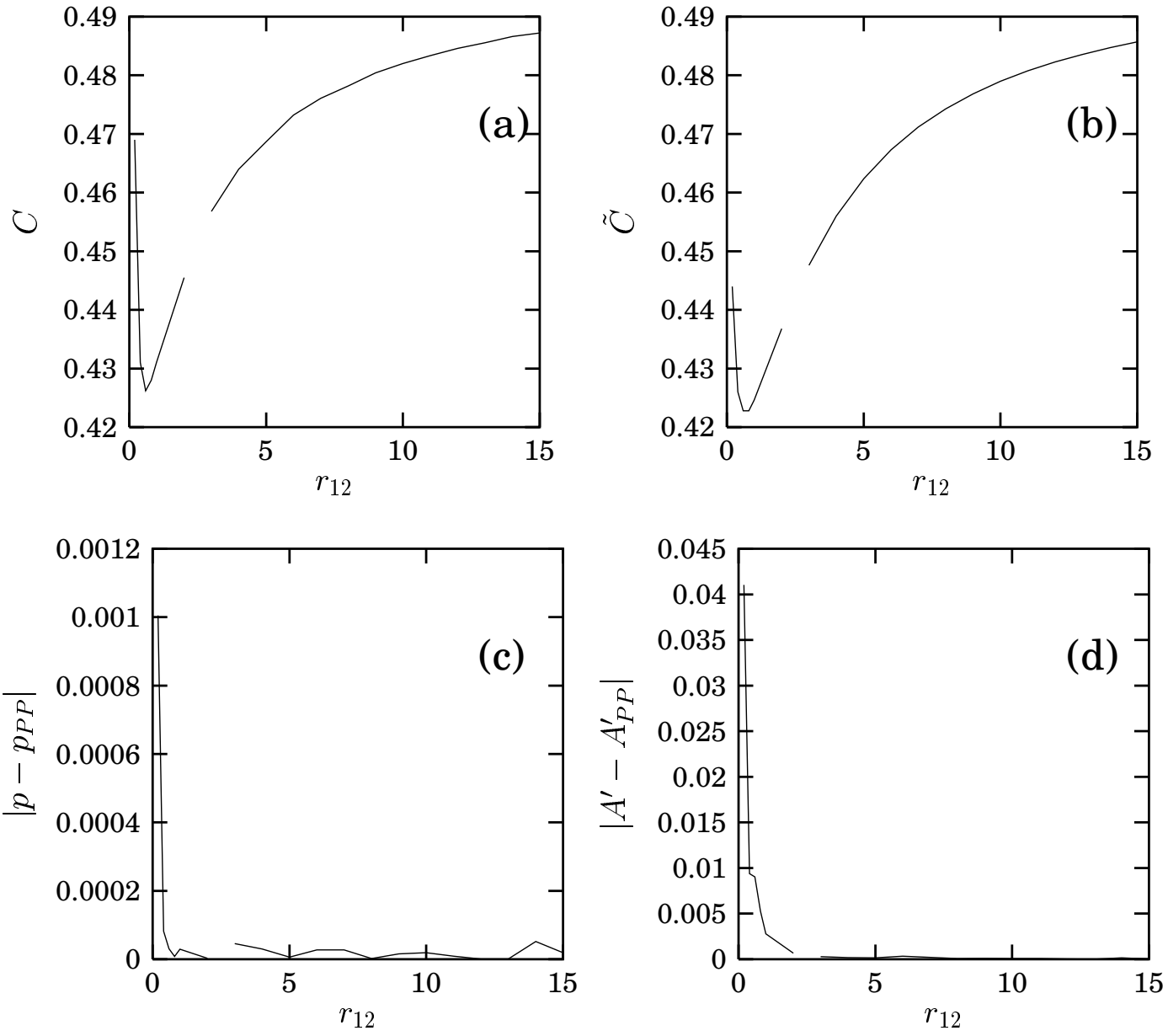


FIG. 4: Plots for the $3s\sigma$ state of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) of (a) $C$ versus $r_{12}$, (b) $\tilde{C}$ versus $r_{12}$, (c) $|p - p_{PP}|$ versus $r_{12}$ and (d) $|A' - A'_{PP}|$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order and the third-order phase-integral results for $p$ as well as for $A'$ coincide. Here $p$ and $A'$ are the phase-integral values obtained in Table IV, while $p_{PP}$ and $A'_{PP}$ are the corresponding numerically exact values obtained by Ponomarev and Puzynina [13] and quoted in Table IV. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

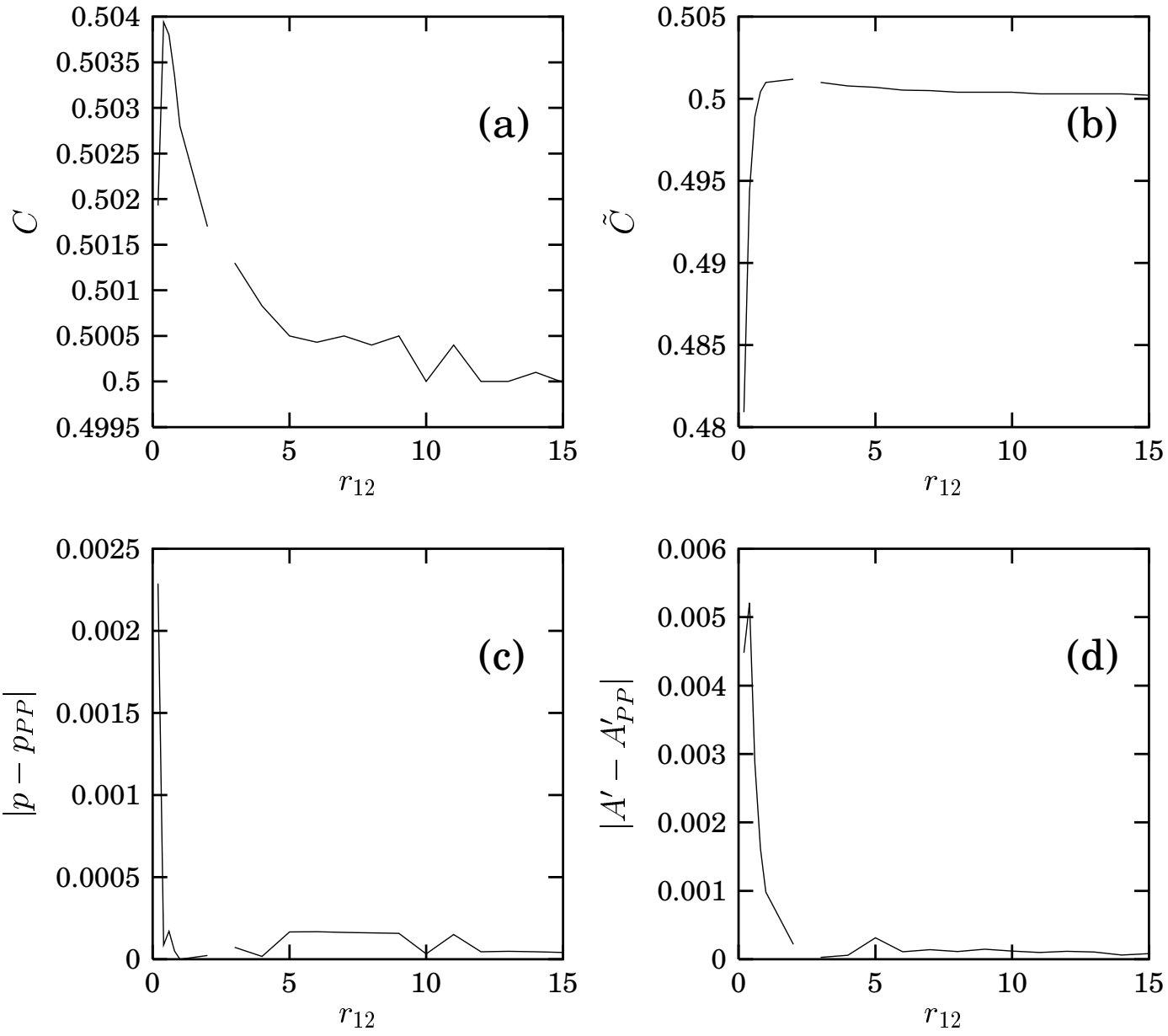


FIG. 5: Plots for the $1s\sigma$ state of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) of (a) $C$ versus $r_{12}$, (b) $\tilde{C}$ versus $r_{12}$, (c) $|p - p_{PP}|$ versus $r_{12}$ and (d) $|A' - A'_{PP}|$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order and the third-order phase-integral results for $p$ as well as for $A'$ coincide. Here $p$ and $A'$ are the phase-integral values obtained in Table V, while $p_{PP}$ and $A'_{PP}$ are the corresponding numerically exact values obtained by Ponomarev and Puzynina [13] and quoted in Table V. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

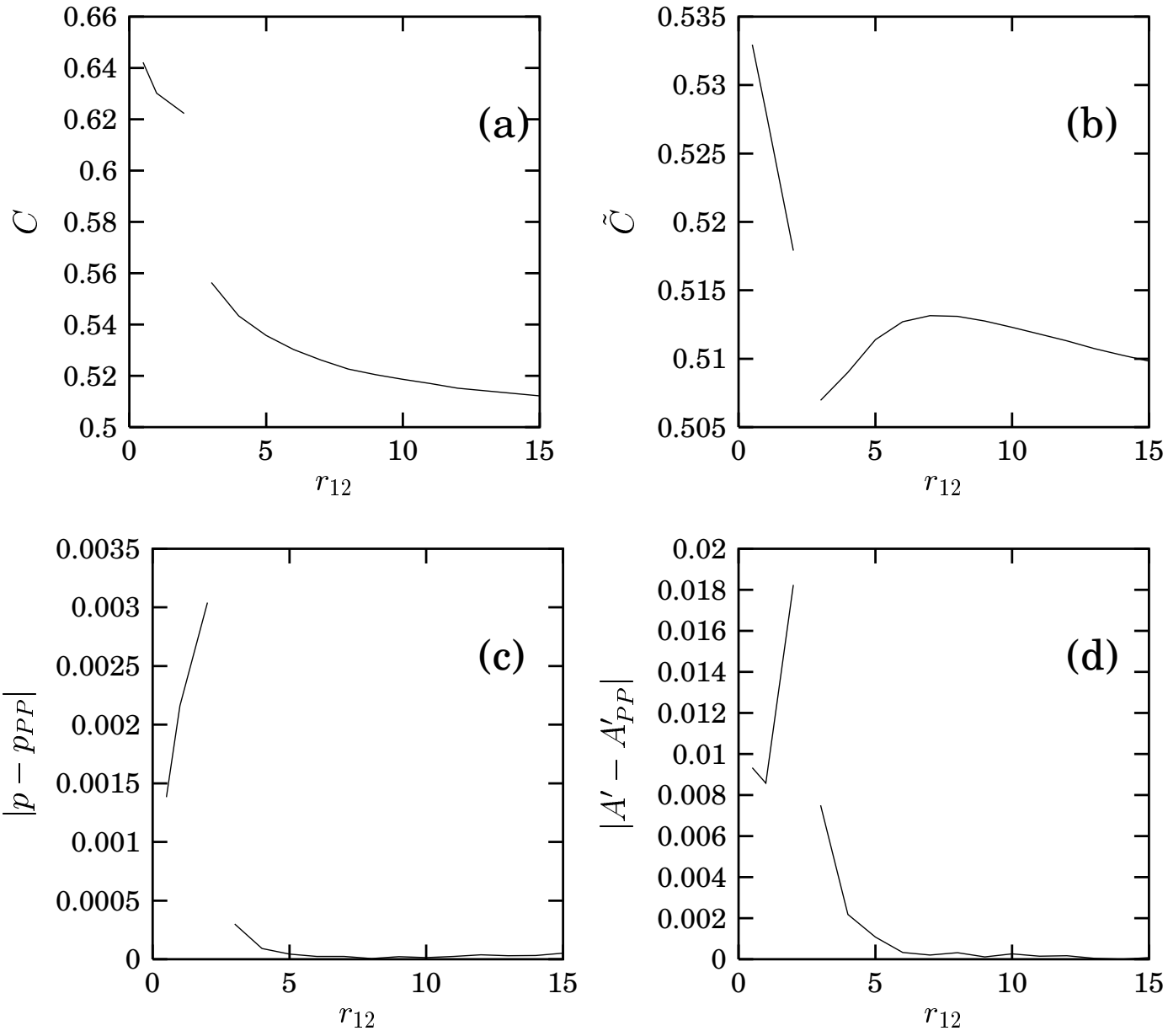


FIG. 6: Plots for the $4d\sigma$ state of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) of (a) $C$ versus $r_{12}$, (b) $\tilde{C}$ versus $r_{12}$, (c) $|p - p_{PP}|$ versus $r_{12}$ and (d) $|A' - A'_{PP}|$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order and the third-order phase-integral results for $p$ as well as for $A'$ coincide. Here $p$ and $A'$ are the phase-integral values obtained in Table VI, while $p_{PP}$ and $A'_{PP}$ are the corresponding numerically exact values obtained by Ponomarev and Puzynina [13] and quoted in Table VI. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

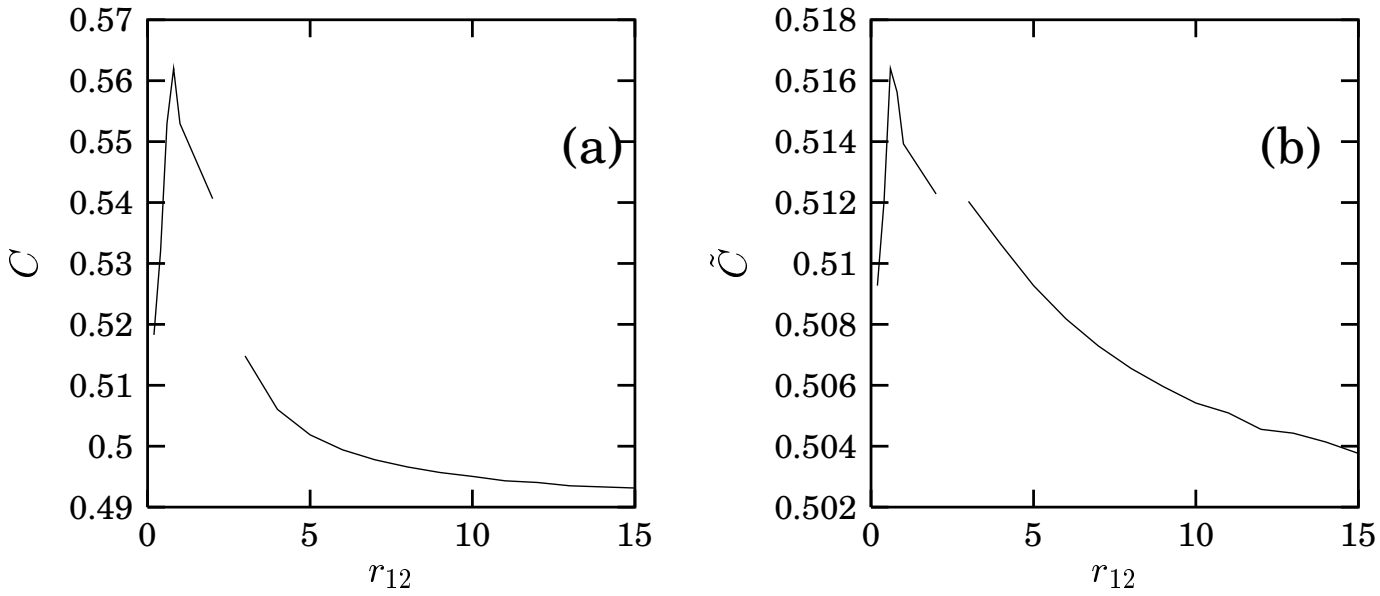


FIG. 7: Plots for the $1s\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) $C$ versus $r_{12}$ and (b) $\tilde{C}$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order phase-integral results and the numerically exact results obtained by Winter *et al.* [4] coincide. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

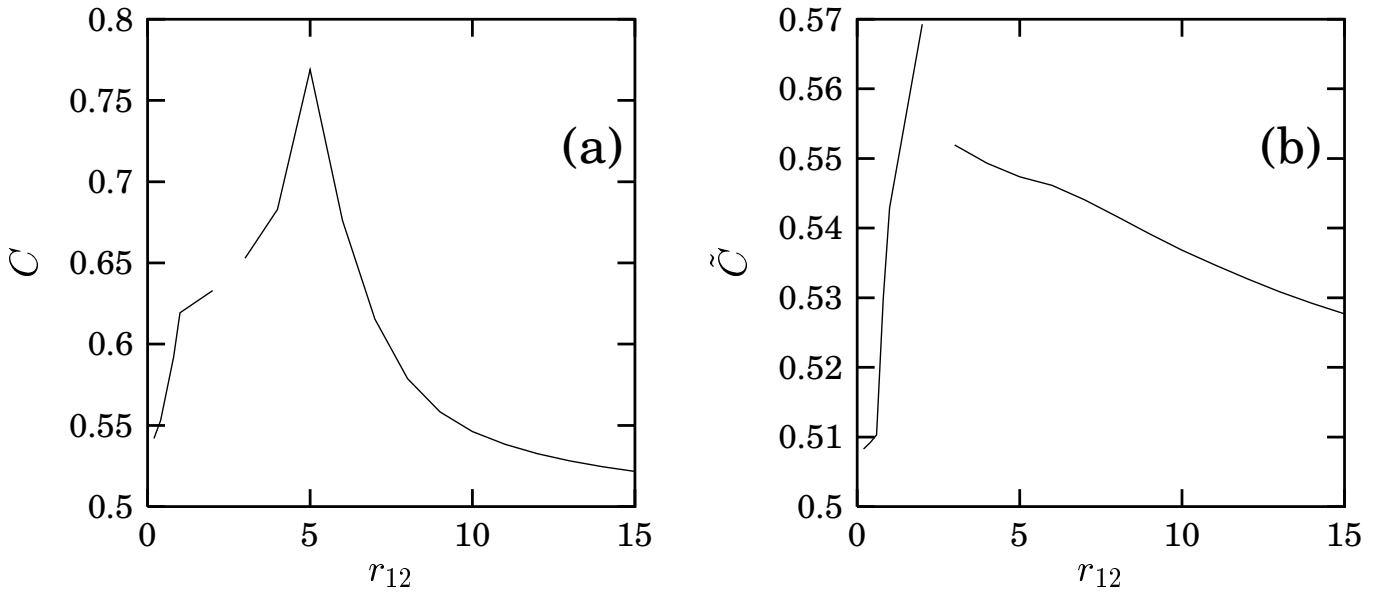


FIG. 8: Plots for the $2p\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) $C$ versus $r_{12}$ and (b) $\tilde{C}$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order phase-integral results and the numerically exact results obtained by Winter *et al.* [4] coincide. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

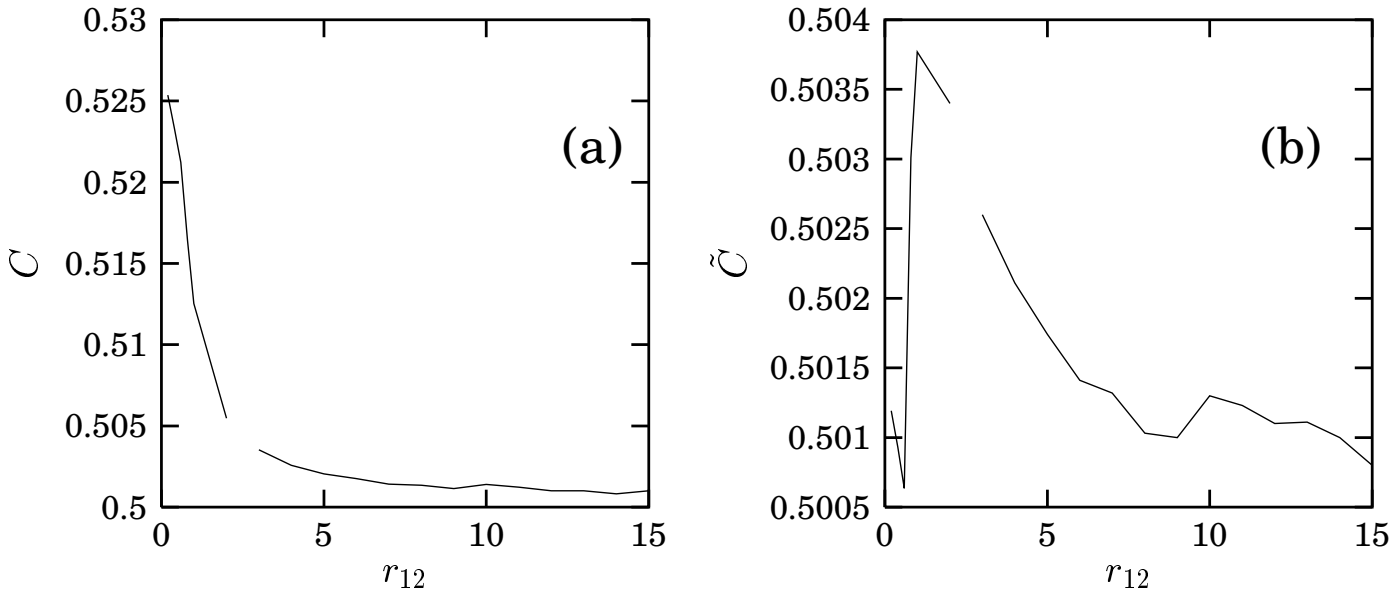


FIG. 9: Plots for the $1s\sigma$ state of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) of (a) $C$ versus $r_{12}$ and (b) $\tilde{C}$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order phase-integral results and the numerically exact results obtained by Ponomarev and Puzynina [13] coincide. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

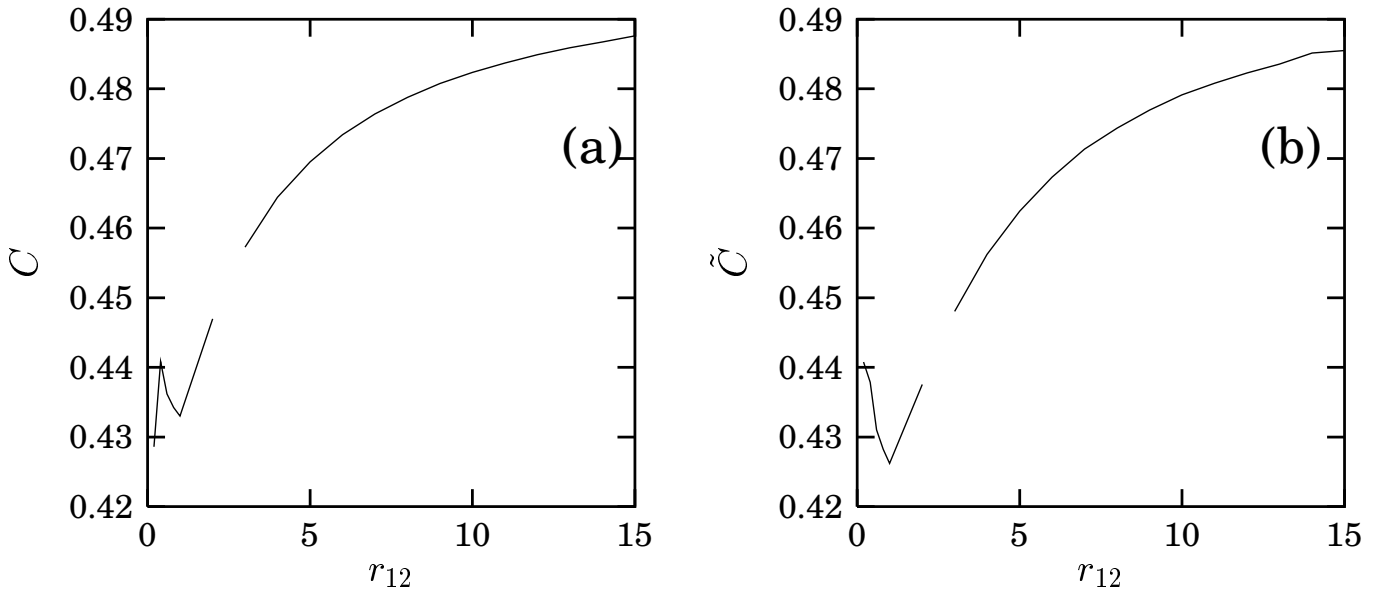


FIG. 10: Plots for the $3s\sigma$ state of the ion $peB^{5+}$ ($Z_1 = 1, Z_2 = 5$) of (a) $C$ versus $r_{12}$ and (b) $\tilde{C}$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order phase-integral results and the numerically exact results obtained by Ponomarev and Puzynina [13] coincide. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

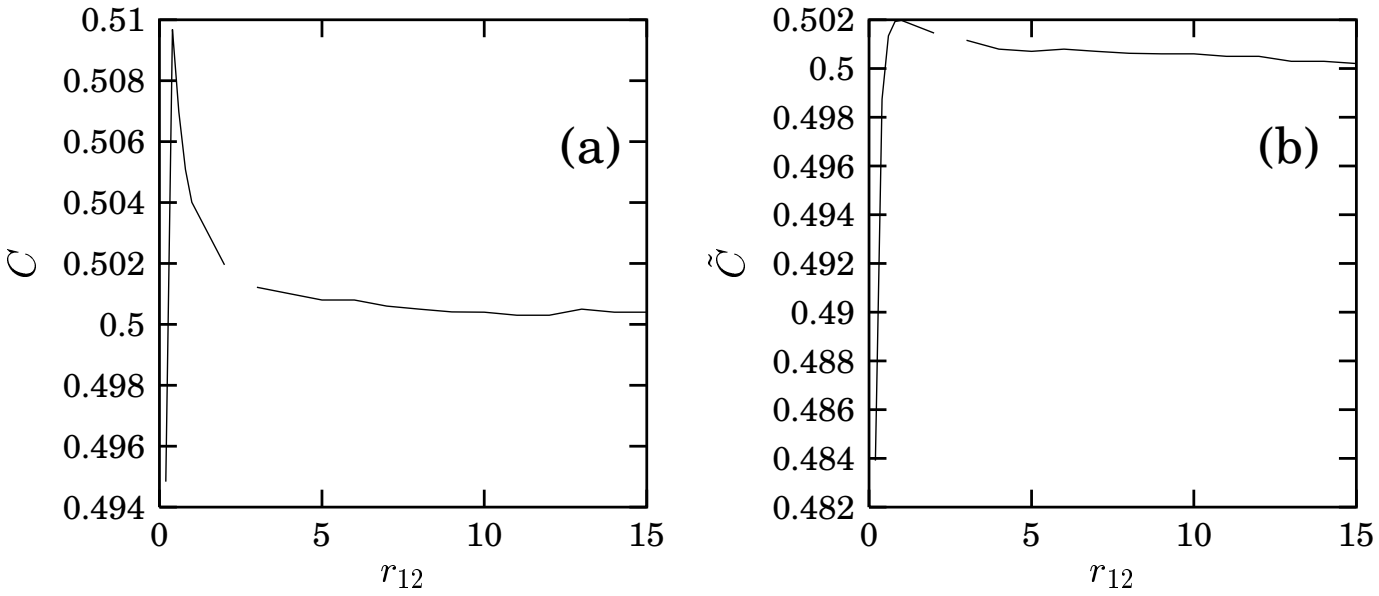


FIG. 11: Plots for the $1s\sigma$ state of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) of (a) $C$ versus $r_{12}$ and (b) $\tilde{C}$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order phase-integral results and the numerically exact results obtained by Ponomarev and Puzynina [13] coincide. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.

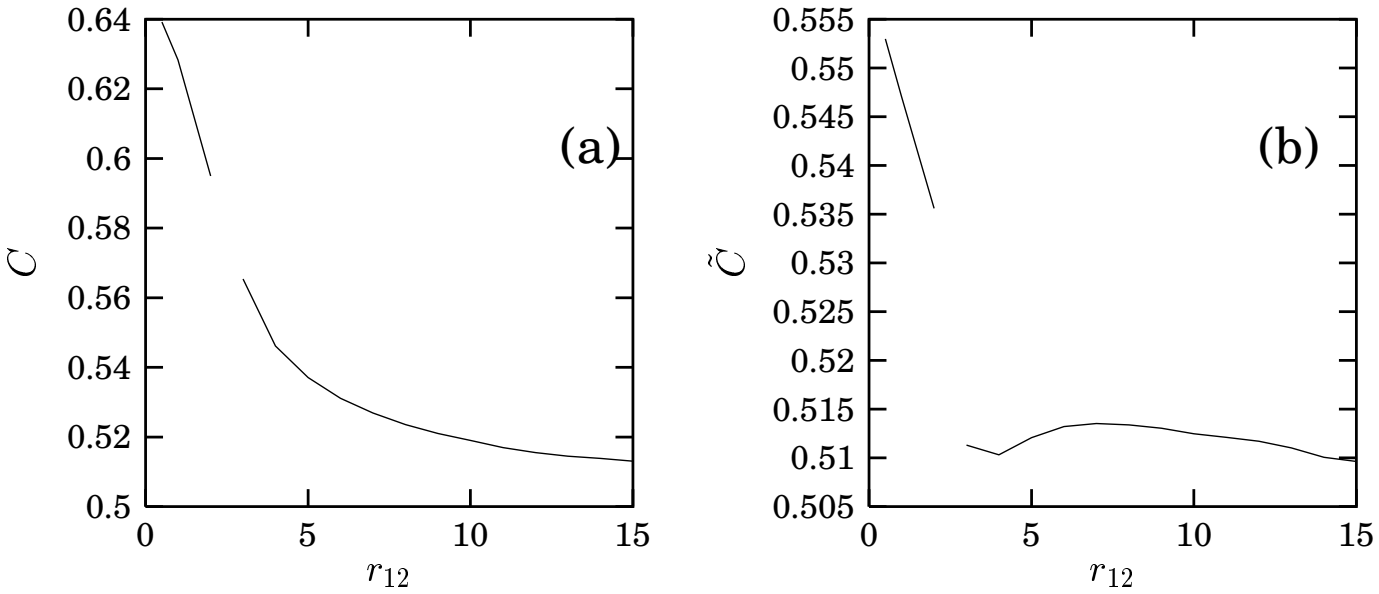


FIG. 12: Plots for the $4d\sigma$ state of the ion $peO^{8+}$ ($Z_1 = 1, Z_2 = 8$) of (a) $C$ versus $r_{12}$ and (b) $\tilde{C}$ versus $r_{12}$, when $C$ and $\tilde{C}$ are determined as functions of $r_{12}$ from the requirement that the first-order phase-integral results and the numerically exact results obtained by Ponomarev and Puzynina [13] coincide. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of $r_{12}$ have been used.