

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

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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.

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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 π^- 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 π^- 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 ξ - and η -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 η -quantization conditions were performed with the use of particular transformations in a rather simple way, while for the quantity \tilde{L} in the ξ -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

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As a consequence, the evaluation of the contour integrals in the cases of the ξ -equation and the η -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 ν_1, ν_2, ν_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 α, β (which may now be different from α), 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 η -part of the quantization conditions in [10]. For the ξ -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 comparison 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 α, β and \bar{K} pertaining to the η -equation: Subbarrier case [Fig. 3(a) in Ref. 11]*

Denoting the zeros η_1, η_2, η_3 and η_4 by a, b, c and d , we write the base function for this case as

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

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

$$\eta = \frac{a - d\nu_1^2 \operatorname{sn}^2 u}{1 - \nu_1^2 \operatorname{sn}^2 u}, \quad (2.2)$$

the parameter ν_1^2 being defined in (2.4) below. Noting that the loop $a \rightarrow b \rightarrow a$, that is $\eta_1 \rightarrow \eta_2 \rightarrow \eta_1$ in the η -plane, denoted by $\Gamma_{a,b}$, which represents the contour Λ_α in Fig. 3(a) of [11], corresponds to $0 \rightarrow K \rightarrow 2K$ in the u -plane, one finds that the first-order contribution to α is

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

where

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

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

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

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

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 ν_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 α is found to be

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

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 ν_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 β . The loop $d \rightarrow c \rightarrow d$, that is $\eta_4 \rightarrow \eta_3 \rightarrow \eta_4$ in the η -plane, denoted by $\Gamma_{d,c}$ and represented by the contour Λ_β in Fig. 3(a) of [11], corresponds to $0 \rightarrow K \rightarrow 2K$ in the u -plane, and hence the first- and third-order contributions to β are

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

and

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

where now

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

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

Similarly one obtains

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

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

where now

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

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

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

According to eq. (3.18a) in [11] the integrals α' and β' 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 ξ -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 η -equation.

2.2.1. The quantities $\alpha, \beta, \bar{K}, L$ and L' pertaining to the η -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 η_2 and η_3 by c and c^* , we have the base function

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

Defining

$$c = b_1 - ia_1, \quad c^* = b_1 + ia_1, \quad (2.14)$$

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

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

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

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

Here we exploit the fact that the Jacobian elliptic functions are doubly periodic, one of the periods being complex. Thus the loop $d \rightarrow a_1 + ib_1 \rightarrow d$, that is $\eta_4 \rightarrow \eta_3 \rightarrow \eta_4$ in the η -plane, denoted by Γ_{d,c^*} , for the contour Λ_β in Fig. 4(a) of [11], corresponds in the u -plane to the path $0 \rightarrow K + iK' \rightarrow 2K + 2iK'$, 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 β

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

where

$$\nu_1 = \frac{A - B}{A + B}, \quad (2.18a)$$

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

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

$$g = \frac{1}{\sqrt{AB}}, \quad (2.18d)$$

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

Similarly one can treat the corresponding integrals in the first-order expressions for α , 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

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

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

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

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

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

and

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

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

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

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

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

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

$$Z = 2\nu_1(\nu_1\nu_2 + \nu_1\nu_3 + 4\nu_2\nu_3), \quad (2.23c)$$

where the parameters ν_1, ν_2, ν_3, g and k^2 are defined in (2.18a-e).

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

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

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

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

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

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

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

where ν_1, ν_2, ν_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 α' and β' associated with the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 4(a) in [11] are obtained from α and β by means of the relations (3.18a) in [11], that is, $\alpha' = \alpha + \frac{\Delta\pi}{2}$ and $\beta' = \beta + \frac{\Delta\pi}{2}$. The integrals L and L' associated with the contours Λ_L and $\Lambda_{L'}$ in Fig. 4(a) in [11] can be obtained from α and β 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 ξ -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 $a \rightarrow -1$ and $d \rightarrow +1$ in the case of the η -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 α , β and \bar{K} pertaining to the η -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 α , β and K , respectively. Here the base function reads as

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

The first- and third-order contributions to α are

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

and

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

where

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

Similarly the first- and third-order contributions to β are

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

and

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

with

$$\nu^2 = \frac{1-b}{1-c}, \quad (3.5)$$

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

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

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

and

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

with

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

and g defined in (3.3).

3.1.2. *The quantities \tilde{L} and \tilde{L}' pertaining to the ξ -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 α, β and \bar{K} pertaining to the η 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

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

and

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

where

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

with

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

and

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

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

We now have

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

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

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

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

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

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

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 σ -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.

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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

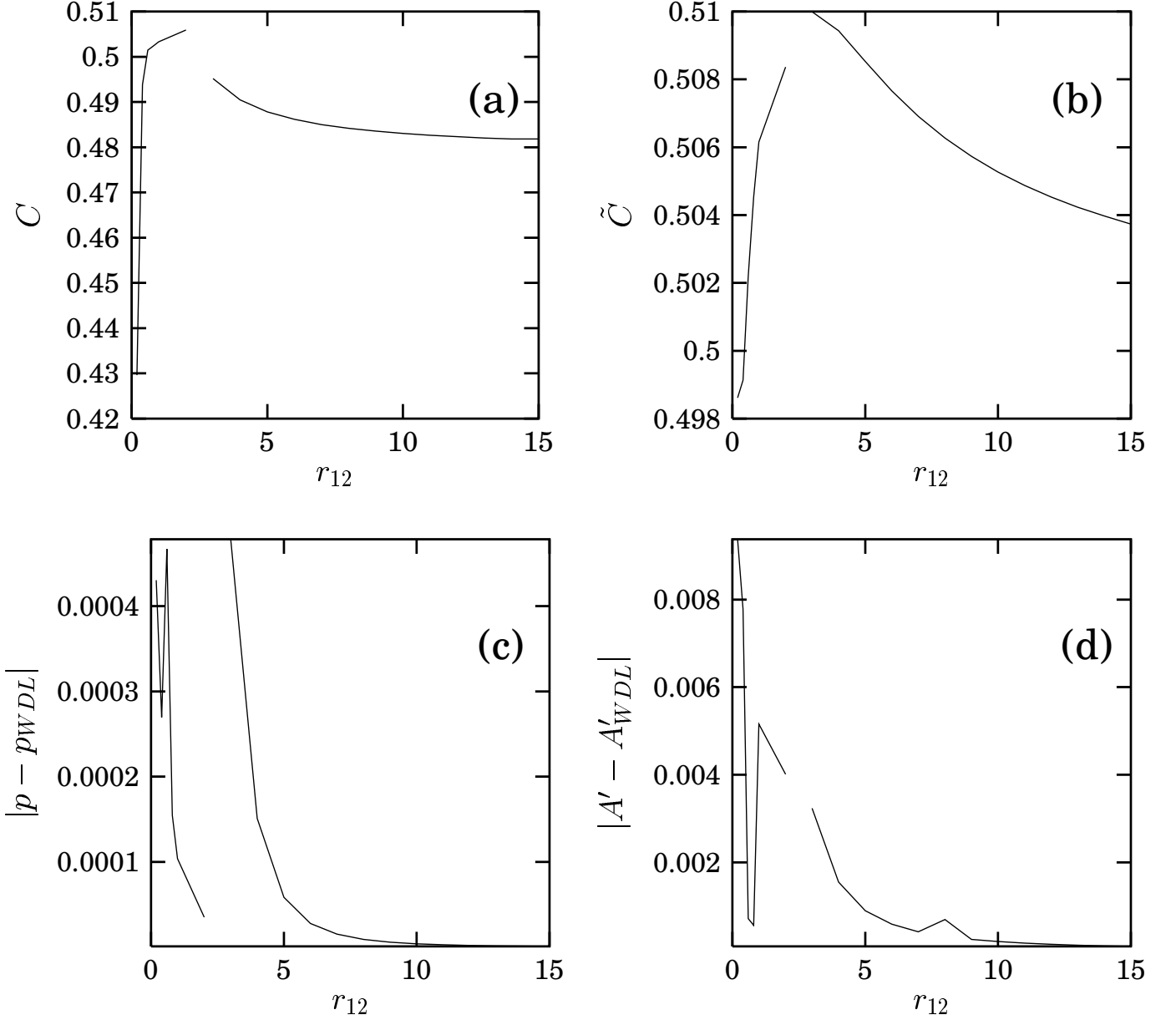


FIG. 1: Plots for the $1s\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) C versus r_{12} , (b) \tilde{C} versus r_{12} , (c) $|p - p_{WDL}|$ versus r_{12} and (d) $|A' - A'_{WDL}|$ versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the 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.

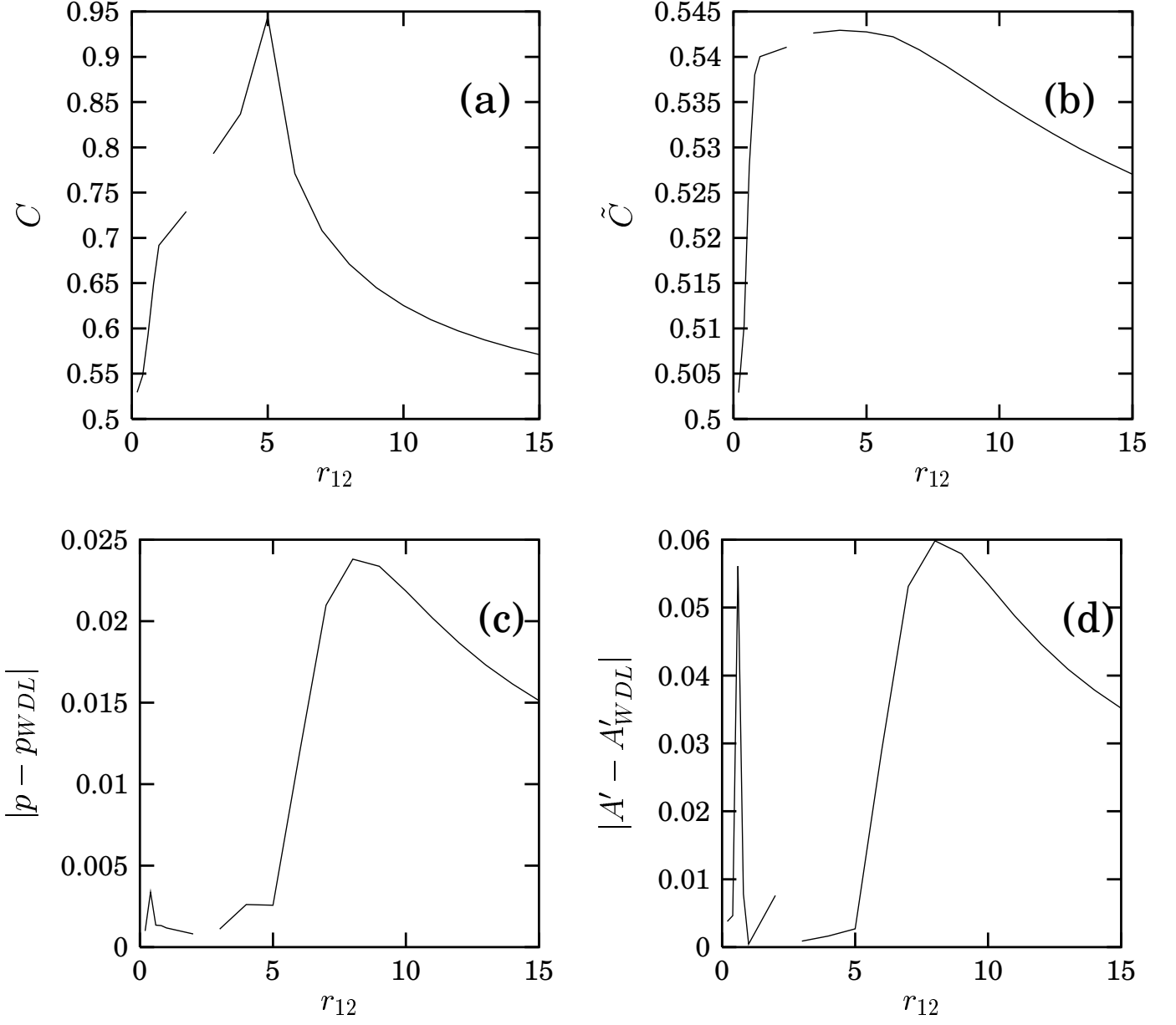


FIG. 2: Plots for the $2p\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) C versus r_{12} , (b) \tilde{C} versus r_{12} , (c) $|p - p_{WDL}|$ versus r_{12} and (d) $|A' - A'_{WDL}|$ versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the 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.

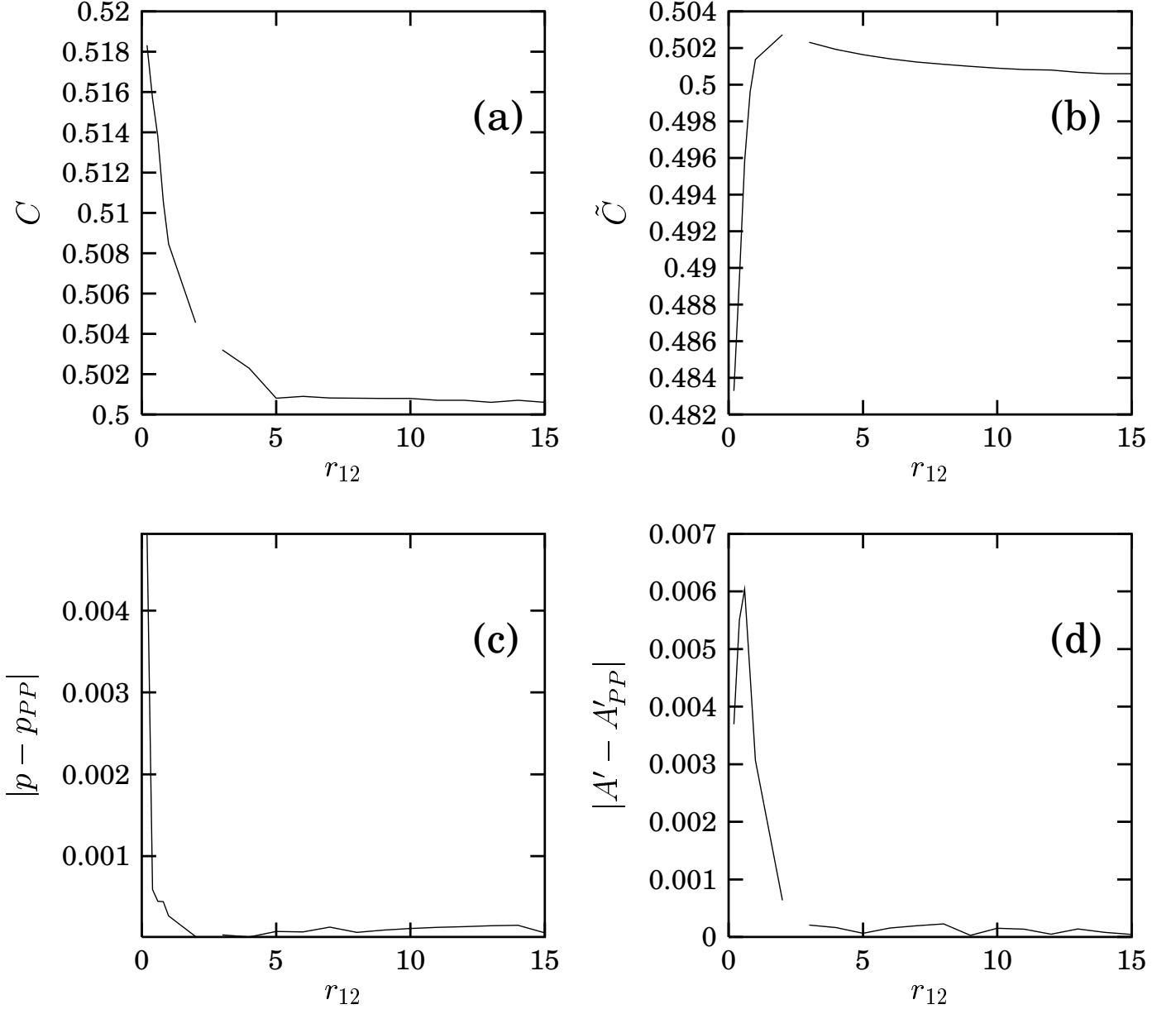


FIG. 3: Plots for the $1s\sigma$ state of the ion peB^{5+} ($Z_1 = 1, Z_2 = 5$) of (a) C versus r_{12} , (b) \tilde{C} versus r_{12} , (c) $|p - p_{PP}|$ versus r_{12} and (d) $|A' - A'_{PP}|$ versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order 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.

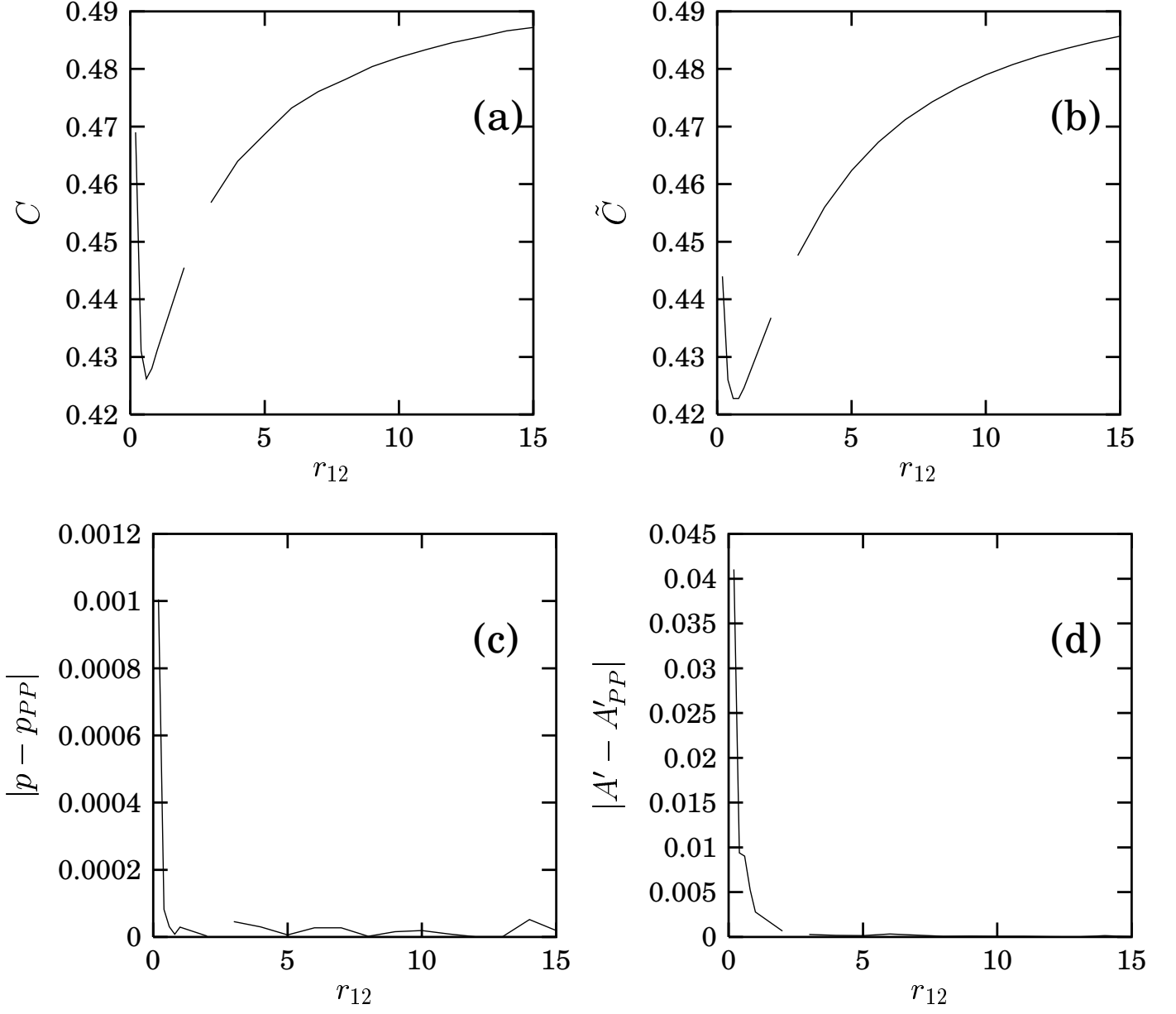


FIG. 4: Plots for the $3s\sigma$ state of the ion peB^{5+} ($Z_1 = 1, Z_2 = 5$) of (a) C versus r_{12} , (b) \tilde{C} versus r_{12} , (c) $|p - p_{PP}|$ versus r_{12} and (d) $|A' - A'_{PP}|$ versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order 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.

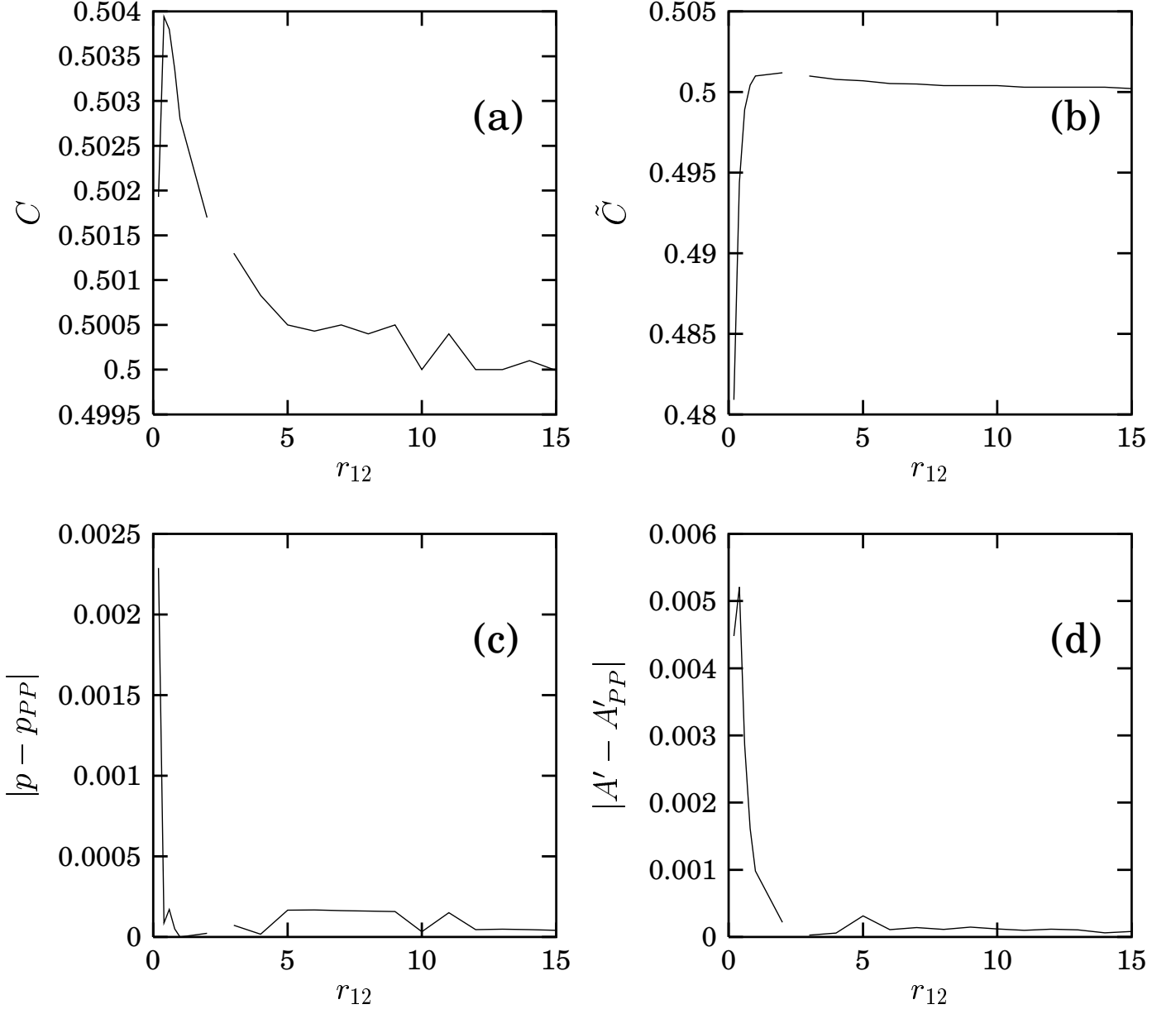


FIG. 5: Plots for the 1σ state of the ion peO^{8+} ($Z_1 = 1, Z_2 = 8$) of (a) C versus r_{12} , (b) \tilde{C} versus r_{12} , (c) $|p - p_{PP}|$ versus r_{12} and (d) $|A' - A'_{PP}|$ versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order 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.

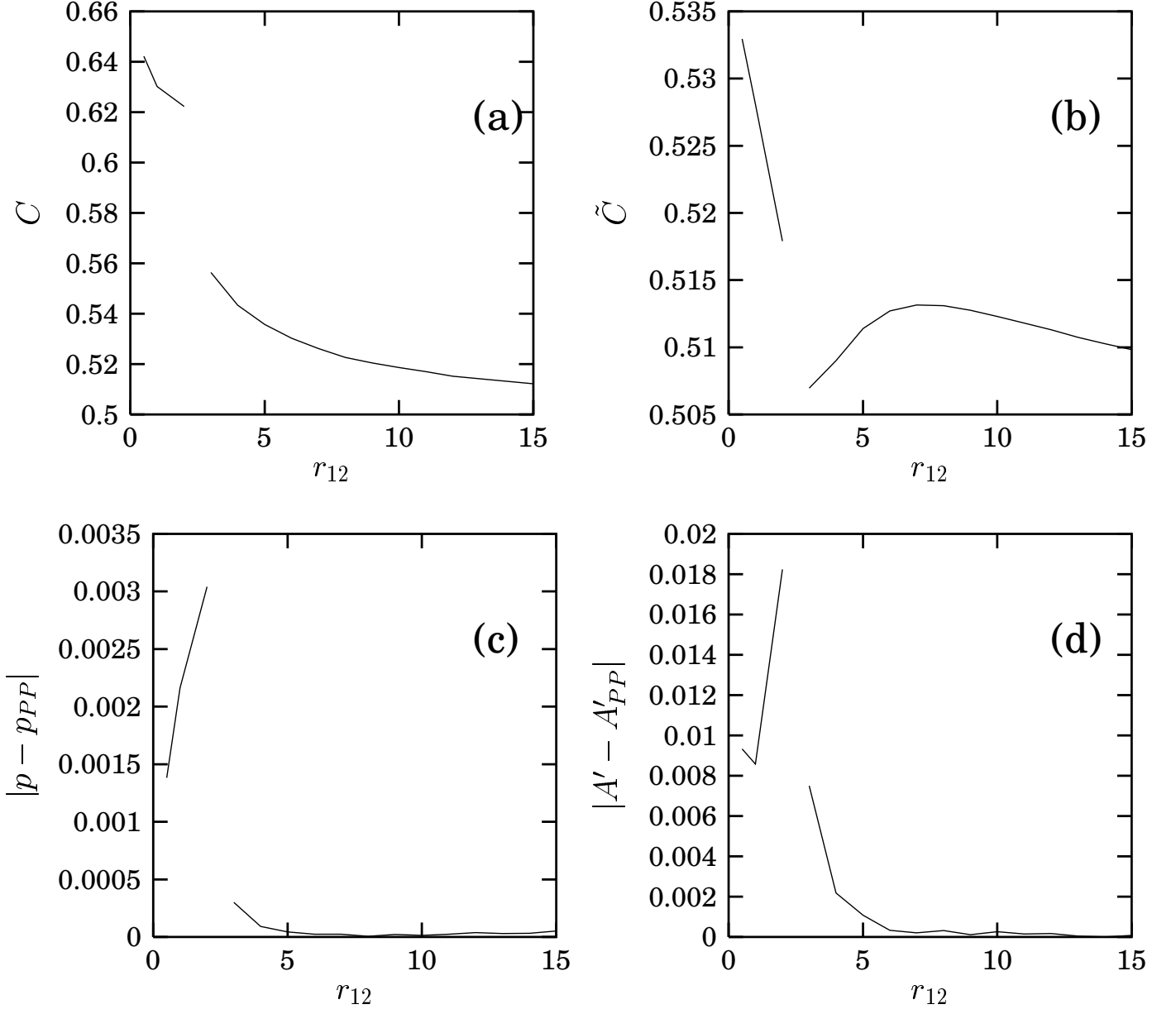


FIG. 6: Plots for the $4d\sigma$ state of the ion peO^{8+} ($Z_1 = 1, Z_2 = 8$) of (a) C versus r_{12} , (b) \tilde{C} versus r_{12} , (c) $|p - p_{PP}|$ versus r_{12} and (d) $|A' - A'_{PP}|$ versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order 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.

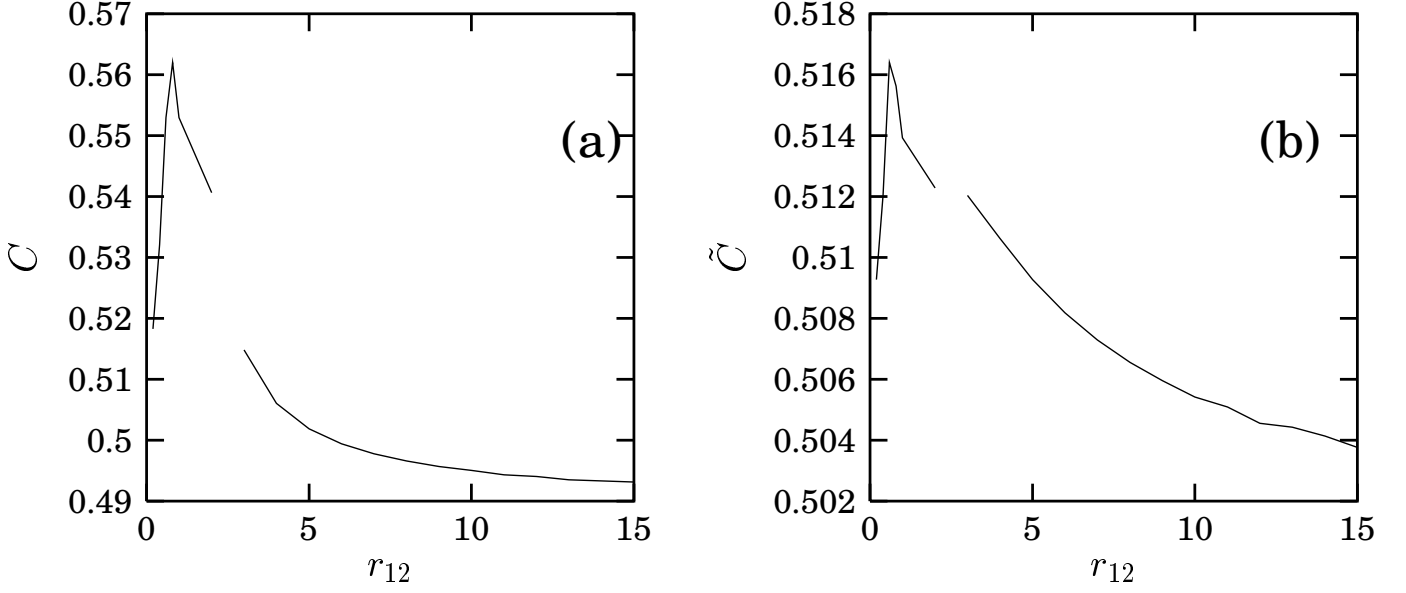


FIG. 7: Plots for the $1s\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) C versus r_{12} and (b) \tilde{C} versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order phase-integral results and the numerically exact results obtained 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.

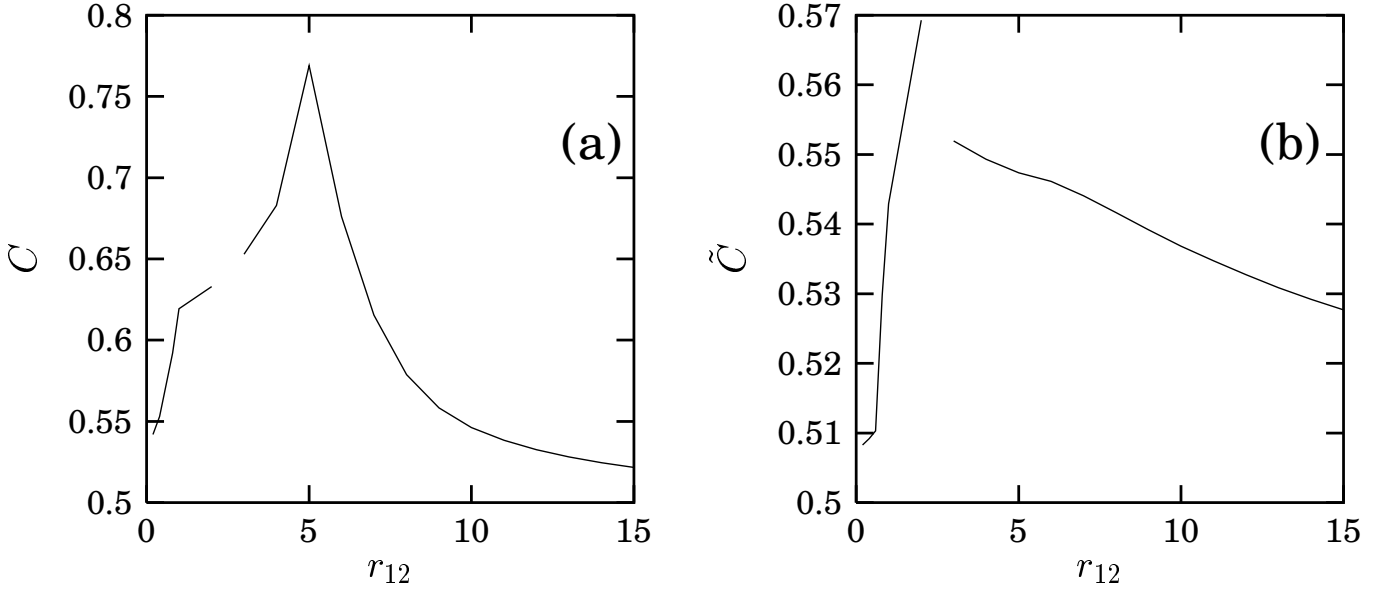


FIG. 8: Plots for the $2p\sigma$ state of the ion $peHe^{2+}$ ($Z_1 = 1, Z_2 = 2$) of (a) C versus r_{12} and (b) \tilde{C} versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order phase-integral results and the numerically exact results obtained 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.

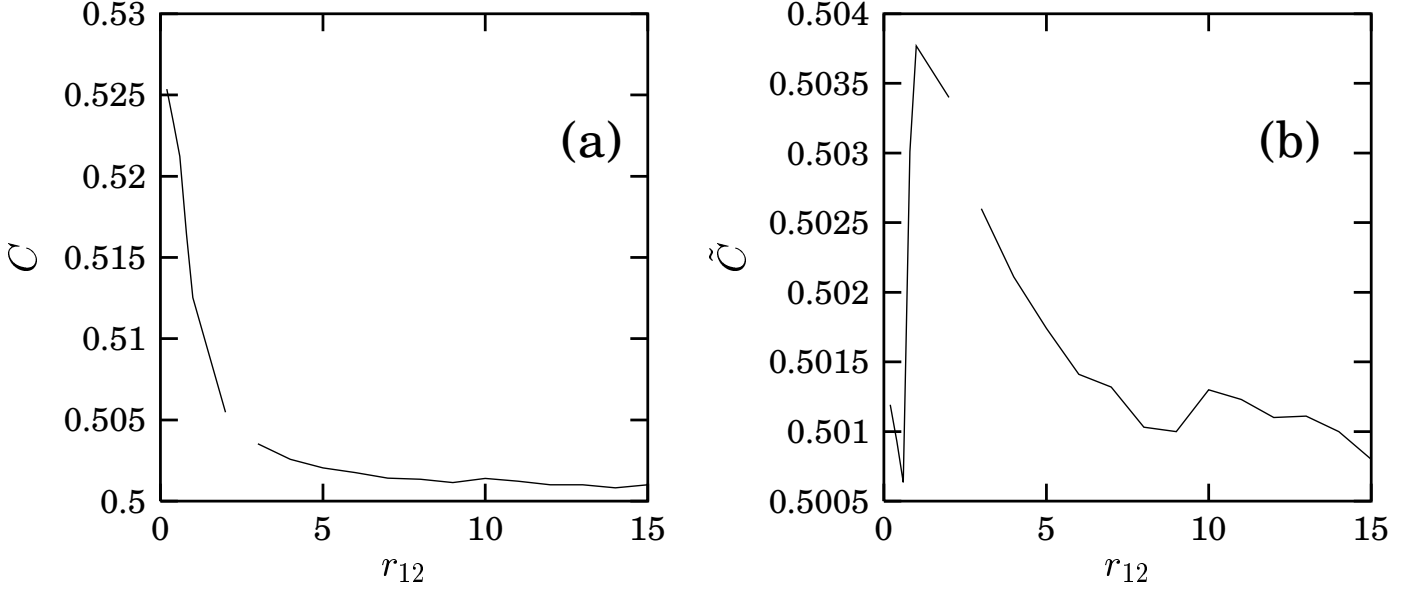


FIG. 9: Plots for the $1s\sigma$ state of the ion peB^{5+} ($Z_1 = 1, Z_2 = 5$) of (a) C versus r_{12} and (b) \tilde{C} versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order phase-integral results and the numerically exact results obtained 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.

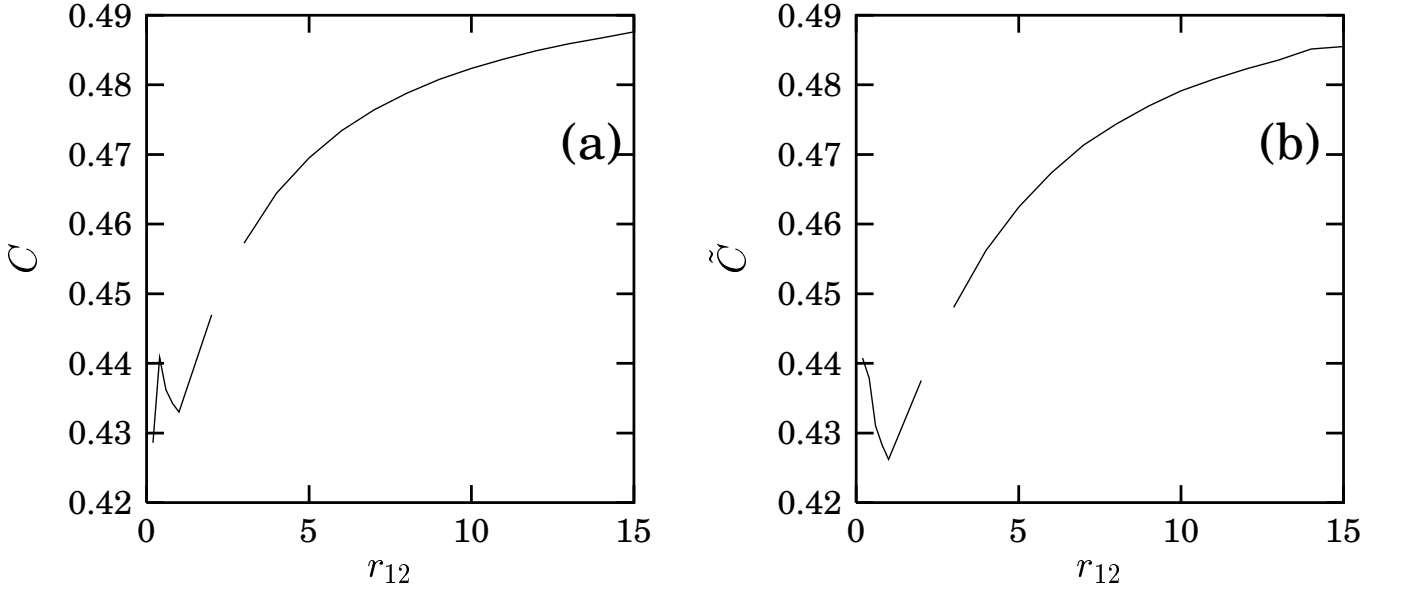


FIG. 10: Plots for the $3s\sigma$ state of the ion peB^{5+} ($Z_1 = 1, Z_2 = 5$) of (a) C versus r_{12} and (b) \tilde{C} versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order phase-integral results and the numerically exact results obtained 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.

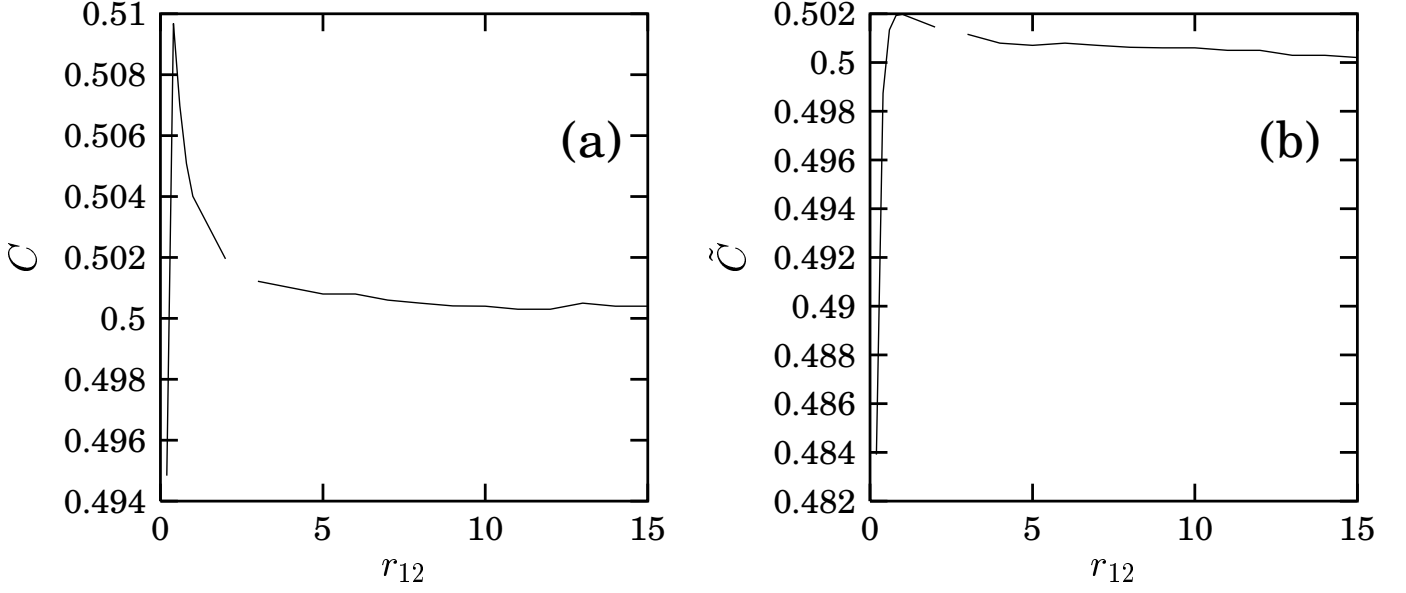


FIG. 11: Plots for the $1s\sigma$ state of the ion peO^{8+} ($Z_1 = 1, Z_2 = 8$) of (a) C versus r_{12} and (b) \tilde{C} versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order phase-integral results and the numerically exact results obtained 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.

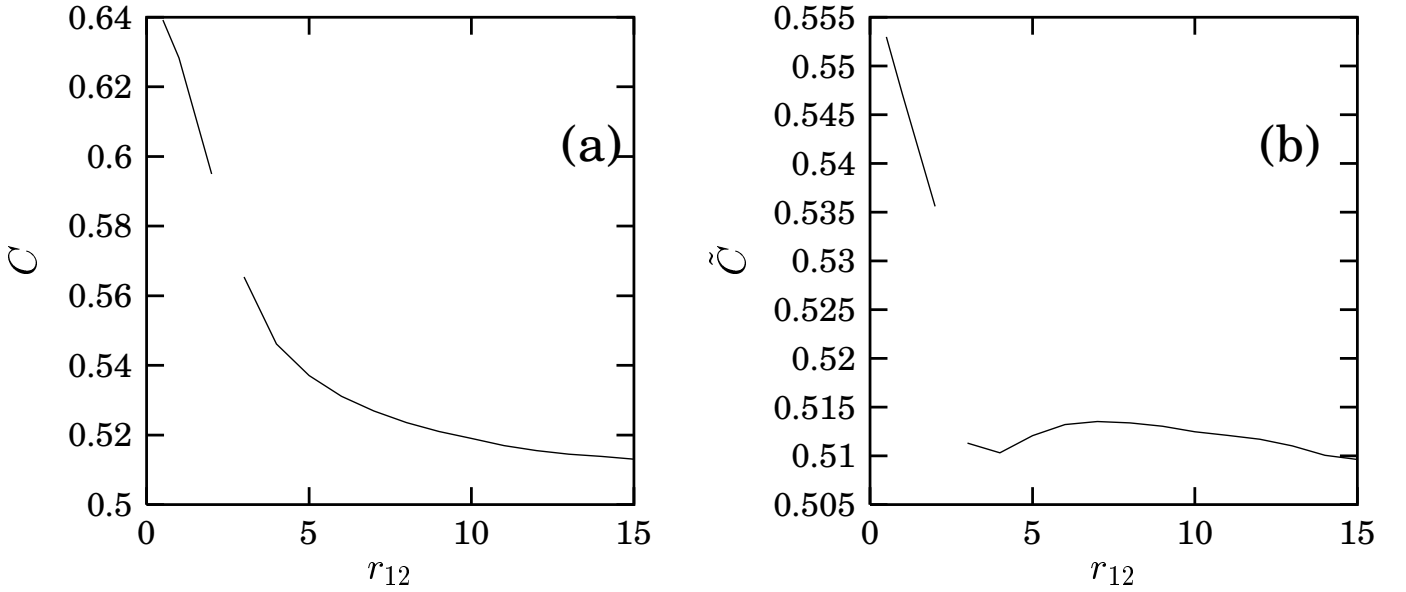


FIG. 12: Plots for the $4d\sigma$ state of the ion peO^{8+} ($Z_1 = 1, Z_2 = 8$) of (a) C versus r_{12} and (b) \tilde{C} versus r_{12} , when C and \tilde{C} are determined as functions of r_{12} from the requirement that the first-order phase-integral results and the numerically exact results obtained 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.