

Fine-structure effects in relativistic calculations of the static polarizability of the helium atom

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We use the relativistic configuration-interaction method and the model potential method to calculate the scalar and tensor components of the dipole polarizabilities for the excited states $1s3p^3P_0$ and $1s3p^3P_2$ of the helium atom. The calculations of the reduced matrix elements for the resonant terms in the spectral expansion of the polarizabilities are derived using two-electron basis functions of the relativistic Hamiltonian of the atom, a Hamiltonian that incorporates the Coulomb and Breit electron–electron interactions. We formulate a new approach to determining the parameters of the Fuss model potential. Finally, we show that the polarizability values are sensitive to the choice of the wave functions used in the calculations.

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1. INTRODUCTION

The anticrossing of atomic levels in an external field constitutes an effective method for precise measurements of the fine- and hyperfine-structure intervals and other spectroscopic constants, such as the exchange energy and the diagonal and off-diagonal matrix elements of the spin–orbit coupling operators. In a recent paper, Schumann *et al.*¹ studied the $0^- \times 0^-$ anticrossing of the $1s3p^3P_J$ ($J=0,2$) levels of helium by methods of high-resolution laser spectroscopy. At the anticrossing point, the error in measuring the fine-structure interval $\delta = E_{3^3P_0} - E_{3^3P_2}$ amounted to ± 5 MHz, and the use of microwave devices makes it possible to reduce this value by a factor of at least 100. Nevertheless, the degree of accuracy already achieved makes it possible to draw important conclusions concerning the optimum choice of theoretical approaches describing the effect of 100–200 kV cm⁻¹ electric fields on the spectrum of the helium atom.

In particular, the widely used semiempirical approach, which makes it possible to analyze the observed spectrum in terms of averaged values of the atomic Hamiltonian with allowance for relativistic corrections (either spin-dependent or spin-independent) of order α^2 Ry (Refs. 2 and 3), with α the fine-structure constant, does not require allowing for

higher-order perturbation effects, which are needed for a meaningful interpretation of the results of measurements. For this reason, Schumann *et al.*¹ justified the need to employ methods of quantum mechanics and quantum electrodynamics to analyze the results of measurements of the δ -to- $\delta^{(0)}$ ratio ($\delta^{(0)} = 8772.517(16)$ MHz is the fine-structure interval in a zero field⁴) at the point of anticrossing of the $1s3p^3P_0$ and $1s3p^3P_2$ levels of helium. Another interesting result of that paper was the possibility of studying the effects of spin–spin mixing of helium levels with different values of orbital angular momentum L but the same parity.^{5,6}

The aim of the present paper is to analyze theoretically the contribution of relativistic effects in calculations of the scalar and tensor components of dipole polarizabilities, which determine the shift and splitting of the $1s3p^3P_J$ ($J=0,2$) levels of helium. We employ two alternative approaches based on the relativistic configuration-interaction method⁷ and on the Fuss model potential method.⁸

2. ALLOWING FOR RELATIVISTIC EFFECTS IN CALCULATIONS OF DIPOLE POLARIZABILITIES OF THE HELIUM ATOM

The shift and splitting of a level $|nJLM\rangle$ in a uniform field F is described by the formula

$$\Delta E_{nJLM} = -\frac{1}{2} \alpha_{nJLM} F^2, \quad (1)$$

where the polarizability α_{nJLM} contains a scalar component (α_{nJL}^s) and a tensor component (α_{nJL}^t), i.e.,

$$\alpha_{nJLM} = \alpha_{nJL}^s + \alpha_{nJL}^t \frac{3M^2 - J(J+1)}{J(2J-1)}. \quad (2)$$

As the field strength F increases, the splitting of the level may reach values comparable to the distance between adjacent levels of the same parity (the components of the fine structure of an atomic multiplet). Hence in the case under investigation, i.e., the $1s3p^3P_0$ and $1s3p^3P_2$ levels and a field strength F of several hundred kilovolts per centimeter, the level shift $\Delta E_{nJLM} = E - E_{nJLM}$ can be found by solving the secular equation

$$\det \|\Delta E_{nJLM} \delta_{JJ'} - V_{JJ'}\| = 0. \quad (3)$$

Here the finite off-diagonal matrix elements $V_{JJ'}$ correspond to dipole transitions between the fine-structure components in second-order perturbation theory in the external field F .

To derive a formula describing the dependence of δ on F , we use the solutions of Eq. (3) and the definition of the scalar and tensor components of the polarizability (2). The result is

$$\begin{aligned} \delta &= \sqrt{\left[\delta^{(0)} - \frac{1}{2} F^2 (\alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s + \alpha_{3^3P_2}^t) \right]^2 + 2F^4 (\alpha_{3^3P_2}^t)^2} \\ &\simeq \delta^{(0)} - \frac{1}{2} F^2 (\alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s + \alpha_{3^3P_2}^t) \\ &\quad + \frac{F^4}{\delta^{(0)}} (\alpha_{3^3P_2}^t)^2 + \dots \end{aligned} \quad (4)$$

This expression allows for the principal, or resonant, part of the hyperpolarizability (fourth-order corrections in the external field) of the interacting sublevels of the multiplet 3^3P_J with a zero projection of total angular momentum, $M=0$. The contribution of the nonresonant part to the hyperpolarizability is at most a few percent.⁹ In deriving (4) we allowed for the fact that the matrix element $V_{JJ'}$ is finite at $J'=J \pm 1, J \pm 2$ and contains only a tensor part, which depends on the projection M of the total angular momentum J . If we ignore the multiplet splitting $E_{nJL}^{(0)} - E_{nJ'L}^{(0)}$ in comparison to the energy difference $E_{nJL}^{(0)} - E_{n'J'L}^{(0)}$ between different multiplets with $n' \neq n$, the matrix element $V_{JJ'}$ can be expressed in terms of the tensor polarizability of the $1s3p^3P_2$ state. In this approximation the matrix element V_{02} is given by the formula¹⁾

$$V_{02} = -\frac{F^2}{\sqrt{2}} \alpha_{3^3P_2}^t. \quad (5)$$

The difference of the scalar polarizabilities in Eq. (4), $\alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s$, is determined by the contribution of relativistic effects, which means it is a small quantity of order α^2 .

Note that at $M=0$ the matrix element $V_{JJ \pm 1} \equiv 0$ (see, e.g., Ref. 10), so that the state 3^3P_1 remains isolated, i.e., does not mix with states with $J=0$ and $J=2$.

Equation (4) also implies that the minimum value for δ in an electric field (anticrossing of the fine-structure sublevels) is attained at

$$F = \bar{F} = \sqrt{\frac{2\delta^{(0)}(\alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s + \alpha_{3^3P_2}^t)}{(\alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s + \alpha_{3^3P_2}^t)^2 + 8(\alpha_{3^3P_2}^t)^2}}. \quad (6)$$

The problem of exact *ab initio* relativistic calculations of the quantities $\alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s$ and $\alpha_{3^3P_2}^t$ in Eqs. (4) and (6) is extremely difficult and involves calculating spectral sums over the complete set of unperturbed states. The need for such summation (irrespective of the general approach) emerges in the process of determining the perturbed wave functions or energy shifts of atomic levels in the perturbation-theory setting. In addition to direct summation over the discrete spectrum of intermediate states and integration over the continuous spectrum of intermediate states, which are extremely involved processes in the relativistic case, we basically used two methods to effectively calculate such spectral sums (composite matrix elements), a method for integrating inhomogeneous differential equations and a method that uses the formalism of Green's functions.

In the first approach, the polarizability of the state $|0\rangle$ is given by the formula

$$\alpha_{|0\rangle} = -2\langle \Psi | D | \psi_0 \rangle, \quad (7)$$

in which the perturbed wave function $|\Psi\rangle$ satisfies the inhomogeneous equation

$$(\hat{H} - E_0)\Psi = -D\Psi_0. \quad (8)$$

In (7) and (8), D is the dipole moment operator, and \hat{H} is the relativistic Hamiltonian.

An important advantage of this method is the possibility of using different expressions for the atomic potential in the numerical integration of Eq. (8), and the calculations can be done not only for a purely Coulomb interaction but in the multiconfiguration interaction approximation,⁷ the Hartree–Fock–Dirac approximation,¹¹ and the relativistic random phase approximation with exchange.¹² The most exact relativistic calculations were done by Johnson and Cheng¹³ for the polarizability of the ground state of a heliumlike atom with $2 \leq Z \leq 30$, but at present there are no similar results for excited states of helium with $L \neq 0$.

The effectiveness of the method of Green's functions is largely determined by the existence of appropriate representations of these functions. Since in the relativistic case the expressions for the Green's functions are known only for the Coulomb field, the use of this approach is restricted to problems in which the difference of the potential and the Coulomb potential is insignificant or can be taken into account by perturbation-theory techniques.^{14,15}

To allow for the contribution of relativistic corrections in calculations of the scalar and tensor components of polarizabilities, we used the resonance approximation for the second-order composite matrix elements, i.e., in the spec-

trum of intermediate states we isolated the terms that correspond to transitions in which the principal quantum number does not change.

For instance, for the scalar polarizability of the triplet $|nJLM\rangle$ state,

$$\alpha_{nJL}^s = -\frac{2}{3(2J+1)} \sum_{n'J'L'} \frac{|\langle nJL || \mathbf{r} || n'J'L' \rangle|^2}{E_{nJL} - E_{n'J'L'}}, \quad (9)$$

the resonant term $\alpha_{nJL}^{s(r)}$ in (9) has the form

$$\begin{aligned} \alpha_{nJL}^{s(r)} = & -\frac{2\beta_{nJL}^2}{3} \left\{ \sum_{J'} \frac{L(2J'+1)}{E_{nJL} - E_{nJ'L-1}} \left[\beta_{nJ'L-1} R_{nJL}^{nJ'L-1} \right. \right. \\ & \times \left. \left. \begin{Bmatrix} L & J & 1 \\ J' & L-1 & 1 \end{Bmatrix} \right]^2 + \sum_{J'} \frac{(L+1)(2J'+1)}{E_{nJL} - E_{nJ'L+1}} \right. \\ & \left. \left. \times \left[\beta_{nJ'L+1} R_{nJL}^{nJ'L+1} \begin{Bmatrix} L & J & 1 \\ J' & L+1 & 1 \end{Bmatrix} \right]^2 \right\}. \quad (10) \end{aligned}$$

Here the $\begin{Bmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{Bmatrix}$ are Wigner $6j$ -symbols,¹⁶ and the $R_{nJL}^{nJ'L'}$ are radial matrix elements. In Eq. (10), the effects of singlet–triplet mixing of levels are taken into account by the parameter

$$\beta_{nJL} = \begin{cases} \cos \theta_{nL}, & J=L, \\ 1, & J \neq L, \end{cases} \quad (11)$$

where θ_{nL} is the singlet–triplet mixing angle. Chang¹⁷ noted that θ_{nL} is almost entirely independent of n , and the typical values of θ_{nL} at $L=1,2,3$ are 0.02° , 0.5° , and 30° , respectively. The tensor part of the polarizability has a similar structure and differs from (10) only in angular coefficients; for the sake of brevity we will not write it here.

To calculate $\alpha_{nJL}^{s(r)}$ and $\alpha_{nJL}^{i(r)}$ we used exact relativistic results for the radial integrals, while for the energy denominators we used precise experimental data.¹⁸ Calculations of the other terms in (9) with $n' \neq n$ were done with nonrelativistic values for the radial matrix elements of the dipole moment operator. To this end we used exact numerical data for the oscillator strengths of the s – p and p – d transitions in helium calculated with multiparameter variational wave functions.^{19,20}

This approach is applicable primarily because the contribution of states with $n' = n$ in (9) is numerically predominant and amounts to roughly 95% in the case of excited $1s3p^3P_J$ ($J=0,2$) levels of helium (see Tables II and III below).

3. SELECTION OF THE BASIS WAVE FUNCTIONS AND DISCUSSION OF THE RESULTS OF CALCULATIONS

In recent years the configuration-interaction method has been successfully used to obtain precise wave functions and matrix elements for atoms with a small number of electrons, e.g., heliumlike systems. In the present paper we use the technique developed by Johnson *et al.*^{7,13} to calculate the reduced matrix elements corresponding to the resonant terms in the expansion (10).

The wave function of the initial (I) and final (F) states can be written

TABLE I. Reduced matrix elements of the dipole moment operator.

Transition	Matrix element
$1s3p^3P_0 \rightarrow 1s3s^3S_1$	–6.4797
$1s3p^3P_2 \rightarrow 1s3s^3S_1$	–14.489
$1s3p^3P_0 \rightarrow 1s3d^3D_1$	8.2923
$1s3p^3P_2 \rightarrow 1s3d^3D_1$	1.8542
$1s3p^3P_2 \rightarrow 1s3d^3D_2$	7.1805
$1s3p^3P_2 \rightarrow 1s3d^3D_3$	16.994

$$\Psi_{I(F)} = \sum_{k \geq 1} C_{kl}^{I(F)} \Phi_{kl}. \quad (12)$$

Here the Φ_{kl} are two-particle basis functions with fixed values of total angular momentum J , its projection M , and parity. We found the weighting factors $C_{kl}^{I(F)}$ from the variational principle by using the relativistic no-pair Hamiltonian, which incorporates the Coulomb and Breit electron–electron interaction operators,^{21,22} averaged over the functions (12). To exclude the contribution of negative-energy states (the positron spectrum), the two-particle operators in the relativistic Hamiltonian were multiplied by products of single-particle operators projecting on the subspaces of solutions of the positive-energy Dirac equation.⁷

The wave functions (12) are normalized by the condition

$$\sum_{k \geq 1} |C_{kl}^{I(F)}|^2 = 1. \quad (13)$$

The single-particle basis orbitals employed in the configuration-interaction method incorporates the s , p , d , f , and g partial waves, with a spline approximation used for each wave. Estimates of the convergence rate of the method (for calculations of given accuracy) can be found in Refs. 13 and 22.

The results of relativistic calculations for the reduced matrix elements (without allowance for retardation effects for the dipole moment operator) are listed in Table I.

In Tables II and III we list the results for the contributions of the intermediate S and D states in calculations of the scalar polarizabilities of the $1s3p^3P_J$ ($J=0,2$) states of helium. The difference between the tensor part of the polarizability of the $1s3p^3P_2$ level and the scalar part is that the contributions of the intermediate states $1sn's^3S_1$ and $1sn'd^3D_1$ have opposite signs and that the total contribution of the $1sn'd^3D_3$ states contains an additional numerical factor, $-2/7$.

Table IV summarizes the results of numerical calculations of the scalar and tensor components of helium polarizabilities. The dependence of δ on F near the anticrossing point is plotted in Fig. 1.

Note that the difference $\Delta\alpha$ remains almost the same if we use nonrelativistic variational values for the resonant matrix elements in (10): $\alpha_{3^3P_0}^s = 17\,207$, $\alpha_{3^3P_2}^s = 17\,198$, and $\Delta\alpha = 9$. The explanation is that the principal contribution to $\Delta\alpha$ is provided by the relativistic corrections for the fine structure of the levels in the energy denominators of (12) rather than the relativistic corrections for the matrix elements of the dipole moment operator (see Table I).

TABLE II. Contributions of the *S* and *D* states of the intermediate spectrum to the polarizability of the $1s3p^3P_0$ state of helium.

n'	$1sn's^3S_1 (\lambda_0=0.698)$	$1sn's^3S_1 (\lambda_0=-0.302)$	$1sn's^3S_1$	$1sn'd^3D_1$
2	-0.34	-1.67	-1.57	
3	-2377.93	-2682.56	-2638.45	18 742.21
4	451.87	319.37	312.17	623.53
5	25.38	18.27	17.92	86.01
6	6.36	4.60	4.72	27.16
7	2.59	1.88	1.85	12.29
8	1.34	0.97	0.96	6.72
9	0.79	0.57	0.57	4.13
10	0.51	0.37	0.34	2.59
Total	-1888.6	-2337.7	-2301.50	19 540.63

To test the above results, we did alternative polarizability calculations using the method of the Green's functions of an optical electron to sum over the complete intermediate-states spectrum in (9).

Note that the correct selection of the initial analytical representation of the Green's functions $G_E(\mathbf{r}_1, \mathbf{r}_2)$ plays an important role in specific polarizability calculations, since it makes it possible to obtain the result in the form most rational and convenient for further applications. In this paper we have taken the Green's function for the Fuss model potential from Ref. 14. The angular part of $G_E(\mathbf{r}_1, \mathbf{r}_2)$ is simply the product of spherical harmonics, while for the radial part $g_l(E; r_1, r_2)$ we have taken an expansion in Sturm functions, which have only a discrete spectrum:¹⁵

$$G_E(\mathbf{r}_1, \mathbf{r}_2) = \sum_{lm} g_l(E; r_1, r_2) Y_{lm}(\mathbf{n}_1) Y_{lm}^*(\mathbf{n}_2), \quad (14)$$

$$g_l(E; r_1, r_2) = \frac{4Z}{\nu} \sum_{k=0}^{\infty} \frac{U_{kl}(2Zr_1/\nu) U_{kl}(2Zr_2/\nu)}{k + \lambda_l + 1 - \nu}, \quad (15)$$

where $\nu = Z/\sqrt{-2E}$, and

$$U_{kl}(x) = \sqrt{\frac{k!}{\Gamma(k+2+2\lambda_l)}} x^{\lambda_l} \exp\left(-\frac{x}{2}\right) L_k^{2\lambda_l+1}(x). \quad (16)$$

The radial wave functions $R_{nl}(r)$ are obtained from the residues of the Green's function at the poles of $g_l(E; r_1, r_2)$: $\nu = \nu_{nl} = n_r + \lambda_l + 1$, with $n_r = 0, 1, 2, \dots$ the

radial quantum number, λ_l the effective orbital angular momentum, and ν_{nl} the effective principal quantum number in the formula for the energy of the atomic state $|nl\rangle$,

$$E_{nl} = -\frac{Z^2}{2\nu_{nl}^2}. \quad (17)$$

Here and in (15), Z is the charge of the residual ion. The explicit expression for $R_{nl}(r)$ coincides in form with hydrogenlike wave functions:²³

$$R_{nl}(r) = \frac{2Z^{3/2}}{\nu_{nl}^2} U_{n_r, l}\left(\frac{2Zr}{\nu_{nl}}\right). \quad (18)$$

The parameter λ_l (l may represent a specific set of spin-orbit quantum number, in addition to representing a specific angular momentum) can be found by comparing (17) with experimental values of the lowest state of a valence electron with a given l (see Ref. 23). The radial quantum number n_r of this state is assumed to be zero. As shown by Simons,⁸ λ_l represents the entire experimental spectrum of the atom fairly well (in most cases the weak dependence of λ_l on the position of the energy level can be ignored).

With such a definition of λ_l for atomic series whose lowest states are the ground and the metastable, the error in calculating the radial matrix elements $\langle nl|r^L|n'l\rangle L \geq 1$ with wave functions (18) may reach 50%. In view of this we formulated a modified approach to the definition of n_r and λ_l in these series,²⁴ which allowed us to significantly refine the calculations of the spectroscopic characteristics of atoms in ground and excited states. Here the radial quantum number of the lowest state (ground or metastable) of the series is assumed to be unity, so that the effective orbital angular

TABLE III. Contributions of the *S* and *D* states of the intermediate spectrum to the polarizability of the $1s3p^3P_2$ state of helium.

n'	$1sn's^3S_1$	$1sn'd^3D_1$	$1sn'd^3D_2$	$1sn'd^3D_3$
2	-1.57			
3	-2638.76	187.32	2809.37	15 735.95
4	312.15	6.23	93.52	523.74
5	17.92	0.86	12.90	72.25
6	4.72	0.27	4.07	22.81
7	1.85	0.12	1.84	10.32
8	0.96	0.07	1.01	5.65
9	0.57	0.04	0.62	3.47
10	0.34	0.03	0.39	302.17
Total	-2301.83	194.94	2923.72	16 376.36

TABLE IV. Scalar and tensor polarizabilities of the helium atom.

Quantity	Numerical value
$\alpha_{3^3p_0}^s$	17 203
$\alpha_{3^3p_2}^s$	17 191
$\Delta\alpha = \alpha_{3^3p_0}^s - \alpha_{3^3p_2}^s$	10
$\alpha_{3^3p_2}^t$	351.65
\bar{F}	$0.29\ 343 \times 10^{-4}$ $= 150.99\ \text{kV cm}^{-1}$

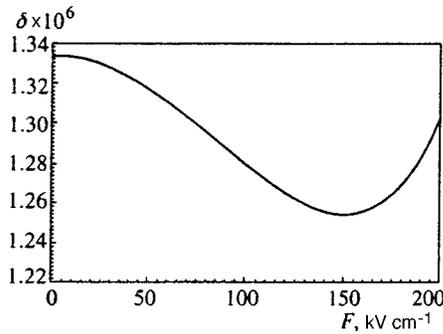


FIG. 1. Dependence of δ (in atomic units) on the electric field strength F in the vicinity of anticrossing \bar{F} .

momentum λ_l is equal to $\nu_g - 2$, with ν_g the effective principal quantum number of the lowest state. Note that the wave function of the lowest level at $n_r = 1$ coincides precisely with the wave function obtained by the quantum-defect method in atoms.²⁵

Thus, the sets of states of an atom with spin-orbit quantum numbers of the ground and metastable levels are, strictly speaking, incomplete since they do not contain states with $n_r = 0$. Hence the radial Green's functions in the subspaces of the series in question contain additional "imaginary" terms with $n_r = 0$ and an effective principal quantum number $\nu_{im} = \nu_g - 1$. The binding energy of the "imaginary" state, defined in (17), is almost ten times higher than the excitation energy of any level in a series, so that its contribution to the optical-transition amplitude can be ignored.

Note also that the wave function of a valence electron in state $|nl\rangle$ has the correct sign in the asymptotic region (which provides the principal contribution to multiple matrix elements) only if we multiply it by an addition phase factor $(-1)^k$, where $k = n - n_r - l - 1$.

The second and third columns of Table II contain the contributions of the intermediate $1sn's^3S_1$ states to the scalar polarizability of the $1s3p^3P_0$ state calculated by the traditional and modified approaches, which yield values of λ_0 equal to 0.698 and -0.302 , respectively. A comparison with the data of precise variational calculations (the fourth column in Table II) suggests that the discrepancy of the final results is less than 2% if the value $\lambda_0 = -0.302$ is used, while calculations with $\lambda_0 = 0.698$ yield an error exceeding 20%.

The results of polarizability calculations based on the use of Green's functions in the method of the Fuss model potential are listed in Table V. The numerical discrepancies of the data of Tables IV and V are due, on the one hand, to the semiempirical approximation of the model potential method and, on the other, to the allowance for the contribution of the continuous spectrum in the Green's functions method. Note that the results for the difference of scalar polarizabilities and for the tensor polarizability of the $1s3p^3P_2$ state differ from those in Table IV only by 10%. To obtain numerical values of the difference of scalar polarizabilities with an accuracy of about 1%, the calculations of the radial integral should be done with an accuracy of five or six figures, since, as Table V implies, the first three signifi-

TABLE V. Scalar and tensor polarizabilities of the helium atom calculated by the model potential method.

Quantity	Numerical value
$\alpha_{3^3P_0}^s$	17 266
$\alpha_{3^3P_2}^s$	17 255
$\Delta\alpha = \alpha_{3^3P_0}^s - \alpha_{3^3P_2}^s$	11
$\alpha_{3^3P_2}^t$	374.16
\bar{F}	0.28458×10^{-4} $= 146.45 \text{ kV cm}^{-1}$

cant figures cancel out. This loss of accuracy can be avoided if we expand the polarizabilities as functions of the energy of an atomic level in a Taylor series. The calculation then reduces to finding the energy derivatives of the polarizabilities, and these can be expressed in terms of third-order dipole matrix elements with two Green's functions, which, in particular, enter into the expression for the hyperpolarizability of the atomic states.²⁶

It is no accident that the numerical results in Tables IV and V are close, since the model potential method yields a correct dependence in the higher-order matrix elements for the energy of the atomic levels,²³ provided that we use the exact (experimental) values for the energies of the fine-structure sublevels. This condition makes it possible to take into account the contributions of relativistic and correlation effects in the model potential method. Furthermore, using this method, one can easily show that the states belonging to a complete set and not taken into account in relativistic calculations (the states belong to the continuum and to the discrete spectrum with $n' > 10$) contribute no more than 0.2% to the numerical values of the quantities considered here.

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¹Here and in the text that follows we use the atomic system of units.

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