COMPARISON BETWEEN ANALYTICAL AND NUMERICAL METHODS AS APPLIED TO CALCULATIONS OF EXCITED ATOMIC STATES

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This article presents a comparison between two approaches for implementing a variational method when calculating excited states of atoms, namely a numerical approach in which the equations arising from the requirement of an extremum of the variational functional (the Hartree–Fock equations) are solved, and an analytical approach in which the energy functional expressed in terms of analytical test functions is minimized. Both approaches are analyzed from the point of view of the approximations used to ensure that the conditions are satisfied for the complete wave function of the excited state being sought to be orthogonal to all wave functions of lower-lying energy states having the same symmetry. The well-known ATOM package is used for numerically solving the Hartree–Fock equations and the MINMAX package is used for the analytical variational calculations. It is shown that the analytical approach based on the minimax method possesses greater possibilities for taking account of relaxation effects. A comparison is made between single-electron wave functions, the matrix elements, and the energies of dipole transitions for a number of excited states of the Ne atom, as calculated using both approaches.

INTRODUCTION

Two approaches can be mentioned from among those for implementing the variational method in atomic theory which have been developed and have mutually complemented and enriched each other. One of these involves numerically solving the equations which arise from the requirement of an extremum of the variational functional. The second approach, let us call it the analytical approach, involves determining some system of optimal variational parameters in terms of which test wave functions and the corresponding energy functionals are expressed.

At present, thanks to the use of powerful computer technology, methods based on numerically solving self-consistent field equations, and in particular the Hartree–Fock equations in various modifications, are widely employed in atomic calculations. The Hartree–Fock equations are actually a consequence of satisfying the conditions for an absolute minimum of the energy functional. The Hartree–Fock solutions therefore most correctly describe states having the lowest energy in their symmetry class.

The task of finding solutions corresponding to excited states is complicated by the need to take account of the conditions for orthogonality of the complete wave function of the excited state being sought to all the wave functions of the states of lower energy having the same symmetry. In this case the variational problem for excited states becomes a problem of finding a conditional minimum at which the imposed orthogonality conditions act as supplementary conditions [1].

In the context of a single-electron approximation, further simplifying assumptions are necessary in order to meet the requirements of the conditions for orthogonality of the complete wave functions. These simplifications are either implemented by "freezing" the shell orbitals of the excited configuration or involve rejecting the orthogonality of the single-electron functions inside the excited configuration.
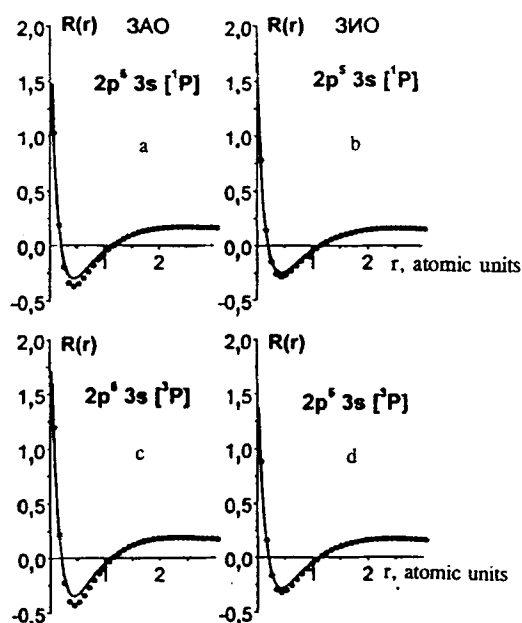
Fig. 1. Wave function of a $3s$ electron for the $2p^53s[^{1,3}P]$ states of the Ne atom, obtained by the numerical (points) and analytical (solid curve) methods using the frozen atom shell and frozen ion shell approximations.

The most widely used are the "frozen" atomic shell and "frozen" ion shell approximations. In the frozen atom shell approximation the wave functions of the shell electrons are selected as given from a calculation of the atomic ground state. Clearly the wave functions and the energy spectrum of the excited states found in this way represent a solution of a nonself-consistent problem.

In the frozen ion shell approximation the shell functions are selected from a calculation of the corresponding ion. However in order to satisfy all the necessary orthogonality conditions in this case one must change to nonorthogonal orbitals in the complete wave function of the excited configuration. It then turns out to be very difficult to solve even the nonself-consistent problem numerically [2-7].

It should also be mentioned that there is a fundamental theoretical problem of providing the limiting properties of the variational energies. The values of the total energies obtained in approximate variational calculations, taking account of the orthogonality conditions, in general fail to possess limiting properties related to the corresponding eigenvalues of the Hamiltonian. This is because the orthogonalization of the functions of excited states is performed on the approximate and not the complete functions of the lower-lying states. For this reason paradoxes of the type of the "collapse" of energy levels [8-10] become possible.

1. MINIMAX METHOD AS A GENERALIZED VARIATIONAL METHOD

It was shown in [11-13] that these difficulties in calculating excited states can be overcome by utilizing the results of a generalized variational method. In particular, it was established that excited states correspond to saddle points in the energy functional. Based on this, a method for calculating excited states having lower-lying states of the same symmetry was formulated in [12, 13]. It was based on a determination of the saddle points of the energy functionals using the minimax method. Conditions were formulated under which the energy of the excited state considered is an upper limit of increased accuracy to the corresponding eigenvalue of the Hamiltonian. It is important that this method can be applied to any class of analytical test functions which satisfy the usual conditions.
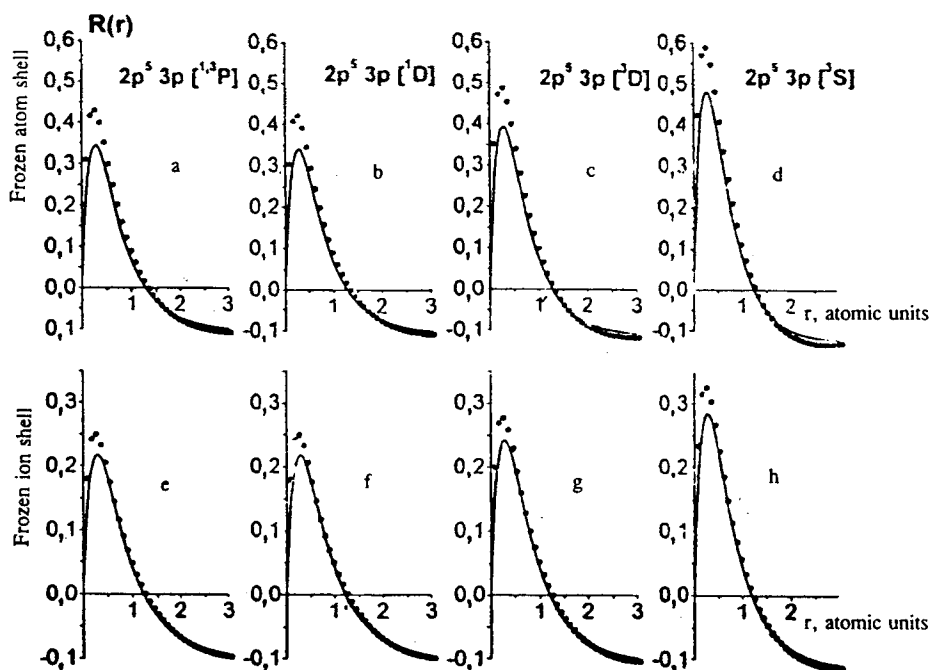
Fig. 2. Wave function of a $3p$ electron for the $2p^53p[^{1,3}P, ^{1,3}D, ^3S]$ states of the Ne atom, obtained by the numerical (points) and analytical (solid curve) methods using the frozen atom shell and frozen ion shell approximations.

The essence of the generalized variational method is as follows. Let $\Phi_\kappa(\{\beta\})$ be a test multielectron wave function of the κ-th excited state which, as well as depending on the spatial and spin variables, depends on a set of variational parameters $\{\beta\}$. Let us utilize $\Phi_i(\{q_i\})$ to denote the orthonormalized wave functions of the lower-lying states having the same symmetry which are functions of their variational parameters $\{q_i\}$. The set of conditions for the orthogonality of the wave functions of the κ-th excited state to all the $(\kappa - 1)$ functions of the lower-lying states having the same symmetry

$$<\Phi_\kappa(\{\beta\})\,|\,\Phi_i(\{q_i\})> = 0, \quad i = 1, 2, \ldots, \kappa-1 \tag{1}$$

forms a system of equations relating the parameters $\{\beta\}$ and $\{q_i\}$. As a result the energy functional of the excited state becomes dependent not only on the parameters $\{\beta\}$ but also on the parameters $\{q_i\}$ of all the functions of the lower-lying states having the same symmetry:

$$E_\kappa = E_\kappa(\{\beta\}, \{q_i\}), \quad i = 1, 2, \ldots, \kappa-1. \tag{2}$$

As part of the minimax approach the energy E_κ of the κ-th excited state is determined by the value of the energy functional found at the saddle point $(\{\beta^0\}, \{q_i^0\})$ from the minimax procedure:

$$E_\kappa = E_\kappa(\{\beta^0\}, \{q_i^0\}) = \max_{\{q_i\}} \min_{\{\beta\}} E\,(\{\beta\}, \{q\}). \tag{3}$$

Equation (3) implies the following sequence of the solution: the maximum value of the energy functional for the parameters $\{q_i\}$ of the lower-lying states is sought from all its values which have a minimum for the parameters $\{\beta\}$ of the desired excited state. Thus, the position of the energy level of the κ-th excited state is strongly dependent on the parameters $\{q_i\}$ of the lower-lying states. The parameters $\{q_i\}$ are called control parameters. It is quite probable that the energy functional $E_\kappa(\{\beta\}, \{q_i\})$ can possess more than one saddle point. Consequently the problem arises of finding the saddle point which corresponds to the upper limit of the eigenvalue of the Hamiltonian. It was shown in [9] that this condition is satisfied by the saddle point at which all the nondiagonal matrix elements of the Hamiltonian fulfill the condition of being equal to zero:

$$<\Phi_i(\{q_i^p\})\,|\,\hat{H}\,|\,\Phi_j(\{q_j^p\})>\,=0, \qquad i\neq j=1,\,2,\,...,\,\kappa-1,$$

$$<\Phi_j(\{q_i^p\})\,|\,\hat{H}\,|\,\Phi_\kappa(\{\beta^0\})>\,=0. \tag{4}$$

The minimax approach is more general than the method of directly seeking a minimum of the energy functional taking account of the supplementary conditions for orthogonality. Here all the functions entering the space of the test functions undergo variation, i.e., both the desired excited state function and the functions of the lower-lying states having the same symmetry. By selecting the appropriate test functions, the minimax approach includes all the other variational methods for calculating the excited states as particular cases. It should be noted that the procedure using Eq. (3) reduces to ordinary minimization for the excited states of lower energy in its symmetry class.

2. EXCITED STATES IN THE NEON ATOM

Here we consider the ground and lower excited states of the $2p^53s$ and $2p^53p$ configurations of the neon atom. In the LS-coupling scheme the $2p^53s$ configurations correspond to the $^{1,3}P$ terms. These terms are the lowest among all the terms of this symmetry and so the task of calculating them is one of finding an absolute minimum. This makes it possible to obtain both numerical wave functions and energies by solving the appropriate self-consistent Hartree−Fock equations and analytical wave functions by directly minimizing the energy functional expressed in terms of analytical test functions. Single-electron functions which are orthogonal inside the configuration can be used for either approach.

The terms $^{1,3}S$, P, D correspond to the $2p^53p$ configuration. The ^3S and $^{1,3}D$ terms also require no special investigation since they are the lowest terms in their symmetry class. The $^{1,3}P$ terms of the configuration considered have lower-lying $^{1,3}P$ terms of the $2p^53s$ configuration. However in the context of the single-electron approximation the complete wave functions of these states are automatically orthogonal, i.e.,

$$<2p^53s\,[^{1,3}P]\,|\,2p^53p\,[^{1,3}P]>\,=0, \tag{5}$$

by virtue of the orthogonality of the single-electron functions φ_{3p} and φ_{3s}. As a consequence of satisfying condition (5), the terms $^{1,3}P$ of the $2p^53p$ configuration can also be considered without explicitly taking account of the conditions for the corresponding wave functions to be orthogonal to the wave functions of the lower-lying $2p^53s$ configuration. Here it is also possible to obtain self-consistent solutions numerically, while from the point of view of the direct variational method the problem reduces to finding the absolute minimum of the energy functional.

For the ^1S term of the $2p^53p$ configuration, the lower-lying term having the same symmetry is the $2p^6[^1S]$ ground state. The condition for orthogonality to this must be explicitly taken into account. In order to ensure that the $2\bar{p}^53p[^1S]$ wave function is orthogonal to the $2p^6[^1S]$ wave function (the bar over the function being introduced to denote the difference between the $2p$ functions from the different configurations), i.e., in order to satisfy the condition

$$<2\bar{p}^53p\,[_1S]\,|\,2p^6\,[^1S]>\,=0 \tag{6}$$

it is necessary for the single-electron functions φ_{2p} from the $2p^6$ configuration and φ_{3p} from the $2\bar{p}^53p$ configuration to be orthogonal. However the $\bar{\varphi}_{2p}$ and φ_{3p} functions inside the $2\bar{p}^53p$ configuration then turn out to be nonorthogonal, i.e.,

$$<\bar{\varphi}_{2p}\,|\,\varphi_{3p}>\,=\lambda\neq0. \tag{7}$$

Thus one must take account of condition (7) when calculating the $2\bar{p}^53p[^1S]$ state, i.e., of the nonorthogonality of the single-electron functions inside the excited configuration. The corresponding system of single-electron equations is then made considerably more complicated so that it becomes questionable whether one can obtain self-consistent solutions by numerical methods.

TABLE 1. Energies of $2p^53p[^{1,3}L]$ — $2p^53s[^{1,3}P]$ Dipole Transitions (eV) in the Ne Atom

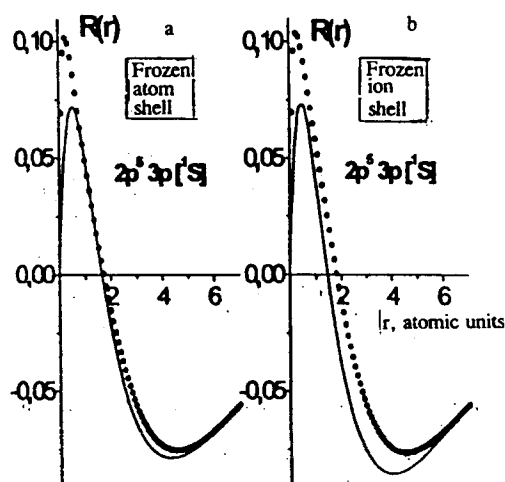| ^{2S+1}L	Variational, frozen atom shell	Variational, frozen ion shell	Numerical	Experimental [17]	Experimental [18]
^1S	2,085	1,857	—	2,120	2,122
^3S	1,640	1,647	1,648	1,736	1,736
^1P	1,794	1,749	1,721	1,878	1,868
^3P	2,018	1,880	1,893	1,992	2,052
^1D	1,754	1,702	1,680	1,856	1,830
^3D	1,886	1,794	1,802	1,962	1,959

Fig. 3. Wave function of a $3p$ electron for the $2p^53p[^1S]$ states of the Ne atom, obtained by the numerical (points) and analytical (solid curve) methods using the frozen atom shell and frozen ion shell approximations.

3. METHOD OF CALCULATIONS

In the present work the well-known ATOM program package [14] was used for numerically solving the Hartree — Fock equations, and the MINIMAX package [15] was used for the analytical variational calculations.

The MINIMAX package makes it possible to determine the saddle points of the energy functionals, to reveal which of these correspond to upper limits and also to perform direct minimization of the energy functionals taking into account supplementary conditions, and to solve the problem of finding the absolute minimum. The use of this package requires a class of test functions to be specified in the form of an energy functional. Generalized hydrogen-like functions were used in the present work, their radial part being of the form

$$R_{nl} = N_{nl} \sum_{i=1}^{\max(2,n-1)} a_i^{nl} r^{m_i} e^{-\gamma_i r}, \quad m_i = \min(l+i, n). \tag{8}$$

Here N_{nl} is a normalization coefficient; $\{a_i^{nl}, \gamma_i\}$ are variational parameters.

The energy functionals for all the terms of the configurations considered, except for the ^1S term of the $2p^53p$ configuration, were given in standard form. The energy functional for the ^1S term of the $2\bar{p}^53p$ configuration, taking condition (7) into account, is of the form

$$E(2\bar{p}^5 3p\,[^1S]) = <2\bar{p}^5 3p\,[^1S]\ |H|\ 2\bar{p}^5 3p\,[^1S]> = [1+5\lambda^2]^{-1}\times$$

$$\times\{2[1+5\lambda^2]\ [I(1s)+I(2s)+5I(2p)+I(3p)+5\lambda\,[2I(2p,\ 3p)+4\lambda I(2p)]\,]+$$

$$+\,[F^0(1s,\ 1s)+F^0(2s,\ 2s)+4F^0(1s,\ 2s)-2G^0(1s,\ 2s)]\,[1+5\lambda^2]+$$

$$+\,2[5F^0(1s,\ 2p)+F^0(1s,\ 3p)+5F^0(2s,\ 2p)+F^0(2s,\ 3p)]+$$

$$+\,10\lambda[2R^0(1s2p,\ 1s3p)+4\lambda F^0(1s,\ 2p)+2R^0(2s2p,\ 2s3p)+$$

$$+\,4\lambda F^0(2s,\ 2p)]-\frac{1}{3}[5G^1(1s,2p)+G^1(1s,\ 3p)+5G^1(2s,2p)+G^1(2s,3p)]+$$

$$+\,[10F^0(2p,\ 2p)-\frac{4}{5}\,F^2(2p,\ 2p)]+5F^0(2p,\ 3p)]-\frac{2}{5}F^2(2p,\ 3p)+$$

$$+\,5G^0(2p,\ 3p)-0,4G^2(2p,\ 3p)+30\lambda^2 F^0(2p,\ 2p)-2,4\lambda^2 F^2(2p,\ 2p)+$$

$$+\,40\lambda R^0(2p2p,\ 2p3p)-3,2\lambda R^2(2p2p,\ 2p3p)\},$$

(9)

where

$$I(nl) = I(nl,\ nl)\,;$$

$$I(n_1 l, n_2 l) = -\frac{1}{2}\int_0^\infty R_{n,l}(r)\left[\frac{d^2}{dr^2}+\frac{2Z}{r}-\frac{l(l+1)}{r^2}\right]R_{n,l}(r)\,r^2\,dr$$

is the radial matrix element of the single-electron operator $h = -(1/2)\nabla^2 - Z/r$, and Z is the nuclear charge of the atom. The radial integrals of the electrostatic interaction are determined in the usual way:

$$F^\kappa(n_1 l_1,\ n_2 l_2) = R^\kappa(n_1 l_1 n_2 l_2,\ n_1 l_1 n_2 l_2),$$

$$G^\kappa(n_1 l_1,\ n_2 l_2) = R^\kappa(n_1 l_1 n_2 l_2,\ n_2 l_2 n_1 l_1),$$

$$R^\kappa(n_1\,l_1\,n_2\,l_2, n_3\,l_3\,n_4\,l_4) = \int\int\frac{r_<^\kappa}{r_>^{\kappa+1}}\times$$

$$\times R_{n_1 l_1}(r_1)\,R_{n_2 l_2}(r_2)\,R_{n_3 l_3}(r_1)\,R_{n_4 l_4}(r_2)\,r_1^2\,r_2^2\,dr_1\,dr_2,$$

where $r_<$ is the smaller and $r_>$ the larger of r_1 and r_2. Expression (9) is a particular case of the more general results obtained for the method of nonorthogonal orbitals [16].

4. DISCUSSION OF RESULTS

Let us compare the numerical and analytical wave functions obtained for the ground and excited states of the Ne atom in the different versions of the calculation. The calculation shows the numerical and analytical wave functions of the inner shells to be practically identical, and the $2p$ functions to be very similar. Small discrepancies between the values of the $2p$ functions close to their maximum results in a difference between the total energies. The numerical Hartree−Fock calculation gives a total energy of the ground state of $E_{num}(2p^6) = -128.547$ atomic units and the analytical calculation gives $E_{anal}(2p^6) = -128.516$ atomic units, so that the difference is 0.031 atomic units (0.02% of the value of the Hartree−Fock energy). These wave functions will henceforth be used in calculations of the excited states in the frozen atom shell approximation.

A similar picture is observed for the Ne$^+$ ion. In this case the numerical and analytical functions, including the $2p$ functions, are practically identical. This is also confirmed by the values of the total energies:

$$E_{num}(2p^5) = -127.8178\ \text{atomic units}\,,\ E_{anal}(2p^5) = -127.8031\ \text{atomic units}$$

We shall henceforth use these functions in calculations of excited states using the frozen ion shell approximation.

The frozen atom shell and frozen ion shell approximations in a certain sense represent limiting cases as regards taking account of relaxation effects in calculations of excited states. Relaxation effects are completely neglected using the frozen atom shell approximation whereas the relaxation accompanying excitation of the atom is overestimated using the frozen ion shell

TABLE 2. Radial Integral $<3p \mid r \mid 3s>$ (atomic units) for $2p^53p[^{1,3}L]$ — $2p^53s[^{1,3}P]$ Dipole Transitions in Ne

^{2S+1}L	Variational, frozen atom shell	Numerical, frozen atom shell	Variational, frozen ion shell	Numerical, frozen ion shell	Numerical, FEAS*	Experimental [18]
^1S	4,314	4,456	4,717	—	4,466	4,522(0,032)
^3S	4,352	4,378	4,576	4,722	4,437	4,587(0,011)
^1P	4,559	4,677	4,699	4,888	4,680	4,731(0,027)
^3P	4,288	4,409	4,516	4,713	4,389	4,378(0,011)
^1D	4,563	4,680	4,708	4,891	4,684	4,720(0,026)
^3D	4,331	4,420	4,574	4,723	4,414	4,462(0,007)

*FEAS (frozen excited atom shell): self-consistent calculation made of the $1s^22s^22p^53p[^{1,3}L]$ states in whose frozen shell configuration $(1s^22s^22p^5)$ the $3s$ wave function is calculated.

approximation. Thus it is the choice of the physical approximation which is decisive for the wave functions of the ground state of both the atom and the ion, especially for the inner shells, and not the method of obtaining them.

Let us now consider the wave functions of an excited electron. Figure 1 gives the $3s$ functions for the $2p^53s^{1,3}P$ terms. It can be seen that the difference between the numerical and analytical $3s$ functions using the frozen atom shell and frozen ion shell approximations is not great. The greatest discrepancies are in a limited region of r values close to the minimum of the function. The wave functions obtained from a self-consistent calculation and by the direct minimization method turn out to be even closer in the case of complete unfreezing.

Figure 2 gives the numerical and analytical $3p$ functions of the $^{1,3}P$, $^{1,3}D$, and ^3S terms, obtained using the frozen atom shell and frozen ion shell approximations. The numerical and analytical $3p$ functions for these terms differ markedly near the values of the maximum of the $3p$ functions, these differences being much greater using the frozen atom shell approximation than using the frozen ion shell approximation. In the case of complete unfreezing the difference between the $3p$ functions remains and is of the same nature as in Fig. 2. Since the numerical functions for these terms are more accurate using the approximation considered, it can be concluded that it is necessary to increase the accuracy of the form of the analytical $3p$ functions given by formula (8).

The picture for the $3p$ function of the ^1S term of the $2p^53p$ configuration (Fig. 3) is somewhat different. It can be seen that the numerical and analytical $3p$ functions using the frozen ion shell approximation differ considerably while using the frozen atom shell approximation the difference is of the same nature as for the other terms. This difference of the functions is explained by the fact that it is possible to obtain self-consistent numerical solutions for this term using the frozen atom shell approximation whereas when using the frozen ion shell approximation self-consistent solutions can be obtained only if one neglects the orthogonality of the $2p^53p[^1S]$ wave function and that of the $2p^6[S]$ ground state. Thus, in this case only the variational method using orbitals which are nonorthogonal inside a configuration enables one to calculate the $2p^53p[^1S]$ state taking account of the complete unfreezing of the shell (i.e., taking the relaxation of the shell into account).

The quality of the wave functions and the suitability of the approximations used to obtain them can be estimated for calculations of the physical characteristics of atoms. We considered as examples the energies and radial matrix elements of dipole transitions between the considered excited configurations of the Ne atom. The corresponding results are given in Tables 1 and 2.

Table 1 gives the energies of dipole transitions in the term system considered, calculated as the difference between the total energies of the corresponding excited states. It can be seen from Table 1 that the numerical and variational values of the transition energies are in reasonable agreement with each other. It is observed that the numerical transition energies lie between the corresponding values of the variational quantities obtained using the frozen atom shell and frozen ion shell approximations. This situation is natural since, as was mentioned above, the frozen atom shell approximation fails to take account of the effect of shell relaxation while the frozen ion shell approximation overestimates it, whereas the relaxation is accurately accounted for in the self-consistent calculation (in the context of the Hartree–Fock approximation). At the same time, the variational method makes it possible to obtain a value of the $[^1S] \rightarrow [^1P]$ transition energy which is in satisfactory agreement with experiment whereas the numerical Hartree–Fock method fails to enable the total energy of the $2p^53p[^1S]$ term to be calculated taking account of the condition of orthogonality to the ground state.

Comparing the dipole radial integrals (Table 2) it can be noted that: 1) the values obtained using the numerical Hartree—Fock approximation are greater than the corresponding values of the variational method for both the frozen ion shell and frozen atom shell approximations; 2) in both the numerical and variational approaches the values of the matrix elements obtained using the frozen atom shell approximation are lower than the corresponding values using the frozen ion shell approximation; 3) the best agreement with the experimental values is obtained for the variational method using the frozen ion shell approximation (except for the transition from the ^3P term) and for the numerical method using the frozen excited atom shell approximation (the values of the latter being close to those using the frozen atom shell approximation).

The features described make it possible to conclude that relaxation effects play an important role in the calculation of atomic characteristics. It can therefore be stated that the choice of the physical model is decisive in calculating the transition probability. At the same time, it follows from Table 1 that the transition energies are more subject to the influence of correlation effects in the initial and final states.

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