Training software apparatus for a plasma physics course

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***Abstract*—The article presents high school educational tool generating problems for a test work on plasma chemistry courses based on the Algorithm for a wave functions fast calculating in the central field aproximation for many-electron atoms based on an iterative procedure similar in ideology to the Hartree-Fock method is described as well as the interface of the resulting task generating program. The work is a first step for a more profound generator which deals with calculating rate constants in plasma.**

Keywords—plasma, task generating, wave function, test works

I. INTRODUCTION

The new state of matter – plasma was descovered in 1879 and the term "plasma" is in use since 1928 [1]). At the moment the rapid development of computer technology supports transition from experimental research and the development of empirical plasma models to a quantitative description on the basis of fundamental theoretical approaches and numerical modeling [2],[3],[4]. Calculating of a large number of elementary radiation and collisional processes competing with each other in the gas discharge requires the use of very laborious methods for describing the plasma as a multicomponent system, which generally persists in a substantially nonequilibrium state [5],[6],[7],[8],[9]. The quantitative models of these processes require knowledge of specific values of the probabilistic characteristics of the elementary processes. Despite the excecive work on collecting and systematizing of experimental material on elementary collisional and radiative processes and development of databases containing processes probabilistic characteristics (see, for example, [10]), the set of elementary processes being considered is usually substantially limited by the set of reliable experimental data [9]. As a result, the use of theoretically obtained data for culculating cross sections and rate constants of collisional processes is significant for plasma physics. Development of reliable and relatively simple methods of such calculations is still demanded.

Calculation of the probabilities of radiation processes, cross sections of collision transitions and corresponding rate constants of plasmachemical reactions is one of the most traditional and developed areas of quantum mechanics [11]. However preparing data for systematic calculations of the kinetics of nonlocal plasma meets some difficuties. First, their computational complexity, is very havy in the preparation of data for the developed multi-channel plasma-chemical models. Second, taking into account a large set of processes close in probability affects the accuracy of calculating.

On the other hand there are numerous applications of gas-discharge plasma: in medicine [12],[13],[14] food industry [15], chemical analysis and environmental monitoring [16], demonstrate actuality of the theme. Though a fast method of culculating wave functions is useful for data preparetion for plasma dynamic simulation as well as for constracting an educational tool to support education of plasma-aware specialists.

II. BASIC THEORY

In the overwhelming majority of cases in the kinetics of low-temperature plasma, collisions of atoms with electrons (ionization and excitation by electron impact, mixing of excited states by electrons, etc.) play a key role, as well as radiation processes. In both cases, accuracy sufficient for plasma applications gained with the use of Born's method [17] where the wave functions of the particles (electrons in collisions and photons in the case of light emission and absorption) are approximated by a plane wave.

Having the first order perturbation, the Born method gives a satisfactory description for the plasma excitation processes important for the plasma kinetics on "optically-resolved" transitions ($\Delta L=\pm 1$, $\Delta S=0$) and ionization by atoms from the ground state by electron impact. Its modifications (taking in account second-order perturbation theory elements and exchange effects) produce results reliable for plasmachemical calculations for the cross sections of collision transitions both between excited levels and "optically forbidden" ($\Delta L \neq \pm 1$) and intercombination ($\Delta S \neq 0$) transitions [18].

Formula for total cross section σ^B of collision transition (in an electron impact) between the states of the atom γ_0 and γ' is:

$$\sigma^{B}_{\gamma_0\gamma} = \pi a_0^2 \frac{8}{k^2(2l+1)} \sum_{\chi} \int_{k-k'}^{k+k'} \left[R_\chi(q)\right]^2 \frac{dq}{q^3}, \qquad (1)$$

Where R_χ is transition matrix element, k and k 'are the momenta of a free electron before and after a collision with an atom, r is the distance from the nucleus to the current point of space measured in relation to a_0 (first Borh radius):

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$$R_\chi(q)=\sqrt{(2\chi+1)(2l+1)(2l'+1)}\begin{pmatrix}\chi & l & l'\\ 0 & 0 & 0\end{pmatrix}\int_0^{r_0}R_{nl}(r)R_{n'l'}(r)j_\chi(qr)dr, \quad (2)$$

R_{nl} (r) are the radial parts of one-electron wave functions that change its state (given by the quantum numbers n and l) of the optical electron; j_χ (qr) is the spherical Bessel function of order χ. Calculation of angular integrals is performed using a standard apparatus of n_j-symbols. Though the knowledge of the radial parts of the wave functions is necassary for calculations. For second-order prcision hrough intermediate ("virtual") states the knowledge of the wave functions not only of the initial and final, but also of all intermediate ("virtual") states [19] is required.

The approach developed by Hartree and Fock in the first half of the twentieth century allows determining stationary electron states in the self-consistent field of the remaining particles is now traditional method of solving the problem of constructing wave functions of an electron in a many-electron atom [20],[21],[22]. It requires sufficiently resource-intensive calculations. The accuracy of the results is often overestimated in comparison with the errors due to the deficit of information on the probabilities of elementary processes by simplifications of plasma-chemical models. In this paper we propouse a variant of constructing semiempirical one-electron wave functions of many-electron atoms. This approach demands low-cost computational resource, and the results of its testing in the course of calculations of atoms with a nuclear charge Z <12 are presented as well as its implementation for educational purposes.

III. Comporisons of Methods for Constructing Semiempirical Wave Functions

A. Semiempirical method

In 1970-x there was developed a simpl semiempirical method [18]in which the experimentally known energy of the electron is substituted as the eigenvalue in the Schrodinger equatin then, the radial part of the wave function of the external ("optical") electron on $R_{nl}(r)$ is obtained as a result of numerical integration of the Schrödinger equation

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}+2\frac{\zeta(r)}{r}+2W\right]\circ R_{nl}(r)=0\ , \quad (3)$$

$\frac{\zeta(r)}{r}$

where – the effective potential of the atomic residue; W is the eigenenergy [23].

The main difficulty of this approach is obtaining the potential of the atomic residue. Its calculation requires knowledge of the wave functions of internal electrons.

B. Hydrogen like atom aproximation

The approximation of analytically described hydrogen-like wave functions is traditionally used for an approximate calculation of the potential of an atomic residue.

$$R_{nl}(r)=g(r)\exp(-kr)=\left(\sum_m a_m r^m\right)\exp(-kr) \quad (4)$$

(3), where the effective charge is equal to the nuclear charge ς (r)=Z, and the coefficients a_m of the polynomial g(r) are calculated from the recurrent formula for the hydrogen atom

$$\begin{cases}a_0=\delta_{l,0}\ ,\\ a_{m+1}=a_m\cdot 2\dfrac{k(m+1)-Z}{(m+1)(m+2)-l(l+1)},\end{cases} \quad (5)$$

where $\delta_{l,0}$ is the Kronecker symbol in the case of the discrete spectrum of the initial states and the delta function for the continuous spectrum.

It uses effective principal quantum number (dute to perturbation of the Coulomb field of the nucleus by contributions from the remaining electrons) associated with the experimental value of the binding energy by a relation analogous to that obtained for hydrogen-like ions: $n^*=(-Z/2W_{exper})^{1/2}$ is used.

Another method for atomic risidue potential determination is based on the use of semi-empirical non-zero functions of Sletter, constructed on the basis of hydrogen-like wave functions (4) for l=n-1, by introducing effective quantum numbers and screening constant [19].

Finally, atoms with bigger number of electrons when individual features of their wave functions becomes insignificant, electron Fermi gas can serve as an atomic residue model. The potential of the atomic residue can be found with numerical integration of the Thomas-Fermi equation [24].

C. A fast method for culculating radial wave function

The approach proposed is a generalization of the above described method of constructing semi-empirical wave functions of an excited electron. Its distinguishing feature is the computation of wave functions in the iteratively corrected self-consistent field, which is calculated not only for the optical electron, but also for all other electrons contributing into the atomic residue. Depending on the availability and reliability of experimental or other reliable information on the binding energies of one or several electrons of a multielectron atom, it is possible to improve iteration procedure. If the value of the electron energy is unknown, it is obtained as a result of processing the procedure of successive iterations.

During the iterative procedure, the an optimal set of values of the effective-value moduli is constructed: $k^*_j=1/n_j^*$ (n_j^* is the effective principal quantum number corresponding to the energy of the electron of the multi-electron atom) and arrays values of the radial component of the wave function corresponding to this value. The criterion of success is the convergence of the vector $K^*=\{k^*_{nl}\}$ and the stabilization of the matrix of values of the wave functions $R^*=\{R_{nl}(r)\}$.

Sredinger equation (3) can be rewriaten for each of the electron shells of a multielectron atom with the current number

p, having a pair of quantum numbers p=(n,l) and the corresponding number of electrons a_p:

$$\frac{1}{r}\frac{d^2}{dr^2}(rR_{nlp})+\left[2U_p(r)-\frac{l(l+1)}{r^2}+2W_{nlp}\right]R_{nlp}=0,$$
$$U_{nlp}(r)=\frac{Z}{r}+(a_p-1)\varphi_p(r)+\sum_{p'\neq p}a_{p'}\varphi_{p'}(r), \quad (6)$$
$$\varphi_{nl}(r)=-4\pi\int_0^\infty\frac{\int_0^r(R_{nl}(r))^2r^2dr}{r^2}dr.$$

Where $U_p(r)$ is the potential of the self-consistent field at the point (r) affecting the electron (the total potential without potential of the carrent electron).

A difference method was used to integrate (6),. The integration region was split into N=200,000 intervals with a self-tuning integration step (the initial value dr=0.015 in the atomic units of the Hartree system). The iterative process folows the scheme:

$$R_{nl}(i)=R_{nl}(i-1)+dR_{nl}(i-1)\cdot dr,$$
$$dR_{nl}(i)=dR_{nl}(i-1)+d^2R_{nl}(i-1)\cdot dr, \quad (7)$$
$$d^2R_{nl}(i)=\frac{-2dR_{nl}(i)}{r}-R_{nl}(i)\left(\frac{2U_{nl}(i)-l(l+1)}{r^2}+2W\right),$$

where R_{nl} (i) is the value of the wave function at the current point; dR_{nl} (i) and d^2R_{nl} (i) are its first and second derivatives. The initial values were given in the form $R_{nl}(0)=1$, $dR_{nl}(0)=1$, d^2R_{nl} (0)=0. After several iterations the result of numerical integration begins to be cosistent with the wave function $R_{nl}(j)$ regardless of the initial values. Backward iterative procedure ensured the coincidence with R_{nl} (i) of numerical values at the initial points i=0,1,2.

Varying the binding energies of the electrons of the atom $W_{nl}=-(1/2)/(n^*)^2$ (or associated with the effective quantum number $k^*_{nl}=1/n^*$) leads to changes in the form of corresponding one-electron wave functions, the number of zeros with (Or) axis and their positions. The target criterion for selecting W_{nl} is the condition of maximum distance from the origin (the nucleus) of the divergence point of the solution of (6) constructed for each of the electrons at the current iteration of the self-consistent solution construction. The set of such maxima is an approximation to the set of eigenvalues of the energy W_{nl}, and the wave functions calculated at these values with the help of the iteration procedure (7), to the eigenfunctions of the given system of equations. This process allows one to find wave functions both for atoms in the ground states, and for excited states and ions. Program testing demonstrated that a stable solution for atoms with $1<Z<10$, is gained after 2-8 iterations, which corresponds to a counting time of 0.5-5 minutes on a personal computer. The increase of atomic number leads to a monotonous increase in the number of necessary iteration and computation time. The library of wave functions, is replenished automatically during the simulation of electronic states of atoms.

D. Genetic Algorithms Approach for Determioning the Energy Eigenvalues

Using genetical algorithm allows futher reducing computational time [25].

At the point of k_p corresponding eigenenergy W_{nl} the function R_{nl} has a the most prolonged area with $|R_{nl}(r)|\le\varepsilon; r\in[r_1,r_2]$ obtained in the numerical integration (7).To identify the eigenvalues, we constructed a function $r_2(k_{nl})$, such that for $r<r_2$ the solution R_{nl} is limited, and for $r>r_{max}$ it is unlimited and monotone increasing in absolute value. A typical graph of the dependence $r_2(k)$, where $k=\sqrt{W/13.4\,(эВ)}$, is a set of relatively narrow maxima (Fig 1).

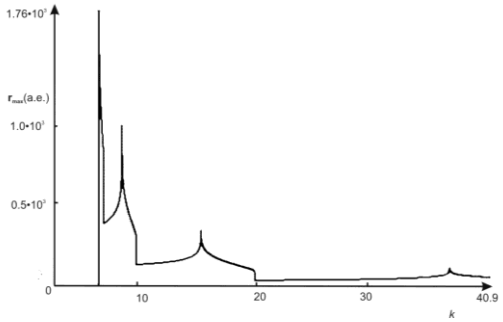

Fig. 1. An example of the dependence r_2 (knl)

Thus, analising r_2 we can detect eigenenergy. For this pupouse the aim function (representing second derivative aproximational formula) C_i

$$C_i=\frac{(r_{i3}-r_{i2})/(k_{i3}-k_{i2})-(r_{i2}-r_{i1})/(k_{i2}-k_{i1})}{k_{i3}-k_{i1}}, \quad (8)$$

Where $k_{j1}<k_{i2}<k_{i3}$. After identifying value of k_p, the surrounding scanned area is excluded from further consideration.

IV. CALCULATING RESULTS

The testing of the described procedure was carried out during calculations of the energies of the ground and excited states of many-electron atoms. In all tests, good agreement was obtained between the results of the calculations with published measurement data or a more rigorous numerical model.

The described algorithm was implemented in the Basic 6 language. Test calculations were carried out on a computer with Intel (R) Core (TM) I5-2537M CPU 1.40GHz CPU, 4 GB memory. The calculation time was varied from a few seconds for H and He atoms, up to two hours for complex multi-electron atoms such as uranium. The number of cycles of successive approximations, after which each of the wave functions changed by less than 0.001, also varied from two cycles for H to 50 for Cu. The practice of calculation showed that the obtained wave functions are independent of the initial values after normalizing. The shape of the wave function is completely determined by the shape of the potential U(r) and

the values of n and l, which rearrange the initial wave function to the one that should correspond to the Schrodinger equation with the selected parameters U(r), n, l, W.

There was performed a test calculation of the ionization energies of the ground states of many-electron atoms having groups of equivalent electrons. For the calculation, no a priori or experimental data on the electron shells of atoms were used. The results of calculations of the ionization energy of atoms from the ground states together with the corresponding experimental values are given in the table.

TABLE I. COMPARISON OF THE RESULTS OF CALCULATIONS OF THE IONIZATION ENERGY OF ATOMS 1-3 GROUPS WITH EXPERIMENTAL DATA

Element	E valus		
	E_{exp}(eV)	E_{culc} (eV)	$(E_{exp}–E_{culc})/E_{exp}$ (%)
H	13,6	13,54	0,44
He	24,6	24,8	–0,81
Li	5,4	4,77	11,67
Be	9,3	7,81	16,02
B	8,3	6,15	25,90
C	11,3	8,2	27,43
N	14,5	10,23	29,45
O	13,6	12,32	9,41
F	17,4	14,5	16,67
Na	5,1	4,47	12,35

To verify the accuracy of calculating the shape of the radial component of the wave function, the results for the hydrogen atom were compared with the results obtained from the well-known recurrence relation (5). The modulus divergence was less than 0.001, which was considered a good approximation for this type of computation.

The calculation of the non-normalized Born cross sections according to formulas (1) - (2), using the developed methods when compared with the experimental values, led to standard overestimations for this type of calculation, not exceeding 20%. When switching to the use of semiempirical wave functions corresponding to the experimental values of the energies of an optical electron, the discrepancy of the results decreased by a factor of 1.5-2.

The results of systematic calculations of the wave functions of light atoms in the ground and excited states demonstrate a qualitatively correct dynamics of the variation of the wave functions as the energy of the optical (excited) electron increases. As expected, the wave function of an optical electron approaches the Rydberg-like state as the state energy grows. Simultaneously with this process, the wave functions of the atomic residue gradually "cling" to the nucleus, which is due to a decrease in the effects of its screening by the electrons of the atomic residue.

The algorithm presented allows calculating radial components of wave function almost for any electron state in any atom that is a useful educational tool for educational process as it is. On the basis of generated values there was a problem generator for student's test works developed that can costruct a number of tests.

V. EDUCATIONAL IMPLEMENTATION

Reactions in plasma (and chemical reactions in genearl) are described by stoichiometric, equation of general form that allows generalized approach to be use when calculating and constricting these equations.

There are test constructed for the general reaction shcems:

- $X + X \rightarrow X + X$ elastic collisions of two atoms
- $X + e^- \rightarrow X + e^-$ elastic scattering of an electron by an atom
- $X + e^- \rightarrow X^+ + 2e^-$ direct ionization of an atom from the ground state by electron impact
- $X^+ + e^- \rightarrow X + h\nu + wall$ two-particle radiative recombination
- $X + e^- \rightarrow X^-$ the formation of a negative ion by electron attachment
- $X^+ + X^- \rightarrow X + X^*$ ion-ion recombination
- $X + e^- \rightarrow X^* + e^-$ excitation of an atom by electron impact
- $X^* + e^- \rightarrow X^+ + 2e^-$ sealed ionization
- $X^* + e^- \rightarrow X + e^-$ collision quenching
- $X^+ \rightarrow X + h\nu$ spontaneous emission
- $X^+ + h\nu \rightarrow X + 2h\nu$ stimulated emission
- $X + h\nu \rightarrow X^*$ photoexcitation
- $X^* + h\nu \rightarrow X^+ + e$ photoionization
- $X^* + X^* \rightarrow X^* + X^+ + e^-$ Penning ionization
- $K + X^+ \rightarrow K + e^-$ emission of electrons from the cathode during ion bombardment

The given schemes of elementary processes in a low-temperature plasma of a gas discharge is a model of real complex procesess. They are convenient for educating process because of its simplicity and presence of elementary processes necessary for the compilation of more real models of one-component plasma. On the other hand, the simplest set of elementary processes presented can be used (and actually used) in simplified plasma calculations in those cases when the set of excited levels of an atom can be approximated by one effective excited level.

Generally, for a selected pair of particles in the collisional process, there are several channels for the reaction. The main

criteria for the elimination of the channel are the following: 1) energy considerations, 2) selection according to the conformity of the process to the requirements of conservation of the angular momentum, 3) a soft requirement for the consideration of collisional and radiative processes that do not co-develop the spin part of the wave function of atoms. The relative simplicity of using the method of constructing wave functions and calculating with their help the probabilistic characteristics of radiation processes and collisions between atom atoms and structureless particles opens up new opportunities for quantitative estimates of the probabilities of reactions proceeding through an unrestricted open channel. This significantly expands the set of training exercises in the field of plasma arc discharges and makes it expedient to create test tasks, which requires active use of computer accounts and/or numerical modeling. Additional chems for collisional transitions from the ground state of atoms:

$$\begin{cases} N_2 + e^- \rightarrow N_2 + e^- \\ N_2 + e^- \rightarrow N_2^+ + 2e^- \\ N_2^+ + 2e^- \rightarrow N_2 + e^- \\ N_2^+ + e^-\big|_{wall} = N_2 + e^-\big|_{wall} \\ cathod + N_2^+ \rightarrow cathod + N_2 + e^- \end{cases} \quad (9)$$

radiative recombination process $X^+ + e \rightarrow X^* + h\nu$

photodetachment $X^- + h\nu \rightarrow X^* + e$; $X + h\nu \rightarrow X^+ + e$

spontaneous de-excitation $X^{*1} \rightarrow X^{*2} + e$

collisional detachment $X^- + X \rightarrow 2X + e + h\nu$

These schemes allows constructing test problems ether on the electron energy, or on the radiation energy, or on reaction possibility.The general algorithm of a generator can be considered as an operator that takes text scheme and valid numerical values and constructs a text of the task.

CONCLUSION

On the basis of the developed algorithms, a working prototype of the program has been created, using otdinary computers for simulation, and able to perform systematic modeling of a large number of elementary processes that are taken into account in plasmachemical models. The use of genetic algorithms to optimize the solution in the case of calculations of atoms with a large number of electrons, accelerates the convergence of the iterative procedure. Test calculations performed to verify the created software module and its operation algorithms consisted in determining the energies of the ground states of many-electron atoms with groups of equivalent electrons on outer shells. The results obtained without using any additional empirical information on the energies of groups of cloud electrons agree with the experimental ones within the limits of accuracy acceptable for input data for numerical simulation of the kinetics of nonequilibrium plasmas. The wave functions constructed in this way are used as input data for the developed software modules for calculating cross sections and rate constants for elementary processes involving electrons and atoms within the framework of the "generalized Born method" [18]. The latter, along with the standard calculations of optically resolved collision transitions in the first order of perturbation theory, includes accounting for substantially more resource-intensive procedures: normalization of cross sections, allowance for exchange processes, and calculation of contributions from transitions through intermediate ("virtual") states, taken into account in the second and higher approximations. The accuracy calculations depends on the number of additional states, which requires solving a large number of problems in the construction of wave functions and makes a practically no-alternative idea of using simplified versions of their variants, walking. Finally, the developed semiempirical approach allows construction of wave functions of optical electrons of simple molecules, information on the rates of electronic excitation and ionization which is extremely necessary for modeling plasmas of gas discharges in air and other gas mixtures important for applications.

Developed eductional tool that uses described above computational approach demonstrates is usefullness for the plasma chemistry lessons.

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