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Study of characteristics elementary atomic processes in the neon-like multicharged ions plasma within an energy approach

We present the theoretical foundations of an advanced relativistic approach to computing the main energy, spectral characteristics of radiative-collisional processes in the plasma (in particular, the Debye plasma) of atomic as the example, neon-like) ions with simultaneous, quantitatively consistent consideration of the complex relativistic, interelectron exchangecorrelation and plasma environment effects. The approach is based on the combination of a relativistic energy approach (S-matrix Gell-Mann and Low formalism), the relativistic gaugeinvariant many-body perturbation theory with optimized Dirac-Fock-Sturm and Debye-Hückel approximations with accounting for the plasma environment effects with possible generalization on the presence of an additional external electromagnetic field. The fundamental point of our approach is the selection of the optimized Dirac-Fock-Sturm zeroth approximation and application of the consistent procedure for constructing a one-quasiparticle representation (basis's of relativistic wave functions) in compliance with the principle of gauge invariance, in particular, by minimizing a gauge-noninvariant contributions to the radiative widths of the atomic (ionic) levels due to the complex exchange-correlation effects. The electron-ion collision strength and the dioelect5ron capture rate etc are determined within the presented theory.

Keywords: Radiative-collisional processes in plasma, Relativistic energy approach, Relativistic many-body perturbation theory, collison strength, dielectron capture rate

Introduction. The theory of radiation processes (transitions, ionization, decay, etc.) is traditionally in the center of attention of theoretical quantum, atomic and molecular physics, laser physics, physics of aerodispersed systems and plasma etc (e.g. [1-7]). In the last decades, the interest has grown even more, when fundamentally important role of elementary radiation and collisional atomic processes involving multi-charged ions, photons in a wide class of physical systems (plasma etc.). We are talking, first of all, about the problems of astrospectroscopy, astrophysics, physics of the Sun and auroras, diagnostics of astrophysical, thermonuclear plasma, topical problems of laser physics, including creation of short-wavelength lasers (e.g. [8-20]). Although a fairly large group of methods for calculating characteristics of radiation and collisional processes has been developed in modern theoretical spectroscopy, including methods of pseudo- and model potential, density functional, various versions of relativistic and QED perturbation theory (PT), standard Hartree-Fock, Dirac-Fock (DF) and even mega-DF methods etc, hitherto the application of most of them faces serious both fundamental and technical problems (e.g. [1-4,13-20]). One should focus on such fundamental shortcomings of most of the mentioned methods as slow convergence of PT series, non-fulfillment of the principle of gauge invariance (appearance of gauge-noninvariant contributions (GNIC) into atomic radiation

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widths), the use of non-optimized bases of wave functions, an insufficiently complete and correct accounting of exchange-correlation effects (e.g. [1-4]).

The aim of the work is the development of the theoretical foundations of an advanced relativistic approach in radiative-collisional spectroscopy of the electronion systems to computing the main energy, spectral characteristics of radiativecollisional processes in plasma with simultaneous, consistent consideration of the complex relativistic, interelectron exchange-correlation and plasma effects.

Relativistic energy approach in radiative-collisional spectroscopy of atomic ions in plasma. In order to formulate an advanced approach, we start from the known consistent theoretical approach to studying relativistic decaying system, namely, relativistic energy formalism in a gauge invariant formulation [21-24] (e.g. [25,26] too). In fact, the known Gell-Mann and Low adiabatic formula with the QED scattering matrix for the energy shifts ΔE of decaying states is used. The whole quantum field procedure is reduced to construction of the secular matrix M and its further diaghonalization [21-24]. The M secular matrix elements are already complex in the PT second order. Their imaginary parts are connected with the radiative-collisional decay probability or cross-section. The total energy shift of the state is usually presented in the form: $\Delta E = \text{Re}\Delta E + i \text{ Im}\Delta E$, Im $\Delta E = -\Gamma/2$, where Γ is interpreted as the level width. The whole calculation of the energies and decay probabilities of a nondegenerate excited state is reduced to calculation and diagonalization of the complex matrix M and definition of matrix of the coefficients with eigen state vectors $B_{ie,iv}^{lK}$ [21-23]. To compute all necessary matrix elements, one should apply the basis's of the relativistic wave functions (look below). The energy approach has been generalized to cover the problems of scattering theory (e.g. [21-26]). Here we briefly outline the main idea considering the collisional de-excitation of the Ne-like ion: $((2j_{iv})^{-1}3j_{ie}[J_iM_i], \varepsilon_{in}) \rightarrow (\Phi_o, \varepsilon_{sc})$. Here Φ_o is the state of the ion with closed shells (ground state of the Ne-like ion); J_i is the total angular moment of the initial target state; indices iv, ie are related to the initial states of vacancy and electron; indices ε_{in} and ε_{sc} are the incident and scattered energies, respectively to the incident and scattered electrons. The initial state of the system is as follows (e.g. [25]): $|I> = a_{in}^+ \sum_{m_i,m_i} a_{ie}^+ a_{iv} \Phi_0 C_{m_{ie},m_{iv}}^{J_i,M_i}$

$$|I> = a_{in}^{+} \sum_{m_{iv}, m_{ie}} a_{ie}^{+} a_{iv} \Phi_{0} C_{m_{ie}, m_{iv}}^{J_{i}, M_{i}}$$

$$\tag{1}$$

Here $C_{m_{l_e},m_{l_e}}^{J_i,M_i}$ is the Clebsh-Gordan coefficient. Final state is as follows: $|F\rangle = a_{sc}^+ \Phi_0$, where Φ_0 is the state of an ion with closed electron shells (ground state of Ne-like ion), | I > represents three-quasiparticle (3QP) state, and | F > represents the onequasiparticle (1QP) state. The justification of the energy approach in the scattering problem is described in Refs. [22-27]. The scattered part of Im ΔE appears first in the atomic PT second order as the integral on energy of the scattered electron ε_{sc} :

$$\int d\varepsilon_{sc} G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc}) / (\varepsilon_{sc} - \varepsilon_{iv} - \varepsilon_{ie} - \varepsilon_{in} - i0)$$
(2)

$$Im\Delta E = \pi G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc})$$
(3)

where G is the combination of the known two-particle matrix elements (e.g. [3, 21]).

Relativistic many-body perturbation theory with the Dirac-Fock-Sturm and **Debye-Hückel approximation.** The most fundamental topic is connected with choice of the corresponding approach to description of relativistic atomic system and further the basis of relativistic wave functions. Namely this point determines a whole approach. In our work we will construct the formalism of relativistic many-body PT with optimized Dirac-Fock-Sturm-Debye-Hückel approximation with accounting for the influence of the plasma environment in the Debye plasma. The technique of conof many-particle structing the formalism PTand the diagrammatization (Feynman diagram technique) of the PT series is well known. We use the ideology presented in details in Refs. [3, 21]. The electronic Hamiltonian for a N-electron ion in a plasma is given in atomic units as follows [25]:

$$H = \sum_{i} \left[\alpha c p - \beta m c^{2} - Z \exp(-\mu r_{i}) / r_{i} \right] + \sum_{i>j} \frac{\left(1 - \alpha_{i} \alpha_{j} \right)}{r_{ij}} \exp(-\mu r_{ij}), \qquad (4)$$

where α nad β (α_i) – Dirac matrices, Z is the charge of the atomic nucleus. The parameter μ in (4) is connected with the plasma parameters: temperature T and charge density n as: $\mu \sim \sqrt{e^2 n / k_B T}$ (as usually, e is the electron charge, κ_B is the Boltzman constant). The density n is given as a sum of the electron density N_e and the ion density N_k of the k-th ion species having the nuclear charge q_k : $n = N_e + \sum_k q_k^2 N_k$.

The fundamental point of our approach is the selection of the optimized Dirac-Fock-Sturm (ODFS) potential as the zero approximation, and application of the procedure for constructing a one-quasiparticle representation in compliance with the principle of gauge invariance, in particular, by minimizing GNIC to the radiative widths of the atomic (ionic)levels. In order to reach that adequate description off characteristics of the atomic elementary processes one requires using the optimized basis's of wave functions. We have applied an effective version [28] (e.g. [29, 30]) of "ab initio" optimization principle for construction of cited basis's, based on relativistic energy approach [22,25]. In the fourth order of QED PT or the second order of the relativistic PT with the DFS approximation there appear diagrams, whose contribution into the Im δ E accounts for the polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the GNICn ΔE_{ninv}). The leading term is as follows [22]:

$$\operatorname{Im} \delta E_{ninv} \left(\alpha - s \mid A_{d} \right) = -C \frac{e^{2}}{4\pi} \iiint dr_{1} dr_{2} dr_{3} dr_{4} \sum \left(\frac{1}{\omega_{mn} + \omega_{\alpha_{2}}} + \frac{1}{\omega_{mn} - \omega_{\alpha_{2}}} \right) \cdot \Psi_{\alpha}^{+} (r_{1}) \Psi_{m}^{+} (r_{2}) \Psi_{s}^{+} (r_{3}) \Psi_{n}^{+} (r_{4}) (1 - \alpha_{1} \alpha_{2}) / r_{12} \cdot \left(\left[\left(\alpha_{3} \alpha_{4} - (\alpha_{3} n_{34}) (\alpha_{4} n_{34}) \right) / r_{34} \cdot \sin \left[\omega_{\alpha_{n}} (r_{12} + r_{34}) + \omega_{\alpha_{n}} \cdot \cos \left[\omega_{\alpha_{n}} (r_{12} + r_{34}) \right] (1 + (\alpha_{3} n_{34}) (\alpha_{4} n_{34}) \right) \right] \Psi_{m} (r_{3}) \Psi_{\alpha} (r_{4}) \Psi_{n} (r_{2}) \Psi_{s} (r_{1})$$

The minimization of the functional Im ΔE_{ninv} leads to the integral differential equation of the DF type, that is numerically solved. In result one can get the optimal one-electron basis of the PT. In our approach it is supposed that the basis is the extended and in the case of the neon-like ions it additionally includes f-orbitals as well as the Sturm complement in order to take into consideration a continuum states. The effective Sturm algorithm is presented in Ref. [25,26] and it is used in our method. In addition to continuum states, there is a need to account for Rydberg states as well. Moreover, in the processes of electron-ion collisions with the participation of multicharged ions in the plasma, the corresponding states converge to the thermalized energy zone of Rydberg and autoionization Rydberg states. Really these states converge to the ionization threshold of each ion in plasma.

Characteristics of electron-ion collision and dielectron capture in plasma.

Let us recall that in the relativistic theory, when constructing the secular matrix M and further transformations, a standard transition is implemented from the representation of a pure j-j scheme of the connection of moments to the presentation of an intermediate scheme of the connection, where quantum numbers I, I' respectively number the states (e.g. [3]). Diagonal elements of the transformed matrix $\langle IK | M | I'K' \rangle$ are then determined in the standard way:

$$< IK | M | IK' > = \sum_{iv',ie'} B_{iv',ie'}^{IK'} < iv',ie',J_i | M | iv,ie,J_i > B_{iv,ie,J_i}^{IK},$$
 (6)

In fact, these matrix elements actually determine the corresponding cross sections of collisions of an electron with an ion, in particular, the cross sections of collisions that are accompanied by the transition of an ion (as an example, we consider a neon-like ion) from a disturbed two-quasiparticle state to the ground state (the socalled collision process where de-excitation): $|IK, \varepsilon_{in}j_{in}\rangle \rightarrow |\Phi_{o}, \varepsilon_{sc}j_{sc}\rangle$.

By definition, the electron-ion collision strength $\Omega(I \to F)$ is related to the corresponding collision cross section σ as follows (e.g.[22,25]):

$$\sigma(I \to F) = \Omega(I \to F) \cdot \pi / \{ (2J_i + 1)\varepsilon_{in}[(\alpha Z)^2 \varepsilon_{in} + 2] \}$$
 (7)

$$\sigma(IK \to 0) = 2\pi \sum_{j_{in}, j_{sc}} (2j_{sc} + 1) \{ \sum_{j_{ie}, j_{iv}} < 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_i > B_{ie, iv}^{IK} \}^2$$
 (8)

$$\sigma(IK \to 0) = 2\pi \sum_{j_{in}, j_{sc}} (2j_{sc} + 1) \{ \sum_{j_{ie}, j_{iv}} < 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_{i} > B_{ie,iv}^{IK} \}^{2}$$

$$< 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_{i} > = \sqrt{(2j_{ie} + 1)(2j_{iv} + 1)} (-1)^{j_{ie} + 1/2} \times \sum_{\lambda} (-1)^{\lambda + J_{i}} \times \frac{1}{\lambda}$$

$$\times \{\delta_{\lambda,J_i} / (2J_i + 1)Q_{\lambda}(sc,ie;iv,in) + \begin{bmatrix} j_{in}...j_{sc}...J_i \\ j_{ie}...j_{iv}....\lambda \end{bmatrix} Q_{\lambda}(ie;in;iv,sc)\}, \qquad (9)$$

where $Q_{\lambda} = Q_{\lambda}^{\text{Qul}} + Q_{\lambda}^{\text{Br}}$ is the sum of the Coulomb and Breit part matrix elements, which are corresponding to the known Coulomb $\sim exp(i|\omega|r_{12})/r_{12}$ and the Breit \sim $exp(i|\omega|r_{12}) \alpha_1\alpha_2/r_{12}$ parts of the relativistic interelectron interaction potential. The details of their computing can be found in Refs. [3, 21-27].

Very important question is connected with the correct determination of normalized cross section. Here it is necessary to perform all calculation with fairly normalized functions f_{in} , g_{in} of an incident electron and f_{sc} , g_{sc} of a scattered electron (e.g. [3]). The corresponding normalizing factors N_{in}^2 , N_{sc}^2 are defined as:

$$N_{in}^{2} = Z\alpha\pi(2j_{in} + 1)\lim_{r \to \infty} \frac{1}{\sqrt{X_{1}X_{2}}Y(f_{in}, g_{in})},$$
 (10)

$$N_{sc}^{2} = Z\alpha / \pi \lim_{r \to \infty} \frac{\sqrt{X_{1}X_{2}}}{Y(f_{sc}, g_{sc})},$$
(11)

where $Y(f,g) = r^{2|k|}(X_1f^2 + X_2g^2)$; f, g are the large and small components of the DF wave function.

Characteristics of a dielectron capture. Dielectron capture as well as an autoionization decays of the Rydberg states are among the most important elementary processes that contribute to the dynamics and kinetics of the population of various states in a plasma. Dielectron traps, in fact, can lower the energy threshold of excitation of the corresponding ion, and thus lead to an increase in the rate of excitation collisions for a given energy distribution of electrons in the plasma. The contribution of this effect will depend on the ratio between different ionization channels of the ion in the plasma, which includes, on the one hand, ionization due to collisions, and photoionization, and on the other hand, Auger decay into the ground state of the ion (e.g.,[21-27]). The cross-section of dielectron capture can be determined by the analytical extension of the electron-ion collision to the region of energy ε_m lower than the collision threshold, where the energy of the scattered (captured) electron becomes negative: $\varepsilon_{sc} = \varepsilon_m - \varepsilon_y$. The rate of dielectron capture can be determined by the formula:

$$C(i-j) = \frac{\pi a_0^2}{(2J_i+1)} \int_{\varepsilon_{in}+\varepsilon_{ji}}^{\infty} d\varepsilon_{in} \frac{Ry}{\varepsilon_{in}} \Omega(i-j;\varepsilon_{in}) F(\varepsilon_{in};T_e)$$
 (12)

$$F(\varepsilon, T) = 2\varepsilon \sqrt{2/(m_e \pi T^3)} \exp(-\varepsilon/T), \qquad (13)$$

where a_0 is the Bohr radius, Ry is the Rydberg energy (in Coulomb units, Ry = 0.5Z²). The function F simulates the energy distribution of plasma electrons. Together with the speed multiplier, it is one of the model elements of the theory. In principle, the theory also allows the use of a non-Maxwellian energy distribution. The fact is that in a real plasma the distribution of time-particles by velocities may differ to one degree or another from the purely Maxwellian one (e.g. [23-25]). In particular, the presence of an external electromagnetic field can cause a distortion of the electron distribution function in the region of high energies (the effect of the flow of so-called fugitive non-thermal electrons), which leads to an increase in the number of particles in the tail of the Maxwellian distribution. In the absence of significant external influence, another situation is possible, when due to collisions accompanied by disruption or ionization, the number of fast electrons turns out to be less than the Maxwellian number. Although differences from the pure Maxwellian distribution are quite common, the case of a purely Maxwellian function is of primary interest in a large number of do-data. In relativistic theory, it is natural to describe the distribution of continuum electrons by the relativistic Maxwell-Boltzmann distribution function (e.g., [3]).

To conlude, we presented a new version of energy approach in radiative-collisional spectroscopy of ions in plasma, based on the relativistic gauge-invariant many-body PT with the optimized Dirac-Fock-Sturm-Debye-Hückel approximation. The approach can be generalized for the case of pr4esense electromagnetic field, correspondingly, the models [31-33] can be used. This topic as well as the application results can be considered in the next work.

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А.А. Свинаренко, М.В. Сміщенко

Вивчення характеристик елементарних атомних процесів у плазмі неоноподібних багатозарядних іонів в рамках енергетичного підходу

КІЦАТОНА

Викладено теоретичні основи удосконаленого релятивістського підходу до визначення основних енергетичних, спектральних характеристик радіаційних процесів та процесів зіткнень у плазмі багатозарядних (неон-подібних) іонів) з одночасним, кількісно послідовним урахуванням складних релятивістських, міжелектронних обміннокореляційних ефектів та ефектів плазмового середовища. Підхід базується на поєднанні релятивістського енергетичного підходу, релятивістської калібрувальноінваріантної багаточастинкової теорії збурень з оптимізованим наближеннями Дірака-Фока-Штурма та Дебая-Хюккеля з урахуванням впливу плазмового середовища, і може бути узагальнений на випадок наявності додаткового зовнішнього електромагнітного поля. Фундаментальним моментом підходу ϵ вибір оптимізованого нульового наближення Дірака-Фока-Штурма та застосування узгодженої процедури побудови одноквазічастинкового відповідно до принципу калібрувальної інваріантності, зокрема , шляхом мінімізації калібрувально-неінваріантних внесків у радіаційні ширини атомних (іонних) рівнів внаслідок впливу складних обмінно-кореляційних ефектів. У рамках представленої теорії визначаються сила (пеерріз) електрон-іонного зіткнення, швидкість діелектронного захоплення тощо.

Ключові слова: радіаційні процеси та процеси зіткнень у плазмі, релятивістський енергетичний підхід, релятивістська калібрувально-інваріантна багаточастинкова теорія збурень, переріз зіткнення, швидкість діелектронного захоплення.