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ГАЗОДИНАМІКА

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Relativistic gauge-invariant theory of determination of autoionization resonances parameters for atomicsystems with accouting for the plasma environment effects

We present the theoretical foundations of an advanced relativistic gauge-invariant theory for computing main energy, spectral characteristics of complex auto ionization resonances for atomic systems with simultaneous, quantitatively consistent consideration of the complex relativistic, interelectron exchange-correlation and plasma environment effects (in particular, the Debye plasma). The approach is based on the combination of a relativistic energy approach (S-matrix Gell-Mann and Low formalism), the relativistic gauge-invariant 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 additionalexternal electromagnetic field. The fundamental advantage of pt presented theory is the selection of the optimized Dirac-Fock-Sturm zeroth approximation and application of the consistent procedure for constructing a one-quasi particle representation (basis's of relativistic wave functions) incompliance with the principle of gauge invariance, in particular, by minimizing a gauge-noninvariant contributions to the radioactive widths of the atomic (ionic) levels due to the complex exchange-correlation effects.

Keywords: *complex autoionization resonances, relativistic energy approach, relativistic many-body perturbation theory, interelectron exchange-correlation and plasma environment effects.*

Introduction. It is known that autoionization states (AS) play a fundamental role in various elementary atomic processes such as autoionization, selective photoionization, electron scattering on atoms, atom- and ion-atom collisions, etc. The presence of AS in ions significantly affects the nature of the radiation spectrum of high-temperature astrophysical and laboratory plasma. Their radiative decay is accompanied by the formation of complex spectra of dielectronic satellites to the resonance lines of ions of the next ionization multiplicity, which contain information on the state of the plasma used for its diagnostics, as well as in studying the physical conditions in the solar corona and other astrophysical objects [1-16]. Knowledge of the properties of AS is also very important for understanding the processes occurring, for example, in laser plasma. Their decay can greatly affect the kinetics of population of excited levels and the intensity of radiation of spectral lines. (e.g. [1-5]).

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-

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Fock (DF) and even mega-DF methods etc, hither to the application of most of them faces serious both fundamental and technical problems (e.g. [1-4, 17-29]). The most known short comings of most of the mentioned method sare a slow convergence of PT series, violation of the principle of gauge invariance (appearance of gauge-noninvariant contributions (GNIC) into atomic radiation widths), the use of non-optimized bases of wave functions, an insufficiently complete and correct accounting of exchange correlation effects, nonaccurate account of the plasma effects (e.g. [1-4]).

Theaimoftheworkisthedevelopmentofthetheoreticalfoundationsofofan advanced relativistic gauge-invariant theory for computing main energy, spectral characteristics of complex autoionization resonances for atomic systems with simultaneous, quantitatively consistent consideration of the complex relativistic, interelectron exchange-correlation and plasma environment effects (in particular, the Debye plasma).

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. In our work we will develop 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 constructing the formalism of many-particle PT and the corresponding diagram matization (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]:

$$H = \sum_i [\alpha cp - \beta mc^2 - Z\exp(-\mu r_i)/r_i] + \sum_{i>j} \frac{\left(1 - \alpha_i \alpha_j\right)}{r_{ij}} \exp(-\mu r_{ij}), \qquad (1)$$

where α and 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 and $\kappa_Б$ 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 PT zeroth approximation, and application of the procedure for constructing a one-quasi particle representation in compliance with the principle of gauge invariance, inparticular, by minimizing GNIC to the radioactive 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. 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] has been used.

In the fourth order of QED PT or the second order of the relativistic PT with the DFS approximations there appear diagrams, whose contribution into the Im δE ac-

counts 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]:

$$\mathrm{Im}\delta E_{ninv}(\alpha - s \mid A_d) = -C\frac{e^2}{4\pi}\iiint\int dr_1 dr_2 dr_3 dr_4 \sum(\frac{1}{\omega_{mn}+\omega_{\alpha_s}} +$$

$$\frac{1}{\omega_{mn}-\omega_{\alpha_s}})\Psi_\alpha^+(r_1)\Psi_m^+(r_2)\Psi_s^+(r_3)\Psi_n^+(r_4)(1-\alpha_1\alpha_2)/r_{12}\cdot \qquad (2)$$

$$\{[(\alpha_3\alpha_4-(\alpha_3 n_{34})(\alpha_4 n_{34}))/r_{34}\cdot\sin[\omega_{\alpha_n}(r_{12}+r_{34})+\omega_{\alpha_n}\cdot$$

$$\cos[\omega_{\alpha_n}(r_{12}+r_{34})](1+(\alpha_3 n_{34})(\alpha_4 n_{34}))]\}\Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1)$$

The minimization of the functional $\mathrm{Im}\Delta E_{ninv}$ 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. The effective Sturm algorithm is presented in Ref. [25, 26] and it is implemented into our theorrtical approach.

Relativistic energy approach to complex autoionization resonances. 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 relativistic case the Gell-Mann and Low formula expressed an energy shift ΔE through the QED scattering matrix including the interaction with as the photon vacuum field as the laser field. The first case is corresponding to definition of the traditional radiative and autoionization characteristics of multielectron atom.

Generally speaking, the majority of complex atomic systems possess a dense energy spectrum of interacting states with essentially relativistic properties. Further one should realize a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix M diagonalization [8-12]. The secular matrix elements are already complex in the second order of the PT. Their imaginary parts are connected with a decay possibility.A total energy shift of the state is presented in the standard form [12]

$$\Delta E = Re\Delta E + iIm\Delta E \quad Im\Delta E = -\Gamma/2 \qquad (3a)$$

where Γ is interpreted as the level width, and the decay possibility $P = \Gamma$. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the M. The *jj*-coupling scheme is usually used. The complex secular matrix M is represented in the form [9, 10]

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)} \qquad (3b)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}, M^{(3)}$ those of the one-, two- and three-QP diagrams respectively. $M^{(0)}$ is a real matrix, proportional to the unit matrix. It determines only the general level shift. We have assumed $M^{(0)} = 0$. The diagonal matrix $M^{(1)}$ can be presented as a sum of the in-

dependent 1QP contributions.

The optimized 1-QP representation is the best one to determine the zeroth approximation. In the second order, there is important kind of diagrams: the ladder ones. These contributions have been summarized by a modification of the central potential, which must now include the screening (anti-screening) effect of each particle by two others.

Let us remind that in the QED theory, the photon propagator D(12) plays the role of this interaction. Naturally, an analytical form of D depends on the gauge, in which the electrodynamic potentials are written. In general, the results of all approximate calculations depended on the gauge. Naturally the correct result must be gauge invariant. The gauge dependence of the amplitudes of the photoprocesses in the approximate calculations is a well known fact and is in details investigated by Grant, Armstrong, Aymar-Luc-Koenig, Glushkov-Ivanov [1, 2, 5, 9]. Grant has investigated the gauge connection with the limiting non-relativistic form of the transition operator and has formulated the conditions for approximate functions of the states, in which the amplitudes are gauge invariant (so called Grant's theorem). In ref. [16] it has been developed a new version of the approach to conserve gauge invariance. Here we applied it to get the gauge-invariant procedure for generating the relativistic DKS orbital bases (abbreviator of our method: GIRPT).

The most important characteristic of the AS (resonances) is, in addition to the AS energy, also the AS width. It should be especially emphasized that in almost all works on the AS theory, the standard Fermi rule is used to calculate the autoionization widths, written in a form slightly different from similar expressions for determining the radiative width. Indeed, remembering the rarely used, but extremely accurate definition of "autoionization resonance" as a "state in the continuum", it is easy to see the way to modify Fermi's golden rule. Indeed, if the autoionization decay in the single-particle approximation can be represented as follows: $(\beta_1 \beta_2 \rightarrow \beta_3 k)$, where βi (i= l, 2, 3) describes the set of quantum numbers of bound states, k is the state of a free electron. In this case, the decay is possible only into a state of a continuous spectrum, coinciding in parity and in the value of the total moment J with the original AS. Then, obviously, the width of the level Γ, associated with autoionization decay, is determined by its connection with the states of the continuous spectrum:

$$\Gamma = 2\pi |\langle i | V | f \rangle|^2 \infty |V(\alpha_1 \alpha_2, \alpha_3 k)|^2, \qquad (4)$$

where $\langle i|$ is the initial, $|f\rangle$ is the final state of the system, V is the operator of interelectron interaction.This approach is standardly used in almost all modern theories of the relativistic multielectron atom, based on methods such as HF, DF, multiconfiguration approximations of these methods, etc. Naturally, the basis for these methods are the well-known, remarkable works of Fano.The shortcomings of the method of calculating the widths of the AS using directly (2) and the corresponding bases of wave functions are also obvious. In our opinion, a more adequate and fundamental approach to calculating the characteristics of the AS should be an approach based on the QED PT. It should be recalled that, of course, in QED PT the autoionization width first manifests itself in the fourth order (the second order of atomic TB). It was emphasized above that in the QED PT series there are known divergent terms, caused, in our case, first of all, by two types of divergences. The first type is the stan-

dard QED ultraviolet divergence associated with integration over the frequencies of virtual photons. For the autoionization width, the ultraviolet divergence first manifests itself in terms of the sixth order of TB; however, in modern atomic spectroscopy there are convenient procedures for eliminating such a divergence (see, for example, [1]). The second type of divergence is associated with the vanishing of the energy denominator upon integration over virtual stationary electron states. This type of divergence is also known in the nonrelativistic theory. This divergence also manifests itself for the first time in the sixth order of TB. As in the previous case, theoretical atomic physics has well-developed procedures for eliminating this type of divergence, in particular, by summing the divergent terms in all orders of the PT. It is very important to emphasize that the contribution of this sum decreases rapidly with increasing nuclear charge.

The fourth-order correction of the PT to the energy of a state, a certain state, say, $n_1^0 j_1^0 n_2^0 j_2^0 [J]$, can be represented as follows:

$$\Delta E^{(4)} = \underset{k_1 k_2}{S} \sum_{\substack{\beta_1\beta_2 \\ \beta_1'\beta_2'}} C^J(\beta_1\beta_2) \frac{V_{\beta_1\beta_2;k_1k_2} V_{k_2k_1;\beta_1'\beta_2'}}{E(n_1^0 j_1^0 n_2^0 j_2^0) - E(k_1k_2) + i0} C^J(\beta_1'\beta_2'). \quad (5)$$

Here, as usual, V is the matrix element of the interelectron interaction. The coefficients $C^J(\beta_1\beta_2)$ provide the correct angular symmetry, for certainty, say, of a two-electron system. The sum $\underset{k_1k_2}{S}$ denotes the double sum and integral over the entire spectrum of one-electron Dirac functions. Naturally, here we mean both the spectrum of bound states and the continuous spectrum, including the "negative" continuum.

The total width is given the expression:

$$\Gamma(n_1^0 j_1^0, n_2^0 j_2^0; J) = \frac{2\pi\varepsilon}{K_0} \sum_{\beta_1\beta_2} \sum_{\beta_1'\beta_2'} C^J(\beta_1\beta_2) C^J(\beta_1'\beta_2') \sum_{\beta\,\beta_K} V_{\beta_1\beta_2;\beta\,\beta_K} V_{\beta_K\beta\,;\beta_1'\beta_2'} \quad (6)$$

where the coefficients C can be determined as follows:

$$C^J(\beta_1\beta_2) = C^J(n_1 j_1 n_1^0 j_1^0; n_2 j_2 n_2^0 j_2^0) A(j_1 m_1; j_2 m_2; JM) \quad (7)$$

$$(j_1 m_1, j_2 m_2 JM) = (-1)^{j_1 - j_2 + M} \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix} \sqrt{2J+1} \quad (8)$$

$$C^J(n_1 j_1 n_1^0 j_1^0; n_2 j_2 n_2^0 j_2^0) = N(n_1^0 j_1^0, n_2^0 j_2^0)[\delta(n_1^0 j_1^0 n_1 j_1)\delta(n_2^0 j_2^0 n_2 j_2) + \\ + (-1)^{j_1 + j_2 + J + 1} \delta(n_1^0 j_1^0 n_2 j_2)\delta(n_2^0 j_2^0 n_1 j_1) \quad (9)$$

$$N(n_1^0 j_1^0; n_2^0 j_2^0) = \begin{cases} \frac{1}{\sqrt{2}} n_1^0 j_1^0 = n_2^0 j_2^0 \\ 1\; n_1^0 j_1^0 \neq n_2^0 j_2^0 \end{cases} \quad (10)$$

The matrix element of the relativistic inter-particle interaction

$$V(r_i r_j) = \exp(i\omega_{ij} r_{ij}) \cdot (1 - \alpha_i \alpha) / r_{ij}. \quad (11)$$

(here α_i –the Dirac matrices) in (3) is determined as follows:

$$V_{\beta_1\beta_2;\beta_4\beta_3} = \sqrt{(2j_{1+1})(2j_{2+1})(2j_{3+1})(2j_{4+1})}(-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \times \\ \times \sum_{a\mu} (-1)^{\mu} \begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix} \begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & -\mu \end{pmatrix} Q_a(n_1 j_1 l_1 n_2 j_2 l_2; n_4 j_4 l_4 n_3 j_3) \quad (12)$$

$$Q_a = Q_a^{Qul} + Q_a^{\mathrm{Br}} \tag{13}$$

Here Q_a^{Qul} and Q_a^{Br} is corresponding to the Coulomb and Breit parts of the interparticle interaction (5). It is worth to remind that the real part of the interaction matrix element can be expanded in terms of Bessel functions and the Coulomb part Q_a^{Qul} can be expressed in the radial integrals R_λ, angular coefficients S_λ. The detailed description of these quantities as well as the detailed algorithms of their computing are presented, e.g. in ref. [21-25].

To conclude, we presented a new advanced relativistic gauge-invariant theory for computing main energy, spectral characteristics of complex autoionization resonances for atomic systems with simultaneous, quantitatively consistent consideration of the complex relativistic, interelectron exchange-correlation and plasma environment effects (in particular, the Debye plasma). The approach is based on the combination of a relativistic energy approach (S-matrix Gell-Mann and Low formalism), the relativistic gauge-invariant 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 (e.g. [31-33]). This topic as well as the application results can be considered in the next work.

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Глушков О.В., Свинаренко А.А.

Релятивістська калібрувально-інваріантна теорія обчислення характеристик автоіонізаційних резонансів для атомних систем з урахуванням впливу плазмового середовища

Викладені теоретичні основи удосконаленої релятивістської калібрувально-інваріантної теорії для обчислення енергетичних та спектральних характеристик складних автоіонізаційних резонансів для атомних систем з одночасним, кількісно узгодженим розглядом складних релятивістських, міжелектронно-обмінно-кореляційних ефектів та ефектів плазмового середовища (зокрема, дебаєвських плазми). Підхід базується на поєднанні релятивістського енергетичного підходу (формалізм S-матриці Гелл-Манна та Лоу), релятивістської калібрувально-інваріантної багаточастинскової теорії збурень з оптимізованими наближеннями Дірака-Фока-Штурма та Дебая-Хюккеля з урахуванням вплив плазмового середовища і з можливим узагальненням на наявність додаткового зовнішнього електромагнітного поля. Фундаментальною перевагою представленої теорії є вибір оптимізованого нульового наближення Дірака-Фока-Штурма та застосування узгодженої процедури побудови одноквазічастинкового представлення (базису релятивістських хвильових функцій) відповідно до принципу калібрувальної інваріантності, зокрема , шляхом мінімізації калібрувально-неінваріантних внесків у радіаційні ширини атомних (іонних) рівнів за рахунок складних обмінно-кореляційних ефектів.

Ключові слова: *комплексні автоіонізаційні резонанси, релятивістський енергетичний підхід, релятивістська калібрувально-інваріантна багаточастинкова теорія збурень, міжелектронні обмінно-кореляція ефекти та ефекти плазмового середовища*