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ADVANCED RELATIVISTIC ENERGY APPROACH TO RADIATION DECAY PROCESSES IN ATOMIC SYSTEMS

We consider the fundamental aspects of the advanced generalized energy approach to relativistic calculation of the radiative decay (transitions) probabilities in heavy neutral atomic systems and multicharged ions. The approach is based on the Gell-Mann and Low S-matrix formalism and the relativistic many-body perturbation theory (PT) with using the optimized one-quasiparticle representation and an accurate account of the relativistic and correlation. In relativistic case the Gell-Mann and Low formula expresses an energy shift through the electrodynamical scattering matrix including the interaction with as the laser field as the photon vacuum field. The last case is corresponding to definition of the traditional radiative transitions probabilities for atoms and ions.

1. Introduction

Accurate radiative decay widths and probabilities, oscillator strengths of atomic and ionic line transition are of a great interest for astrophysical analysis, laboratory, thermonuclear plasma diagnostics, fusion research, laser physics etc [1–160].

Spectral lines are usually characterized by their wavelength and oscillator strength. Typically, transition probabilities are known less accurately than wavelengths. Moreover, for many spectral lines of heavy atoms and especially multicharged ions the radiative transition probabilities are not reliably known at all. Radiative transition probabilities have been mainly determined from calculations and to a much smaller extent from experiment [1,2]. Many theoretical methods use techniques which include extensive configuration interaction or multi-configuration treatments [2-22]. The well known multi-configuration Hartree-Fock method (the relativistic effects are often taken into account in the Pauli approximation or Breit Hamiltonian etc) allowed to obtain the useful spectral data on light and not heavy atomic systems [8]. The multi-configuration (MC) Dirac-Fock (DF) method is the most reliable version of calculation for multielectron systems with a large nuclear charge. In these calculations the effects are taken into account practically precisely [3-17]. The calculation program of Desclaux (the Desclaux program, Dirac package) is compiled with proper account of the one- and two-particle relativistic, a finiteness of the nucleus size etc. In last decades a consistent quantum-electrodynamical (QED) techniques have been implemented to atomic theory calculations (look [17]). It should be given special attention to two very general and important computer systems for relativistic and QED calculations of atomic and molecular properties developed in the Oxford group and known as GRASP ("GRASP", "Dirac"; "BERTHA", "QED", "Dirac") (see [3–7] and references there). Besides, the well known density functional theory (DFT), relativistic coupled-cluster approach and model potential approaches in heavy atoms and ions should be mentioned too [18-24].

In order to determine the transition probabilities one usually uses usually a standard amplitude approach. Each of theoretical approaches to calculation of transition probabilities contains critical factors (configuration interaction or multiconfiguration treatment, spectroscopic coupling

schemes and relativistic corrections, exchange-correlation corrections convergence of probabilities results and of the dipole length and velocity forms, accuracy of transition energies etc) which need to be adequately taken care of to get reliable results.

The purpose of this paper is to review the fundamental ideas of the generalized relativistic energy approach to calculation of the radiative decay characteristics for atoms and multicharged ions, in particular, transition probabilities and oscillators strengths, line strengths etc. The bases of the energy approach to one-electron ions have been considered by Labzovsky et al [25]. Originally the energy approach to radiative and autoionization processes in multielectron atoms and ions has been developed by Ivanova-Ivanov et al [23,24] (the PC code "Superatom-ISAN"). More accurate, advanced version of the relativistic energy approach has been further developed in Refs. [26,27]). The energy approach is based on the Gell-Mann and Low S-matrix formalism combined with the relativistic perturbation theory (PT). In relativistic case the Gell-Mann and Low formula expressed an energy shift ΔE through the electrodynamical scattering matrix including interaction with as the photon vacuum field as a laser field. The first case is corresponding to determination of radiative decay characteristics for atomic systems. Earlier we have applied the corresponding generalized versions of the energy approach to many problems of atomic, nuclear and even molecular spectroscopy, including, cooperative electron-gamma-nuclear "shake-up" processes, electron-muon-beta-gamma-nuclear spectroscopy, spectroscopy of atoms in a laser field etc [28-34].

2. Relativistic energy approach to radiative decay processes

Generally speaking, the majority of complex atomic systems possesses a dense energy spectrum of interacting states with essentially relativistic properties. In the theory of the non-relativistic atom a convenient field procedure is known for calculating the energy shifts ΔE of degenerate states. This procedure is connected with the secular matrix *M* diagonalization [24-26]. In constructing *M,* the Gell-Mann and Low adiabatic formula for ΔE is used. A similar approach, using the Gell-Mann and Low formula with the electrodynamic scattering matrix, is applicable in a theory of relativistic atom; the approach is consistently electrodynamical. In contrast to the non-relativistic case, the secular matrix elements are already complex in the second order of the PT (first order of the interelectron interaction). Their imaginary parts are connected with the radiation decay (radiation) probability. The total energy shift of the state is usually presented in the form:

$$\Delta \mathrm{E} = \mathrm{Re}\,\Delta E + i\,\mathrm{Im}\,\Delta E \qquad \mathrm{Im}\,\Delta E = -\Gamma/2 \quad (1)$$

where Γ is interpreted as the level width, and the decay possibility $\mathrm{P} = \Gamma$.

In this approach, the whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the complex matrix *M*. In the papers of different authors, the $\mathrm{Re}\,\Delta E$ calculation procedure has been generalized for the case of nearly degenerate states, whose levels form a more or less compact group. One of these variants has been previously [23,26] introduced: for a system with a dense energy spectrum, a group of nearly degenerate states is extracted and their matrix *M* is calculated and diagonalized. If the states are well separated in energy, the matrix *M* reduces to one term, equal to ΔE. The non-relativistic secular matrix elements are expanded in a PT series for the interelectron interaction.

The complex secular matrix *M* is represented in the form [23]:

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

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- quasiparticle diagrams respectively. $M^{(0)}$ is a real matrix, proportional to the unit matrix. It determines only the general level shift. It is usually assumed $M^{(0)} = 0$. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent one-quasiparticle contributions. For simple systems (such as alkali atoms and ions) the one-quasiparticle energies can be taken from the experiment. Substituting these quantities into (2) one could have summarized all the

contributions of the one -quasiparticle diagrams of all orders of the formally exact relativistic PT. However, the necessary experimental quantities are not often available. The first two order corrections to $\mathrm{Re}\,M^{(2)}$ have been analyzed previously [23,35] using the Feynman diagrams technique.

The contributions of the first-order diagrams have been completely calculated. In the second order, there are two kinds of diagrams: polarization and ladder ones. The polarization diagrams take into account the quasiparticle interaction through the polarizable core, and the ladder diagrams account for the immediate quasiparticle interaction.

An effective form for the two-particle polarizable operator has been proposed in Ref. [28]; it has the following form:

$$V^{d}_{pol}(r_1 r_2) = X\left\{\int \frac{dr'\left(\rho_c^{(0)}(r')\right)^{1/3}\theta(r')}{|r_1 - r'|\cdot|r' - r_2|} - \right.$$
$$\left. - \int \frac{dr'\left(\rho_c^{(0)}(r')\right)^{1/3}\theta(r')}{|r_1 - r'|}\int \frac{dr''\left(\rho_c^{(0)}(r'')\right)^{1/3}\theta(r'')}{|r'' - r_2|}\Big/\left\langle\left(\rho_c^{(0)}\right)^{1/3}\right\rangle\right\},$$
$$\left\langle\left(\rho_c^{(0)}\right)^{1/3}\right\rangle = \int \boldsymbol{d}\ \left(\rho_c^{(0)}(r)\right)^{1/3}\theta(r), \qquad (3)$$
$$\theta(r) = \left\{1 + \left[3\pi^2\cdot\rho_c^{(0)}(r)\right]^{2/3}\Big/c^2\right\}^{1/2}$$

where ρ_c^0 is the core electron density (without account for the quasiparticle), X is numerical coefficient, c is the light velocity. The similar approximate potential representation has been received for the exchange polarization interaction of quasiparticles. Some of the ladder diagram contributions as well as some of the three-quasiparticle diagram contributions in all PT orders have the same angular symmetry as the two-quasiparticle diagram contributions of the first order. These contributions have been summarized by a modification of the central potential, which must now include the screening (anti-screening) of the core potential of each particle by the two others (look details in Refs. [23,26,35]). The additional potential modifies the one-quasiparticle orbitals and energies. Then the secular matrix can be approximated as follows: $M \sim \tilde{M}^{(1)} + \tilde{M}^{(2)}$, where $\tilde{M}^{(1)}$ is the modified one-quasiparticle matrix (diagonal), and $\tilde{M}^{(2)}$ the modified two-quasiparticle one. $\tilde{M}^{(1)}$ is calculated by substituting the modified one-quasiparticle energies), and $\tilde{M}^{(2)}$ by means of the first PT order formulae for $M^{(2)}$, putting the modified radial functions of the one-quasiparticle states in the radial integrals (look below)

Let us remind that in the QED theory the photon propagator D(12) plays the role of interparticle interaction. Naturally the analytical form of D(12) depends on the gauge, in which the electrodynamical 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 (look Refs. [1,3,26]). 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 of the photoprocesses are gauge invariant. These results remain true in the energy approach because the final formulae for the probabilities coincide in both approaches.

3. Imaginary part of the secular matrix and transition probability

Within the relativistic energy approach the radiative processes are determined by the imaginary part of the interaction (1b) between the active quasiparticle and the electrodynamic vacuum of the electronic field. The presence of the polarizable core can be effectively accounted for by modification of (1b). This corresponds to a modification of the radiation transition operator in the traditional amplitude approach. A local form of the modified transition operator has been previously treated by Hibbert, Migdalec, Ivanova-Ivanov et al (look, for example, see Refs. [9,21,23,24,26]). An integral form of the additional polarization interaction, including the imaginary part, has been deduced on the base of the analysis of the second-order (the QED PT fourth order) polarization diagrams. In result one could take into account for the corresponding corrections to $\mathrm{Im}\,\Delta E$. The detailed description of the accounting for the correlation corrections of the PT high orders within the Green functions method (with the use of the Feynman diagram's technique) is given in Refs. [23,24, 34,35], where additional details can be found. The corresponding form of the polarizable operator is given below.

The probability is directly connected with imaginary part of electron energy of the system, which is defined in the lowest order of the PT as follows [23]:

$$\mathrm{Im}\,\Delta E = -\frac{e^2}{4\pi}\sum_{\substack{\alpha>n>f\\[\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n\alpha n}, \tag{4}$$

where $\sum^{-}_{\alpha>n>f}$ for electron and $\sum^{-}_{\alpha<n\le f}$ for vacancy. The potential V is as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \tag{5}$$

The individual terms of the sum in (5) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha_n} = \frac{1}{4\pi}\cdot V^{|\omega_{\alpha_n}|}_{\alpha_n\alpha_n} \tag{6}$$

The corresponding oscillator strength is defined as:

$$gf = \lambda_g^2\cdot\Gamma_{\alpha_n}/6.67\cdot10^{15}, \tag{7}$$

where g is the degeneracy degree, l is a wavelength in angstroms (Å). When calculating the matrix elements (5), one should use the angle symmetry of the task and write the corresponding expansion for $\sin|w|r_{12}/r_{12}$ on spherical harmonics as follows:

$$\frac{\sin|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}^{\infty}(\lambda)J_{\lambda+1/2}(|\omega|r_1)J_{\lambda+1/2}(|\omega|r_2)P_\lambda(\cos\widehat{r_1 r_2}) \tag{8}$$

where J –is the Bessel function of first kind and (l) = 2l + 1. This expansion is corresponding to usual multipole expansion for probability of the radiative transition. Substitution of the expansion (11) to matrix element of interaction gives the following expression:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2}\times \times\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1 j_3 & \lambda\\ m_1 - m_3 & \mu\end{pmatrix}\times\mathrm{Im}\,Q_\lambda(1234) \tag{9}$$

$$Q_\lambda = Q^{\mathrm{Qul}}_\lambda + Q^{\mathrm{Br}}_\lambda. \tag{10}$$

where j_i are the entire single electron momentums, m_i – their projections; Q^{Cul}_λ and Q^{Br}_λ are connected with the Coulomb and Breit magnetic parts of the operator (1b). The total radiation width of the one-quasiparticle state is presented in the form:

$$\Gamma(\gamma) = -2\,\mathrm{Im}\,M^1(\gamma) = -2\sum_{\lambda nlj}(2j+1)\,\mathrm{Im}\,Q_\lambda\left(n_\gamma l_\gamma j_\gamma nlj\right)$$
$$Q_\lambda = Q^{Cul}_\lambda + Q^{Br}_\lambda. \tag{11}$$

The individual terms of the $\sum_{\eta lj}$ sum correspond to the partial contribution of the $n_\lambda l_\lambda j_\lambda \to nlj$ transitions; $\sum_\lambda$ is a sum of the contributions of the different multiplicity transitions. The detailed expressions for the Coulomb and Breit parts can be found in Refs. [23,35]. The imaginary part Q^{Cul}_λ contains the radial R_l and angular S_l integrals as follows (in the Coulomb units):

$$\begin{aligned}\mathrm{Im}\,Q^{\mathrm{Qul}}_\lambda(12;43) = Z^{-1}\,\mathrm{Im}\{&R_l(12;43)S_\lambda(12;43)+\\ &+R_\lambda(\tilde1 2;4\tilde3)S_\lambda(\tilde1 2;4\tilde3)+\\ &+R_\lambda(1\tilde2;\tilde43)S_\lambda(1\tilde2;\tilde43)+\\ &+R_\lambda(\tilde1\tilde2;\tilde4\tilde3)S_\lambda(\tilde1\tilde2;\tilde4\tilde3)\}\end{aligned} \tag{12}$$

In the non-relativistic limit there remains only the first term in (14) depending only on the large component $f(r)$ of the one-electron Dirac functions:

$$\begin{aligned}&\mathrm{Im}\,R_\lambda(12;43) = \frac{1}{2}(2\lambda+1)\pi X_\lambda(13)X_\lambda(24)\\ &X_\lambda(12) = \int dr\, r^{3/2} f_1(r) J^{(1)}_{\lambda+1/2}\left(r\alpha Z|\omega| f_2(r)\right)\end{aligned} \tag{13}$$

The angular coefficient has only a real part:

$$S_\lambda(1243) = \{\lambda l_1 l_3\}\{\lambda l_2 l_4\}\begin{pmatrix} j_1 & j_3 & \lambda\\ 1/2 & -1/2 & 0\end{pmatrix}\begin{pmatrix} j_2 & j_4 & \lambda\\ 1/2 & -1/2 & 0\end{pmatrix} \tag{14}$$

$\{\lambda l_1 l_3\}$ means that λ, l_1 and l_3 must satisfy the triangle rule and the sum $\lambda + l_1 + l_3$ must be an even number. The rest terms in (12) include the small components of the Dirac functions. The tilde designates that the large radial component f must be replaced by the small one g, and instead of $l_i, \tilde l_i = l_i - 1$ should be taken for $j_i < l_i$ and $\tilde l_i = l_i + 1$ for $j_i > l_i$. The Breit (magnetic) part can be expressed as follows:

$$Q^{Br}_\lambda = Q^{Br}_{\lambda,\lambda-1} + Q^{Br}_{\lambda,\lambda} + Q^{Br}_{\lambda,\lambda+1} \tag{15}$$

The corresponding imaginary part (15) is as follows:

$$\begin{aligned}\mathrm{Im}\,Q_\lambda^{\mathrm{Br}}(12;43) = Z^{-1}\,\mathrm{Im}\{&R_l\left(12;\widetilde{4}\widetilde{3}\right)S_\lambda\left(12;\widetilde{4}\widetilde{3}\right)+\\ &+R_\lambda\left(\widetilde{1}\widetilde{2};43\right)S_\lambda\left(\widetilde{1}\widetilde{2};43\right)+\\ &+R_\lambda\left(\widetilde{1}2;\widetilde{4}3\right)S_\lambda\left(\widetilde{1}2;\widetilde{4}3\right)+\\ &+R_\lambda\left(1\widetilde{2};4\widetilde{3}\right)S_\lambda\left(1\widetilde{2};4\widetilde{3}\right)\}\end{aligned} \tag{16}$$

The angular part S_λ^l has the form

$$S_\lambda^l\left(12;43\right)=\left(2\lambda+1\right)S_\lambda^l\left(13\right)S_\lambda^l\left(24\right)\left(-1\right)^{\lambda+l+1} \tag{17}$$

The total probability of a λ - pole transition is usually represented as a sum of the electric P_λ^E and magnetic P_λ^M parts. The electric (or magnetic) λ - pole transition $\gamma \to \delta$ connects two states with parities which by λ (or λ +1) units. In our designations:

$$P_\lambda^E(\gamma \to \delta) = 2(2j+1)Q_\lambda^E(\gamma\delta;\gamma\delta) \tag{18}$$

$$Q_\lambda^E = Q_\lambda^{Qul} + Q_{\lambda,\lambda-1}^{Br} + Q_{\lambda,\lambda+1}^{Br} \tag{19}$$

$$P_\lambda^M(\gamma \to \delta) = 2(2j+1)Q_\lambda^M(\gamma\delta;\gamma\delta) \tag{20}$$

$$Q_\lambda^M = Q_{\lambda,\lambda}^{Br} \tag{21}$$

In the numerical calculations the transition probability, as usually, is expanded to the series on the known parameter *aw* as follows:

$$\begin{aligned}&Q_\lambda^{Qul} \approx (\alpha\omega)^{(\lambda)},\ Q_{\lambda,\lambda-1}^{Br} \approx (\alpha\omega)^{\lambda},\\ &Q_{\lambda\lambda}^{Br} \approx (\alpha\omega)^{\lambda+3},\ Q_{\lambda,\lambda+1} \approx (\alpha\omega)^{\lambda+5}.\end{aligned} \tag{22}$$

In a case of the two-quasi-particle states (for example, this is a case of the Ne-like ions, where the excited state can be represented as stale with the two quasiparticles – electron and vacancy above the closed shells core $1s^22s^22p^6$) the corresponding probability has the following form (say, transition: $j_1 j_2[J] \to \bar{j}_1 j_2[\bar{J}]$):

$$P(\lambda \mid j_1 j_2[J], \bar{j}_1 j_2[\bar{J}]) = (\bar{J})\begin{Bmatrix}\lambda \ldots J \ldots \bar{J}\\ j_2 \ldots \bar{j}_1 \ldots j_1\end{Bmatrix} P(\lambda \mid 1\,\bar{1})(\bar{j}_1) \tag{23}$$

It should be noted that that all calculation is usually carried out in the *jj*-coupling scheme representation. The transition to the intermediate coupling scheme has been realized by diagonalization of the secular matrix. Indeed, only $\mathrm{Re}\,M$ should be diagonalized. The imaginary part is converted by means of the matrix of eigenvectors $\{C_{mk}\}$, obtained by diagonalization of $\mathrm{Re}\,M$:

$$\mathrm{Im}\,M_{mk} = \sum_{ij} C_{mi}^*\, M_{ij}\, C_{jk} \tag{24}$$

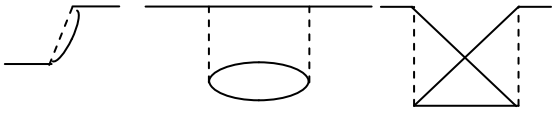
M_{ij} are the matrix elements in the *jj*-coupling scheme, and M_{mk} in the intermediate coupling scheme representation. This procedure is correct to terms of the order of $\mathrm{Im}\,M/\mathrm{Re}\,M$. Further let us also underline that the tedious procedure of phase convention in calculating the matrix elements of different operators is avoided in the energy approach, although the final formulae, of course, must coincide with the formulae obtained using the traditional amplitude method operating with the amplitudes of the processes. Therefore, the energy approach simplifies the analysis of complex atomic processes including processes with the interference of different kinds of channels (i.e. radiation and autoionization ones).

4. The one-quasiparticle optimized representation

The problem of the searching for the optimal one-electron representation is one of the oldest in the theory of multielectron atoms. Two decades ago Davidson had pointed the principal disadvantages of the traditional representation based on the self-consistent field approach and suggested the optimal "natural orbitals" representation. Nevertheless , there remain insurmountable calculational difficulties in the realization of the Davidson program (look, for example, Ref.[12]). One of the simplified recipes represents, for example, the DFT method [18,19].

Unfortunately, this method doesn't provide a regular refinement procedure in the case of the complicated atom with few quasiparticles (electrons or vacancies above a core of the closed electronic shells). For simplicity, let us consider now the one-quasiparticle atomic system (i.e. atomic system with one electron or vacancy above a core of the closed electronic shells). The multi-quasiparticle case doesn't contain principally new moments. In the lowest, second order, of the QED PT for the D*E* there is the only one-

quasiparticle Feynman diagram a (fig.1), contributing the ImDE (the radiation decay width).



(a) (b) (c)

Figure 1. a: second other PT diagram contributing the imaginary energy part related to the radiation transitions; b and c: fourth order polarization diagrams.

In the next, the fourth order there appear diagrams, whose contribution into the ImDE account for the core polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). Let us examine the multielectron atom with one quasiparticle in the first excited state, connected with the ground state by the radiation transition. In the PT zeroth approximation one can use the one-electron bare potential:

$$V_N(r)+V_C(r), \qquad (25)$$

with $V_N(r)$ describing the electric potential of the nucleus, $V_C(r)$, imitating the interaction of the quasiparticle (initial or any other appearing in the real and virtual processes) with the core of closed shells.

The perturbation in terms of the second quantization representation reads as follows:

$$-V_C(r)\, y^+(r)\, y(r) \; - \; j_m(x)\, A^m(x). \qquad (26)$$

The core potential $V_C(r)$ is related to the core electron density $r_C(r)$ in a standard way. The latter fully defines the one electron representation. Moreover, all the results of the approximate calculations are the functionals of the density $r_C(r)$. Here, the lowest order multielectron effects, in particular, the gauge dependent radiative contribution for the certain class of the photon propagator gauge is treating. This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criteria in the searching for the optimal one-electron basis of the PT. Besides, this procedure derives an undoubted profit in the routine spectroscopic calculations as it provides the way of the refinement of the atomic characteristics calculations, based on the "first principles" . Remember that the closeness of the radiation probabilities calculated with the alternative forms of the transition operator is commonly used as a criterion of the multielectron calculations quality. It is of special interest to verify the compatibility of the new optimization principle with the other requirements conditioning a "good" one-electron representation.

The imaginary part of the diagram a (fig.1) contribution has been presented previously as a sum of the partial contributions of *a-s* transitions from the initial state *a* to the final state *s* [26]:

$$\mathrm{Im}DE_a\,(\mathrm{a}) = \sum_S \; \mathrm{Im}\; DE\ (a\text{-}s;\ \mathrm{a}). \qquad (27)$$

Two fourth order polarization diagrams b,c (fig.1) should be considered further. The contributions being under consideration, are gauge-dependent, though the results of the exact calculation of any physical quantity must be gauge independent . All the non-invariant terms are multielectron by their nature.

Let us take the photon propagator calibration as follows:

$$D = D_T + CD_L,$$

$$D_T = d_{mn} / (k - k^2),$$
$$D_L = - k_m k_n / (k - k^2). \qquad (28)$$

Here C is the gauge constant; D_T represents the exchange of electrons by transverse photons, D_L that by longitudinal ones. One could calculate the contribution of the a,b,c diagrams (fig.1) into the Im DE taking into account both the D_T and D_L parts. The a diagram (fig.1) contribution into the Im DE related to the *a -s* transition reads as

$$-\frac{e^2}{8\pi}\iint \mathrm{d}r_1\mathrm{d}r_2 y_a^+(r_1)\, y_s^+(r_2)\mathrm{x}$$
$$\mathrm{x}\ \frac{1-\alpha_1\alpha_2}{} \sin(w_{as} r_{12}) y_a(r_2) y_s(r_1), \qquad (29)$$

for $D = D_T$ and

$$- \frac{e^2}{8\pi}\int\int \mathrm{d}r_1\,\mathrm{d}r_2\, y_a^+(r_1)\, y_s^+(r_2)\ \{[(1- a_1 n_{12} a_2 n_{12})/ r_{12}]\sin(w_{as} r_{12}) + w_{as}\,(1+ a_1 n_{12} a_2 n_{12})' \cos(w_{as} r_{12})\}\, y_a(r_2) y_s(r_1), \qquad (30)$$

for $D=D_{\mathrm{L}}$, where w_{as} is the a -s transition energy. According to the Grant theorem [1], the $D_{mn,\mathrm{L}}$ contribution vanishes, if the one-quasiparticle functions y_a , y_s satisfy the same Dirac equation. Nevertheless this term is to be retained when using the distorted waves approximation, for example. Another very important example represents the formally exact approach based on the bare Hamiltonian defined by its spectrum without specifying its analytic form [26,34]. Here the non-invariant contribution appears already in the lowest order. When calculating the forth order contributions some approximations are inevitable.

These approximations have been formulated in Refs.[26], where the polarization corrections to the state energies have been considered.

Let us consider the direct polarization diagram b (fig.1) as an example. After the some transformations the formal expression for the sought for value looks as

$$\mathrm{Im}\, E_{ninv}(\alpha - s \mid A_d) = -C\frac{e^2}{4\pi}\iiint\int dr_1 dr_2 dr_3 dr_4 \sum \Big(\frac{1}{\omega_{mn}+\omega_{\alpha_s}} + \frac{1}{\omega_{mn}-\omega_{\alpha_s}}\Big)\Psi_\alpha^+(r_1)\Psi_m^+(r_2)\Psi_s^+(r_3)\Psi_n^+(r_4)(1-\alpha_1\alpha_2)/r_{12}\cdot \{[(\alpha_3\alpha_4 - (\alpha_3 n_{34})(\alpha_4 n_{34}))/r_{34}\cdot \sin[\omega_{\alpha_n}(r_{12}+r_{34}) + \omega_{\alpha_n}\cdot \cos[\omega_{\alpha_n}(r_{12}+r_{34})](1+(\alpha_3 n_{34})(\alpha_4 n_{34}))]\}\Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1), \qquad (31)$$

and the upper continuum electron states; $m \pounds f$ indicates the finite number of states in the core and the states of the negative continuum (accounting for the electron vacuum polarization).

All the vacuum polarization and the self-energy corrections to the sought for values are omitted. Their numerical smallness compared with the other relativistic corrections to the different atomic characteristics had been verified by the numerous calculations. The renormalization procedure is not needed here. Nevertheless the second-order vacuum polarization and self-energy corrections can be additively added to the complex state energy. The remaining expression includes summation over the bound and upper continuum atomic states. To evaluate this sum, we use the analytic relation between the atomic electron Fermi level and the core electron density $r_{\mathrm{c}}(r)$, appropriate to the homogeneous nonrelativistic electron gas (the Tomas- Fermi approximation). Now the sum $\sum_{n>f,\ m<f}$ can be calculated analytically, its value becomes a functional of the core electron density. The resulting expression looks as the correction due to the additional nonlocal interaction of the active quasiparticle with the closed shells. Nevertheless, its calculation is reducible to the solving of the system of the ordinary differential equations (1-D procedure) [26]. The most important refinements can be introduced by accounting for the relativistic and the density gradient corrections to the Tomas- Fermi formula (see Refs. [23,26]). The same program is realized for other polarization diagrams. The minimization of the functional Im dE_{ninv} (b+c) leads to the integro-differential equation for the r_{c} (the DF or Dirac-Kohn-Sham-like equations for the electron density) that are numerically solved. In result we obtain the optimal one-quasiparticle representation, which is further used in calculation of the radiative (autoionization) transition characteristics (7)-(10).

5. Conclusion

We have considered the fundamental blocks of the generalized energy approach to relativistic calculation of the radiative decay (transitions) probabilities in heavy neutral atomic systems and multicharged ions. The approach is based on the Gell-Mann and Low S-matrix formalism and the gauge-invariant relativistic many-body perturbation theory (PT) with using the optimized one-quasiparticle representation and an accurate account of the relativistic and exchange-correlation effects. In relativistic case the Gell-Mann and Low formula expresses an energy shift ΔE through the electrodynamical scattering matrix including the interaction with the photon vacuum field. This case is corresponding to definition of the traditional radiative transitions probabilities for atoms and ions. Obviously, the same program can be realized in order to give adequate quantitative description of interaction of atomic systems

with a laser field and further computing the radiation emission and absorption lines parameters, the corresponding lines moments etc. [28,29].

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ADVANCED RELATIVISTIC ENERGY APPROACH TO RADIATION DECAY PROCESSES IN ATOMIC SYSTEMS

Abstract.

We consider the fundamental aspects of the generalized energy approach to relativistic calculation of the radiative decay (transitions) probabilities in heavy neutral atomic systems and multicharged ions. The approach is based on the Gell-Mann and Low S-matrix formalism and the relativistic many-body perturbation theory (PT) with using the optimized one-quasiparticle representation and an accurate account of the relativistic and correlation. In relativistic case the Gell-Mann and Low formula expresses an energy shift ΔE through the electrodynamical scattering matrix including the interaction with as the laser field as the photon vacuum field. The last case is corresponding to definition of the traditional radiative transitions probabilities for atoms and ions.

Key words: energy approach, atomic systems and multicharged ions, radiative transitions, Gell-Mann and Low S-matrix formalism

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РЕЛЯТИВИСТСКИЙ ЭНЕРГЕТИЧЕСКИЙ ПОДХОД К ОПИСАНИЮ ПРОЦЕССОВ РАДИАЦИОННОГО РАСПАДА В АТОМНЫХ СИСТЕМАХ

Резюме.

В работе рассмотрены фундаментальные аспекты обобщенного релятивистского энергетического подхода в релятивистской теории радиационных распадов (переходов) вероятностей в тяжелых нейтральных атомных системах и многозарядных ионов. Подход базируется на S-матричном формализма Гелл-Манна и Лоу и релятивистской многочастичных теории возмущений с выполнением оптимизированного одинквазичастинквого представления и аккуратным учетом релятивистских и корреляционных поправок. В релятивистском случае формула Гелл-Манна и Лоу выражает энергетический сдвиг через электродинамическую матрицу рассеяния, в том числе, с учетом взаимодействия как с полем лазерного излучения, так и полем фотонного вакуума. Последний случай соответствует определению традиционных вероятностей радиационных переходов для атомов и ионов

Ключевые слова: энергетический подход, атомные системы и многозарядные ионы, радиационные переходы, S-матричный формализм Гелл-Манна и Лоу

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РЕЛЯТИВІСТСЬКИЙ ЕНЕРГЕТИЧНИЙ ПІДХІД ДО ОПИСУ ПРОЦЕСІВ РАДІАЦІЙНОГО РОЗПАДУ В АТОМНИХ СИСТЕМАХ

Резюме.

У роботі розглянуті фундаментальні аспекти удосконаленого релятивістського енергетичного підходу в релятивістській теорії радіаційних розпадів (переходів) ймовірностей у важких нейтральних атомних системах і багатозарядних іонів. Підхід базується на S-матричному формалізму Гелл-Манна та Лоу і релятивістської багаточастинковій теорії збурень з імплементацією оптимізованого одинквазічастинквого представлення і акуратним урахуванням релятивістських і кореляційних поправок. У релятивістському випадку формула Гелл-Манна і Лоу виражає енергетичний зсув через електродинамічну матрицю розсіювання, в тому числі, з урахуванням взаємодії як з полем лазерного випромінювання, так й полем фотонного вакууму. Останній випадок відповідає визначенню традиційних ймовірностей радіаційних переходів для атомів та іонів

Ключові слова: енергетичний підхід, атомні системи і багатозарядні іони, радіаційні переходи, S-матричний формалізм Гелл-Манна та Лоу