Chapter 5

Relativistic Perturbation Theory Formalism to Computing Spectra and Radiation Characteristics: Application to Heavy Elements

Alexander V. Glushkov, Olga Yu. Khetselius,
Andrey A. Svinarenko, Vasily V. Buyadzhi,
Valentin B. Ternovsky, Anna A. Kuznetsova and
Petr G. Bashkarev

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Abstract

Fundamentals of gauge-invariant relativistic many-body perturbation theory (PT) with optimized ab initio zeroth approximation in theory of relativistic multi-electron systems are presented. The problem of construction of optimal one-electron representation is directly linked with a problem of the correct accounting for multielectron exchange-correlation effects and gauge-invariance principle fulfilling in atomic calculations. New approach to construction of optimal PT zeroth approximation is based on accurate treating the lowest order multielectron effects, in particular, the gauge-dependent radiative contribution for the certain class of photon propagator (for instance, the Coulomb, Feynman, Babushkin ones) gauge. This value is considered to be a typical representative of important multielectron exchange-correlation effects, whose minimization is a reasonable criteria in the searching for optimal PT one-electron orbital basis. This procedure derives an undoubted profit in the routine many-body calculations as it provides the way of refinement of the atomic characteristics calculations, based on the "first principles". The relativistic density-functional approximation is taken as the zeroth one. There have taken into account all exchange-correlation corrections of the second order and dominated classes of the higher orders diagrams (polarization interaction, quasiparticles screening, etc.). New form of multi-electron polarization functional is used. As illustration, the results of computing energies, transition probabilities for some heavy ions are presented.

Keywords: relativistic many-body perturbation theory, density-functional approximation, exchange-correlation effects, radiative transitions, oscillator strengths, heavy atoms

1. Introduction

Perturbation theory (PT) formalism has a long history in studying different multielectron (more generally, multifermion) systems, including different atomic, molecular, and nuclear properties. Really, one should say about formalism of the many-body PT as, a rule, usually it applies to studying different properties of the multiparticle systems, for instance, ionization and excitation energies, spectra, electron exchange-correlation energies, hyperfine structure, radiative and autoionization decay rates (transition probabilities, oscillator, and lines strengths), as well as the influence of an external electromagnetic fields. In the last few decades, the PT methods have been refined with a sophisticated and comprehensive approach of more correct treatment of the exchange-correlation effects, electron-nuclear dynamics, and so on [1–44]. Rephrasing the known interesting quote by Bartlett and Musiał [3, 4] and earlier by Wilson, one could say that *the PT methods are an emerging computational area that is sixty years ahead of lattice gauge theory… and a rich source of new ideas and new approaches to the computation of many fermion systems*. The old multibody quantum theoretical approaches often take place, which have been primarily developed in a theory of a superfluity and/or a superconductivity, and generally speaking in a theory of solids, became the powerful tools for developing new conceptions in many-body (multielectron) atomic, nuclear, and molecular calculations [1–7].

A number of the PT versions include a synthesis of cluster expansions, Brueckner's summation of ladder diagrams, the summation of ring diagrams Gell-Mann, and an infinite-order generalization of manybody PT (Kelly, 1969; Ivanov-Tolmachev, 1969–1974, Bartlett and Silver, 1974–1976, etc.; see review in Ref. [7]). Using quantum-field methods in atomic and molecular theory allowed obtaining a very powerful approach for the correct treatment of the exchange-correlation effects in many-electron systems. In this context, it is useful to remind about such sophisticated methods as a coupled-cluster theory, the Green-functions method, configuration interaction methods, and so on. Only with this property are applications to solids or the electron gas possible, and, even for small atoms and molecules, its effects are numerically quite essential. When relativistic effects became essential in the studied multielectron (fermion) system, naturally it is necessary to formulate a formalism of the relativistic many-body PT. In the first attempts, an account for the relativistic effects had been reduced to treating the Darwin, mass-velocity, and spin-orbit effects, which have to be added to the nonrelativistic solution and provide different approximations lying between the Schrödinger equation and the four-component Dirac equation [2, 6, 7]. Among recent developments in this field, special attention should be given to two very general and important computer systems for relativistic and QED calculations of atomic and molecular properties developed in the Oxford, Troitsk, and other groups (known as "GRASP," "Dirac," "BERTHA," "QED," "Superatom," etc.; Ref. [1–13] and references therein). For example, a new relativistic molecular structure theory within the QED framework with accounting of the electron correlation and higher-order QED effects has been formulated and further realized as the BERTHA program. The master system of equations includes the so-called Dirac-Hartree-Fock-Breit self-consistent field equations. The useful overview of the relativistic electronic structure theory is presented in Refs. [2, 7] from the QED point of view. The next important step is an adequate taking into account the QED corrections. This topic has been a subject of intensive theoretical and experimental interest.

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Hitherto, most many-body PT studies concerned atoms with a simple electron-shell structure, namely atoms of the inert gases and atoms and ions with a single electron (or hole) above (or inside) the closed shells core. The fundamental limitation to extend the many-body procedure beyond such simple atomic systems arises from the complexity of any perturbation expansion if more than just one or two *effective* particles appear in the derivation (see detailed analysis in Ref. [5]). In order to overcome this difficulty, a number of different efficient techniques of complex expansions were developed. As a rule, the atomic PT expansions are expressed in terms of the Feynman-Goldstone diagrams in Rayleigh-Schrödinger PT formulation. Above the most popular and known versions of the PT formalism, one should mention formally exact relativistic many-body PT with the model zeroth approximation by Ivanova-Ivanov et al., relativistic PT with the Hartree-Fock (HF) or Dirac-Fock (DF) zeroth approximations by Johnson et al., Flambaum-Dzuba et al., Safronova and Safronova et al., Khetselius et al., and so on [9–38]).

The searching for the optimal one-electron zeroth representation is one of the oldest in the theory of multielectron atoms and, respectively, in the formulation of the effective PT formalism. 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 [11]. Nevertheless, there remain insurmountable computational difficulties in the realization of the Davidson program (see, e.g., Refs. [11, 12]). One of the simplified recipes represents, for example, a density functional theory (DFT) formalism [8]. Unfortunately, this approach does not provide a regular refinement procedure in the case of the complicated atom with few quasiparticles (QPs) (electrons or vacancies above a core of the closed electronic shells). The problem of construction of the optimal one-electron representation is tightly linked with the problem of the correct accounting for the multielectron exchange-correlation effects. In Refs. [47, 48], the PT lowest-order multielectron effects, in particular, the gauge-dependent radiative contribution (gauge-noninvariant) for the certain class of the photon propagator gauge is treated. This value is considered to be the typical representative of the multielectron exchange-correlation effects contribution. New fundamental idea has been proposed in Refs. [47, 48] in order to construct the optimal PT one-electron basis and is in minimization of the gauge-noninvariant contribution into a radiation width of atomic level. Such an approach allows to determine an effectiveness of accounting of the multielectron exchange-correlation effects and provides the practical way of the refinement of the atomic characteristics calculations, based on the "first principles." Really, the known standard criterion of the multielectron computing quality in atomic spectroscopy is linked with a closeness of the atomic level radiation width values, calculated using two alternative forms of the transition operator (the "length" and the "velocity" forms). It is of special interest to verify the compatibility of the new optimization principle with the other requirements conditioning a "good" one-electron representation. We suppose that this point should be obligatory in formulation of the effective, optimal PT formalism.

In this chapter, we present the theoretical fundamentals of the gauge-invariant relativistic many-body PT with using the optimized one-QP representation in the theory of relativistic multielectron systems [21–23, 47, 48]. All exchange-correlation corrections of the second-order and dominated classes of the higher-orders diagrams (polarization interaction, QPs screening, etc.) [47–67] have

been taken into account. As illustration of application of the presented PT formalism, we list the results of computing energies, transition probabilities (oscillator strengths) in some heavy atoms (ion of Hg+).

2. Relativistic many-body perturbation theory with optimized one-quasiparticle zeroth representation

2.1. General remarks

Our relativistic PT version is constructed on the same principles as the known formally exact PT with model zeroth approximation by Ivanova-Ivanov et al. [33–47]; however, there a few principal points, where our formalism differs from this known theory. At first, this is another definition of the zeroth approximation, namely within the relativistic DFT one [14–17, 19–22]. Second, this is an implementation of the principally new approach to construction of the optimized one-QP representation, which allows correctly to take into account a gauge invariance principle fulfilling.

In nonrelativistic theory of multielectron atoms, a powerful field approach for computing the electron energy shift ΔE of the degenerate states is known, which are usually present in the dense spectra of the complex relativistic atomic multielectron systems **(Tolmachev-Ivanov-Ivanova, 1969–1974)**. The key algorithm of this approach includes construction of the secular matrix M using the known Gell-Mann and Low adiabatic formula and its further diagonalization. The analogous approach using the Gell-Mann and Low formula with an electrodynamic scattering matrix has been developed in a theory of the relativistic atom [33–36]; however, the M matrix elements in the relativistic representation are complex; the corresponding imaginary parts determine the values of radiation widths. According to Ref. [34], the total electron energy shift can be defined as follows:

$$\Delta E \; = \; \mathrm{Re}\,\Delta E + i\,\mathrm{Im}\Delta E \quad \mathrm{Im}\Delta E = \; - \; \Gamma/2. \tag{1}$$

Here, Γ is a radiation width of the atomic level (or a possibility **P** of the radiation decay or transition: P = Γ. Within the general framework, the corresponding energies of a nondegenerated excited states and their radiation decay amplitudes can be determined by means of the computing and further diagonalization of the matrix M. In Refs. [33–37], the ReΔE calculation procedure has been generalized for the case of nearly degenerate states, whose levels form a more or less compact group. Naturally, the matrix M reduces to one term (ΔE) in the case of well-identified and separated energy spectrum. The Gell-Mann and Low formula allow further to obtain the expansion of the M elements into PT series on interelectron interaction and apply the standard Feynman diagrammatic technique. The corresponding PT series is as follows:

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

Here, $M^{(0)}$ is the contribution of the PT all-orders vacuum diagrams (in fact, this is a real matrix, which determines only the general atomic levels shift); $M^{(1)}$, $M^{(2)}$,and $M^{(3)}$ are the

contributions, which correspond to the one-, two- and three-QP PT diagrams, respectively. The diagonal matrix $M^{(1)}$ can be easily calculated as it represents a sum of the one-QP contributions. Generally speaking, computing all the one-QP diagrams contributions within the PT formalism is the most simple procedure. The more complicated problem is computing the $M^{(2)}$ and $M^{(3)}$contributions. Using the Feynman diagrams technique, the authors [33–38] have in detail analyzed the $M^{(2)}$ contributions. Naturally, the fundamental point of the whole consideration is the definition of the PT zeroth approximation.

2.2. The perturbation theory zeroth approximation

We will describe an atomic multielectron system by the relativistic Dirac Hamiltonian (the atomic units are used) as follows [14, 15]:

$$H = \sum_i \{\alpha c p_i - \beta c^2 - Z/r_i\} + \sum_{i>j} \exp(i|\omega|r_{ij})(1 - \alpha_i \alpha_j)/r_{ij}, \tag{3}$$

where Z is a charge of nucleus, α_i, α_j are the Dirac matrices, ω_{ij} is the transition frequency, and c, a light velocity. The interelectron interaction potential (second term in Eq. (3)) takes into account the retarding effect and magnetic interaction in the lowest order on parameter α^2 (α is the fine structure constant). Let us note that in order to account for the nuclear finite size effect (in the zeroth approximation), one could describe a charge distribution in the atomic nucleus $\rho(r)$ by the Gaussian or Fermi (another variant is relativistic mean-field theory of a nucleus) functions and write the Coulomb potential for the spherically symmetric nuclear density $\rho(r|R)$ as [14]

$$V_{nucl}(r|R) = -\Big((1/r)\int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R). \tag{4}$$

Here, R is a nuclear radius. According to the known Ivanova-Ivanov et al. method of differential equations [33–36], computing the potential (20) can be reduced to solving the system of the differential equations. By the way, this method is used by us in further under computing the PT first- and second-order corrections. The zeroth-order Hamiltonian H_0 and perturbation operator can be presented in the standard form as follows [7, 14, 15]:

$$\begin{aligned} H_0 &= \sum_i a_i^+ a_i E_i \\ H_{\text{int}} &= \sum_{ij} a_i^+ a_j V_{ij} + \frac{1}{2}\sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_k a_l \\ V_{ij} &= \int d\vec{r} \cdot \varphi_i(\vec{r})[-V_{MF}(r)] \cdot \varphi(\vec{r}) \\ V_{ijkl} &= \iint d\vec{r}_1 d\vec{r}_2 \, \varphi(\vec{r}_1)\, \varphi(\vec{r}_2)\, V(r_1 r_2)\, \varphi_k(\vec{r}_2)\, \varphi_l(\vec{r}_1), \end{aligned} \tag{5}$$

where $\varphi(\vec{r})$ are one-electron functions (Dirac bispinors), E_i , one-electron energies, and V_{MF} is the central field self-consistent potential of the Coulomb type. The latter can be taken in the

form of the usual Dirac-Fock potential or even any appropriate model potential, which imitates an effect of the electron subsystem. Let us remind that in the relativistic PT by Ivanova-Ivanov et al., the consistent model (as a rule, empirical) potential was taken as $V_{\mathrm{MF.}}$ In our PT version, we use the potential

$$V_{MF} = V^{DKS}(r) = [V^{D}_{Coul}(r) + V_X(r) + V_C(r|a)] \tag{6}$$

Further as $V_X(r)$ we use the standard Kohn-Sham (KS) exchange potential as follows [8]:

$$V^{KS}_X(r) = -(1/\pi)[3\pi^2\rho(r)]^{1/3}. \tag{7}$$

The standard definition of the exchange potential in the density-functional theory is as follows:

$$V_X[\rho(r), r] = \frac{\delta E_X[\rho(r)]}{\delta\rho(r)}, \tag{8}$$

In the relativistic multielectron theory with a Hamiltonian having a transverse vector potential (for describing the photons), one could determine the homogeneous density $\rho(r)$, construct the corresponding exchange energy $E_X[\rho(r)]$, and introduce the following exchange potential [16]:

$$V_X[\rho(r), r] = V^{KS}_X(r) \cdot \left\{\frac{3}{2}\ln\frac{[\beta + (\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\right\}, \tag{9}$$

where $\beta = [3\pi^2\rho(r)]^{1/3}/c$. The corresponding correlation functional is as follows [16, 17]:

$$V_C[\rho(r), r] = -0.0333 \cdot b \cdot \ln[1 + 18.3768 \cdot \rho(r)^{1/3}], \tag{10}$$

where b is the optimization parameter (for details, see below and Refs. [16–19, 47–49] too). Naturally, potential (6) is subtracted from the interelectron potential in Eq. (3) in the perturbation operator. The Dirac equations for F and G components can be written as [14] follows:

$$\begin{aligned} f' &= -(\chi + |\chi|)f/r - \alpha ZVg - (\alpha ZE_{n\chi} + 2/\alpha Z)g, \\ g' &= (\chi - |\chi|)g/r - \alpha ZVf + \alpha ZE_{n\chi}f. \end{aligned} \tag{11}$$

Here, $E_{n\chi}$ is one-electron energy without the rest energy. The boundary values are defined by the first terms of the Taylor expansion:

$$g = \left(V(0) - E_{n\chi}\right)r\alpha Z/(2\chi + 1); \quad f = 1 \; at \; \chi < 0, \tag{12a}$$

$$f = \left(V(0) - E_{n\chi} - 2/\alpha^2 Z^2\right)\alpha Z; \quad g = 1 \; at \; \chi > 0. \tag{12b}$$

The condition $f, g \to 0$ at $r \to \infty$ determines the quantified energies of the state $E_{n\chi}$. The system of Eq. (11) is numerically solved by the Runge-Kutta method ('Superatom" package is used [7, 13–23, 34, 36, 47–67]).

2.3. The perturbation theory first- and second-orders corrections: correlation effects

In the PT first order, one should determine the matrix elements of the PT operator with the relativistic Coulomb-Breit potential, which are the contributions of the following type [36]:

$$\begin{aligned} M_1^{(2)} &= \langle\, n_1 l_1 j_1 \quad n_2 l_2 j_2[J]\,|V_{\text{int}}|\, n_4 l_4 j_4 \quad n_3 l_3 j_3[J]\,\rangle \\ &= P_1 P_2 (-1)^{1+j_2+j_4+J}[(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)]^{1/2} \\ &\times \sum_{i,\,k}\sum_{a} \begin{Bmatrix} j_i j_k J \\ j_2 j_1 a \end{Bmatrix} \left(\delta_{i,3}\delta_{k,4} + (-1)^J \delta_{i,4}\delta_{k,3}\right) \cdot Q_\lambda, \end{aligned} \tag{13}$$

where

$$P_1 = \begin{cases} 1 & \text{if} \quad n_1 l_1 j_1 \neq n_2 l_2 j_2 \\ 1/2 & \text{if} \quad n_1 l_1 j_1 = n_2 l_2 j_2 \end{cases},\ P_2 = \begin{cases} 1 & \text{if} \quad n_3 l_3 j_3 \neq n_4 l_4 j_4 \\ 1/2 & \text{if} \quad n_3 l_3 j_3 = n_4 l_4 j_4 \end{cases}. \tag{14}$$

The value of the Q_λ can be expressed through the radial Slater-like integrals and presented as a sum of the Coulomb and Breit parts: $Q_\lambda = Q_\lambda^{Qul} + Q_\lambda^{Br}$, which corresponds to a partition of the interelectron potential into the Coulomb and Breit ones in the second term of Eq. (1). Let us remind that, for instance, the Coulomb part in Eq. (13) is expressed through the radial integrals and angle coefficients as follows:

$$\begin{aligned} Q_\lambda^{Qul} = \frac{1}{Z}\Big\{ & R_l(1243) S_\lambda(1243) + R_l(\tilde{1}24\tilde{3}) S_\lambda(\tilde{1}24\tilde{3}) + \\ & + R_l(1\tilde{2}4\tilde{3}) S_\lambda(1\tilde{2}4\tilde{3}) + R_l(\tilde{1}\tilde{2}4\tilde{3}) S_\lambda(\tilde{1}\tilde{2}4\tilde{3}) \Big\}. \end{aligned} \tag{15}$$

In the nonrelativistic limit, there remains only the first term in Eq. (15) depending only on the large component *f*(*r*) of the one-electron Dirac functions. For example, its imaginary part is as follows [36]:

$$\begin{aligned} \text{Im}\, R_\lambda(12;43) &= \frac{1}{2}(2\lambda+1)\pi X_\lambda(13) X_\lambda(24) \\ X_\lambda(12) &= \int dr\, r^{3/2} f_1(r) J^{(1)}_{\lambda+1/2}\left(r\alpha Z|\omega| f_2(r)\right) \end{aligned} \tag{16}$$

The angular coefficient has only a real part:

$$S_\lambda(12;43) = S_\lambda(13) S_\lambda(24) \qquad S_\lambda(13) = \{\lambda l_1 l_3\} \begin{pmatrix} j_1 & j_3 & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \tag{17}$$

Here, $\{\lambda l_1 l_3\}$ 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 Eq. (16) include the small components of the Dirac functions. The tilde in Eq. (13) 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 by the similar way (see details in Refs. [13–16]).

Then, exchange-correlation effects can be treated within the PT formalism as effects of the second and higher PT orders. In the second order, one should especially note the polarization and ladder diagrams. In **Figures 1** and **2**, we list some important diagrams of the second order describing the effects of the polarization interaction of quasiparticles and screening of the external quasiparticles (or antiscreening in the case, say, of an electron and a vacancy).

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 approach to accounting the polarization contributions is in adding the effective two-QP polarizable operator into the first-order matrix elements. The corresponding polarization operator can be taken in the following form [50]:

$$V^d_{\mathrm{pol}}(r_1 r_2) = X \left\{ \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3} \theta(r')}{|r_1 - r'| \cdot |r' - r_2|} - \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3} \theta(r')}{|r_1 - r'|} \int \frac{dr'' \left(\rho_c^{(0)}(r'')\right)^{1/3} \theta(r'')}{|r'' - r_2|} \Big/ \left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle \right\} \tag{18a}$$

$$\left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle = \int dr \left(\rho_c^{(0)}(r)\right)^{1/3} \theta(r), \tag{18b}$$

$$\theta(r) = \left\{ 1 + [3\pi^2 \cdot \rho_c^{(0)}(r)]^{2/3} / c^2 \right\}^{1/2} \tag{18c}$$

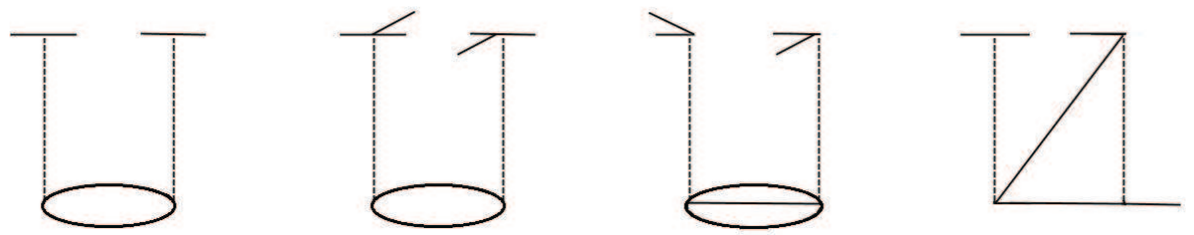

Figure 1. Some diagrams of the second order, taking into account the exchange and polarization interaction of quasiparticles and electrons of the closed shells core.

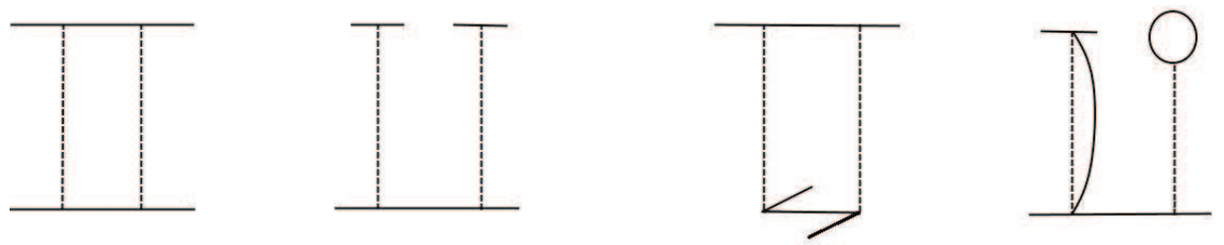

Figure 2. Some diagrams of the second order, describing a direct interaction of the two or three external quasiparticles.

where ρ_c^0 is the core electron density (without account for the quasiparticle), X is the numerical coefficient, and c is the light velocity. The similar approximate potential representation has been received for the exchange polarization interaction of quasiparticles (see details in Refs. [7, 14–19]). The polarization potential Eqs. (18a)–(18c) generalizes the corresponding nonrelativistic operator, which has been derived in Ref. [36].

In order to take into account the ladder diagrams contributions as well as some of the three-quasiparticle diagram contributions in all PT orders, we use the special procedure, which includes a modification of the mean-filled potential, which describes the effects of screening (antiscreening) of the core potential of each QP by the others (see details in Refs. [7, 14–19, 33–38]). Introduction of the additional screening potential into the Dirac equations for the large and small components changes the 1-QP energies and orbitals. It results in the corresponding modification of the diagonal 1-QP matrix $\tilde{M}^{(1)}$ and further 2-QP one too; $\tilde{M}^{(2)}$ is computed using the PT first-order formulae and the modified radial 1-QP wave functions.

2.4. Optimization of the relativistic orbitals basis

In order to obtain a precise description of the spectral characteristics of multielectron atomic systems, within the PT framework one should generate the optimized relativistic orbitals basis (see "Introduction" section) [1–7, 9–15]. The powerful ab initio approach to construction of the optimized PT basis has been developed in Ref. [48] and reduced to consistent treating gauge-dependent multielectron contributions $\mathrm{Im}\Delta E_{\mathrm{ninv}}$ of the lowest relativistic PT corrections to the atomic level radiation width and their further functional minimization.

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 multiquasiparticle case does not contain principally new moments. In the PT lowest, second order for the ΔE, there is only one-quasiparticle Feynman diagram B (see **Figure 3**), contributing the $\mathrm{Im}\Delta E$ (the radiation decay width).

In the fourth order of QED PT (the second order of the atomic PT), the diagrams appear, whose contribution to the $\mathrm{Im}\Delta E_{\mathrm{ninv}}$ accounts for the multielectron exchange-correlation (polarization) effects (diagrams A_d, A_{ex}; **Figure 3**). This multielectron contribution is dependent on the photon propagator gauge (the gauge-noninvariant contribution). Let us remind about the known criterion of the correctness of the atomic-computing radiation transition probabilities using the alternative forms for the transition operator ("length" and "velocity" transition operator forms). Their closeness of the "length" and "length" transition probabilities values

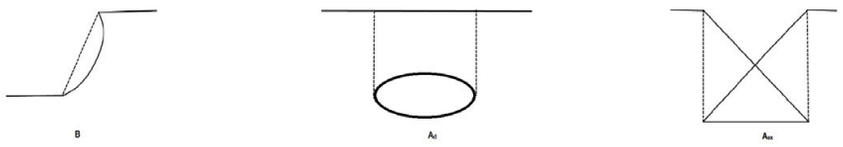

Figure 3. B: second other PT diagram contributing the imaginary energy part related to the radiation transitions; A_d and A_{ex}: QED PT fourth (atomic PT second)-order polarization diagrams.

confirms the correctness of the relativistic orbitals basis construction. Correspondingly, their noncoincidence is provided by multielectron by their nature and gauge-noninvariant terms.

In Ref. [48], the gauge-noninvariant contribution to an imaginary part of the electron energy has been calculated, which is as follows:

$$\begin{aligned}&\mathrm{Im}\Delta E_{ninv}(\alpha - s|A_d) = -C\frac{e^2}{4\pi}\int\int\int\int dr_1 dr_2 dr_3 dr_4 \sum(\frac{1}{\omega_{mn}+\omega_{\alpha_s}}+\\&\frac{1}{\omega_{mn}-\omega_{\alpha_s}})\Psi^+_\alpha(r_1)\Psi^+_m(r_2)\Psi^+_s(r_3)\Psi^+_n(r_4)(1-\alpha_1\alpha_2)/r_{12}\cdot\\&\{[(\alpha_3\alpha_4-(\alpha_3 n_{34})(\alpha_4 n_{34}))/r_{34}\cdot\sin[\omega_{\alpha_n}(r_{12}+r_{34})+\omega_{\alpha_n}\cdot\\&\cos[\omega_{\alpha_n}(r_{12}+r_{34})](1+(\alpha_3 n_{34})(\alpha_4 n_{34}))]\}\Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1)\end{aligned} \tag{19}$$

where C is the gauge constant, and f is the boundary of the closed shells.

Realizing a principle of minimization of the functional $\mathrm{Im}\Delta E_{\mathrm{ninv},}$ one could obtain the Dirac-Kohn-Sham (DKS)-like equations for an electron density. Their numerical solution allows to obtain the optimized basis of the one-QP relativistic orbitals. The corresponding procedure is described in detail, for example, in Refs. [18–23]. All details of the presented PT formalism can be found in Refs. [7, 14–20, 47–49].

2.5. Radiation decay probability as an imaginary part of the electron energy shift. Method of calculation

The method of computing the radiation decay (transition probabilities, oscillator strengths) probabilities within the relativistic energy approach is presented in, for instance, Refs. [16–19, 33–35, 47, 48]. Here, we only note that a probability is directly linked with the imaginary part of electron energy shift, which is defined in the PT lowest order as follows:

$$\mathrm{Im}\Delta E = -\frac{e^2}{4\pi}\sum_{\substack{\alpha>n>f\\[\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n\alpha n}, \tag{20}$$

where $\sum_{\alpha>n>f}$ is for electron and $\sum_{\alpha<n\le f}$ for vacancy, and $V^{|\omega_{\alpha n}|}_{\alpha n\alpha n}$ is determined as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \tag{21}$$

The individual terms of the sum Eq. (21) represent the contributions of different channels and probability, for instance, of the dipole α-n transition as $P_{\alpha n}\sim\frac{1}{4\pi}V^{|\omega_{\alpha_n}|}_{\alpha n\alpha n}$; the probability with accounting for the core polarization correction is $P_{\alpha_n}\sim\frac{1}{4\pi}\cdot\{V^{|\omega_{\alpha_n}|}_{\alpha n\alpha n}+(V^{d+ex}_{pol})_{\alpha n\alpha n}\}$. The total probability of a λ-pole transition is usually represented as a sum of the electric P^E_λ and magnetic P^M_λ

parts. The electric (or magnetic) λ-pole transition $\gamma \to \delta$ connects two states with parities which by λ (or $\lambda + 1$) units. In our designations,

$$\begin{aligned} P^E_\lambda(\gamma \to \delta) &= 2(2j+1)Q^E_\lambda(\gamma\delta;\gamma\delta) \qquad Q^E_\lambda = Q^{Cul}_\lambda + Q^{Br}_{\lambda,\ \lambda-1} + Q^{Br}_{\lambda,\ \lambda+1} \\ P^M_\lambda(\gamma \to \delta) &= 2(2j+1)Q^M_\lambda(\gamma\delta;\gamma\delta) \qquad Q^M_\lambda = Q^{Br}_{\lambda,\ \lambda}. \end{aligned} \tag{22}$$

In a case of the two-quasiparticle states (for instance, the excited atomic state is treated as a state with the two QP: electron and vacancy above the closed shells core), the corresponding probability has the following form (say, transition: $\mathrm{j}_1 j_2[J] \to \bar{j}_1 j_2[\bar{J}]$):

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

It is worth noting that all relativistic atomic calculations are usually carried out in the *jj*-coupling scheme. The transition to the intermediate-coupling scheme is realized by diagonalization of the M matrix, but usually only ReM should be diagonalized. The important simplified moment of the procedure is connected with converting the imaginary part by means of the matrix of eigenvectors $\{C_{mk}\}$, obtained by diagonalization of ReM:

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

where M_{ij} are the matrix elements in the *jj*-coupling scheme, and M_{mk} in the intermediate-coupling scheme representation. The procedure is correct to terms of the order of Im M/Re M.

In conclusion, 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, certainly, must coincide with the formulae obtained using the traditional amplitude quantum-mechanical method. All other details can be found in Refs. [7, 16–19, 33–36, 47–50].

3. Some results and conclusions

As illustration of the application of the above presented formalism, we present the results of computing energies, transition probabilities (oscillator strengths) in the heavy multielectron ion of Hg^+. A great interest to studying similar systems (Hg) is explained by the importance of the corresponding data, for instance, for laser effect studying. The collision of atoms of the Mendeleev table second raw with ions of helium (other inert gases) leads to creating ions in the excited states which is important for creating the inverse populations and laser effect. The available literature data on radiative characteristics are definitely insufficient. An account of the relativistic and correlation effects has a critical role in the cited systems as the studied transitions occur in the external shells in a strong field of atom with large Z. Within the relativistic PT, the Hg^+ states can be treated one- and three-QP states of electrons (6s) and

vacancy ($5d^{-1}$) above the core of the closed shells $5d^{10}6s^2$. The interaction "quasiparticle core" is described by the potential (6). The polarization interaction of the quasiparticles through the core is described by the two-particle effective potential Eqs. (18a)–(18c). All calculations are performed using the modified atomic code "Superatom-ISAN."

In **Tables 1–3**, we present the experimental (NIST) [32] and theoretical energies, electric E1 ($5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$), and E2 ($5d^96s^2$ ($D_{5/2}$, $D_{3/2}$)-$5d^{10}6s$ ($S_{1/2}$)) probabilities of the transitions in the spectrum of Hg^+. The theoretical results are obtained within the Hartree-Fock, Dirac-Fock methods by Ostrovsky-Sheynerman, relativistic PT theory with the empirical model potential zeroth approximation (RPT-MP) [18, 31], and our optimized RPT using relativistic energy approach (RPT-EA).

The standard HF and DF approaches in the single-configuration approximations do not allow to obtain very accurate results. Using the empirical transition energies significantly improve the theoretical results as in fact it means an account for very important interparticle correlations effects. In our approach, the corresponding exchange-correlation effects (the polarization

Method	E_{6s}	$7P_{1/2}$-$6S_{1/2}$	$7P_{3/2}$-$6S_{1/2}$	$7P_{1/2}$-$7S_{1/2}$	$7P_{3/2}$-$7S_{1/2}$	$D_{3/2}$-$S_{1/2}$
HF	−1.07	0.721	0.721	0.095	0.095	0.863
DF	−1.277	0.904	0.922	0.109	0.127	0.608
RPT-MP	−1.377	0.986	1.019	0.114	0.147	0.462
RPT-EA	−1.378	0.987	1.020	0.115	0.148	0.462
Exp.	−1.378	0.987	1.020	0.115	0.148	0.461

Theoretical data—Hartree-Fock (HF), Dirac-Fock (DF) [31]; relativistic PT with the empirical model potential approximation (RPT-MP) [18]; relativistic PT-RPT-EA (this work); experimental data—Moore (NBS, Washington) [32] (see text).

Table 1. The energies of the $5d^96s^2(D_{5/2},D_{3/2})$-$5d^{10}6s$ ($S_{1/2}$), $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$, $5d^96s^2(D_{5/2},D_{3/2})$-$5d^{10}6s$ ($S_{1/2}$) transitions in Hg^+ (Ry).

Method	$7P_{3/2}$-$6S_{1/2}$	$7P_{1/2}$-$6S_{1/2}$	$7P_{3/2}$-$7S_{1/2}$	$7P_{1/2}$-$7S_{1/2}$	$7P_{3/2}$-$6S_{1/2}$
HF	4.75×10^6	4.75×10^6	3.65×10^7	3.65×10^7	3.65×10^7
DF	8.45×10^7	1.67×10^7	6.89×10^7	6.89×10^7	4.71×10^7
DF (E_{exp})	1.17×10^8	2.04×10^7	1.10×10^8	1.10×10^8	5.52×10^7
RPT-MP	1.49×10^8	2.31×10^7	1.41×10^8	1.41×10^8	6.33×10^7
RPT-EA	1.51×10^8	2.33×10^7	1.43×10^8	1.43×10^8	6.35×10^7
Exp.	1.53×10^8	2.35×10^7	1.44×10^8	1.44×10^8	6.37×10^7

HF, Hartree-Fock data; DF, Dirac-Fock data; DF (E_{exp}), DF data using the experimental transitions energies [31]; relativistic perturbation theory with the empirical model potential approximation RPT-MP [18]; relativistic PT-RPT-EA (this work); experimental data—Moore (NBS, Washington) [32] (see text).

Table 2. Probabilities of the transitions $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}6s(S_{1/2})$, $5d^{10}7p(P_{1/2},P_{3/2})$-$5d^{10}7s(S_{1/2})$ in Hg^+ (in s^{-1}).

Method	$D_{3/2}$-$S_{1/2}$	$D_{5/2}$-$S_{1/2}$
HF	1360	1360
DF	257.0	77.4
DF (E_{exp})	63.9	13.3
RPT-MP	54.54	11.8
RPT-EA	54.52 (0.2%)	11.7 (0.2%)
Exp.	53.5 ± 2.0	11.6 ± 0.4

HF, Hartree-Fock data; DF, Dirac-Fock data; DF (E_{exp}), DF data using the experimental transitions energies [31]; relativistic perturbation theory with the empirical model potential approximation (RPT-MP) [18]; relativistic PT-RPT-EA (this work); experimental data—Moore (NBS, Washington) [32] (see text).

Table 3. The E2 probabilities of the $5d^96s^2(D_{5/2},D_{3/2})$-$5d^{10}6s$ ($S_{1/2}$) transition in Hg^+ (in s^{-1}).

interaction of the QPs, mutual screening and anti-screening corrections, etc.) are taken into account more accurately. The core polarization correction to the transition probability is of great importance as it changes significantly the probability value (~15–40%). It should be also noted that the gauge-noninvariant contribution to radiation width is very small (0.2%; see **Table 2** in the line "EA") that means equivalence of the calculation results in the standard amplitude approach with using the length and velocity forms for transition operator. From the other side, this is an evidence of the successful choice of the PT zeroth approximation and accurate account of the multi-particle correlation effects.

We have presented the fundamentals of the new relativistic many-body PT formalism with construction of the optimized one-QP representation in the theory of relativistic multielectron systems. The relativistic density-functional approximation with the Kohn-Sham potential is taken as the zeroth one and all exchange-correlation corrections of the second-order and dominated classes of the higher-orders diagrams (polarization interaction, QPs screening, etc.) have been taken into account. In order to reach the corresponding optimization, we have used a procedure of the accurate treating of the PT lowest-order multielectron effects, in particular, the gauge-dependent radiative contribution for the certain class of the photon propagator gauge. The corresponding contribution is considered to be the typical representative of the important multielectron exchange-correlation effects, whose minimization is reasonable criteria in the searching for the optimal PT one-electron basis. This procedure derives an undoubted profit in the routine many-body calculations as it provides the way of the refinement of the atomic (molecular) characteristics calculations, based on the "first principles." The presented relativistic PT formalism can be further generalized, in particular, by the way of accounting for the radiation, QED (the Lamb shift self-energy and vacuum polarization corrections, for instance in the effective Uhling-Serber approximation with account for the Källen-Sabry and Wichmann-Kroll corrections), and nuclear (the Bohr-Weisskopf and Breit-Rosenthal-Crawford-Schawlow effects, nuclear finite size correction, magnetic moment distribution, etc.) effects [13–23].

Author details

Alexander V. Glushkov*, Olga Yu. Khetselius, Andrey A. Svinarenko, Vasily V. Buyadzhi, Valentin B. Ternovsky, Anna A. Kuznetsova and Petr G. Bashkarev

*Address all correspondence to: glushkovav@gmail.com

Odessa State Environmental University, Odessa, Ukraine

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