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Quantum Geometry: Relativistic energy approach to cooperative electron-nuclearγ-transition spectrum

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Abstract An advanced relativistic energy approach is presented and applied to calculating parameters of electron-nuclear γ-transition spectra of nucleus in the atom. The intensities of the spectral satellites are defined in the relativistic version of the energy approach (S-matrix formalism). and gauge-invariant quantum-electrodynamical perturbation theory with the Dirac-Kohn-Sham density-functional zeroth approximation.

Keywords Quantum geometry · S-matrix formalism · cooperative spectra · Quantization of quasi-stationary states

Mathematics Subject Classification (2000) 55R05 · 53B05

1 Introduction

A development of the consistent methods of calculating a spectra of energy eigen values, sets of the eigen functions, different spectral and dynamical parameters (collision cross-section, decay probabilities etc) for relativistic Hamiltonian of the heavy relativistic many-body systems with direct, consistent account of the relativistic and nuclear effects is still actual and fundamentally important problem of the modern quantum geometry and relativistic quantum theory of the many-fermion systems (see, for example, [1]–[15]).

Any alteration of the quantum state must be manifested in the quantum transitions, for example, in a spectrum of the γ-radiation of a nucleus. It is well known that it is possible the transfer of part of a nuclear energy to atom or molecule under radiating (absorption) the γ quanta by a nucleus [3]–[5]. The first references to the neutral recoil are due to Migdal and Levinger, who evaluated

approximately the ionization of an atom undergoing sudden recoil in due to neutron impact and in a radioactive disintegration respectively. The neutral recoil situation differs radically from processes involving a charged particle for which the sudden recoil approximation is often invalid [4]. Simple, as a rule, non-relativistic quantum-mechanical models (c.f. [3]–[5]) have been developed to evaluate the excitation or ionization of an atom induced a sudden recoil of its nucleus occurring when a neutral particle is either emitted or captured. The most consistent approach to considered problems must be based on the quantum electrodynamics (QED).

The nuclear emission or absorption spectrum of an atom possesses a set of electron satellites, which are due to an alteration of the state of the electron shell [3]. The latter is provided by a shaking of the shell resulting from the interaction between the nucleus and γ-quantum or by a direct interaction between γ-quantum and electrons. This paper is going on our studying the co-operative dynamical phenomena (c.f. [3]–[5]) due the interaction between electron shells and nuclei nucleons and devoted to formulation of an advanced relativistic energy approach to calculating parameters of electron-nuclear γ-transition spectra of nucleus in the atom. The intensities of satellites are defined in the relativistic version of the energy approach (S-matrix formalism) [16]. Decay and excitation probabilities are linked with imaginary part of the energy of the 'nuclei nucleons-electron shells-field' system. For radiate decays it is manifested as effect of retarding in interaction and self-action and calculated within QED perturbation theory with the Dirac-Kohn-Sham zeroth approximation. Such an scheme is a new original element of the whole approach.

2 Advanced energy approach to QED theory of co-operative electron-nuclear processes

Following [3]–[5], we consider the following model of atomic system: rigid nuclear core (c), above core proton (p) and electron (e). The masses of three particles are equal correspondingly: $\mu_c M$, $\mu_p M$, $\mu_e M$, where M – mass of all atom; $\mu_c + \mu_p + \mu_e = 1$; the space co-ordinates of the particles are denoted as r_c, r_p, r_e. The charge of nuclear core is z. Besides, the value of z^* denotes an effective charge for Coulomb field of the optically active electron in ion. Naturally, the majority of the excited states of nuclei have the multi-particle character. As exclusion, one may consider the first excited states with one or two quasi-nucleons or quasi-vacancies above 'even-even' core. These states are more suitable for theoretical consideration as the one-particle model could be used. It is very im-

portant to underline that a generalization on the multi-particle case does not lead to qualitatively new results as the dynamical (radial) parts of the nuclear matrix elements do not enter into expressions for relative intensities of the electron satellites and ground line of the nuclear transition. QED is needed here as for obtaining the correct formula as carrying out the precise calculations.

Within the QED energy approach the main our purpose is calculating the imaginary part of energy of the excited state for atomic system. Detailed description of an approach was given earlier (c.f. [5]–[15]). Here we consider only the key elements of the calculation procedure. Following the quasi-potential method, we introduce the bare interaction as follows:

$$V(r_c, r_p, r_c) = v(r_{pc}) - Ze^2/r_{ec} - e^2/r_{pe}. \tag{1}$$

Here $v(r_{pc})$ imitates the interaction of the proton with the core (nuclear and Coulomb); other interactions are obvious. Then imaginary part of the energy of the excited state for three-quasi-particle system Ψ_I in the lowest QED perturbation theory order can be written as follows:

$$\begin{aligned} \mathrm{Im}E = e^2 \mathrm{Im} i \lim_{\gamma\to 0} \iint d^4x_1 d^4x_2 e^{\gamma(t_1+t_2)} \left(D(r_{c_1t_1}, r_{c_2t_2}) \times \right. \\ \times \langle\Psi_I|(j_c(x_1)j_c(x_2))|\Psi_I\rangle + D(r_{p_1t_1}, r_{p_2t_2}) \langle\Psi_I|(j_p(x_1)j_p(x_2))|\Psi_I\rangle + \\ \left. + D(r_{e_1t_1}, r_{e_2t_2}) \langle\Psi_I|(j_e(x_1)j_e(x_2))|\Psi_I\rangle \right). \end{aligned} \tag{2}$$

Here $D(r_1t_1, r_2t_2)$ is the photon propagator; j_c, j_p, j_e are the four-dimensional components for the current operator for particles: core, protons, electrons; $x = (r_c, r_p, r_e, t)$ includes the space co-ordinates of three particles and time (equal for all particles); γ is the adiabatic parameter. For the photon propagator the exact electrodynamical expression is used:

$$D(12) = -\frac{i}{8\pi^2}\frac{1}{r_{12}} \int\limits_{-\infty}^{\infty} d\omega e^{i\omega t_{12} + i|\omega| r_{12}}. \tag{3}$$

In expressions (2), (3) the summation of the directions of the photon polarization are fulfilled. Below we are limited by the lowest order of the QED perturbation theory, i.e. the next QED corrections to ImE will not be considered. Note also that the expression (2) describes the one-photon processes. Further we need the one-quasi-particle state wave functions of the electrons in the atomic shell and nucleons in a nucleus. Here we firstly use the relativistic solutions of the Dirac-Kohn-Sham equation whose radial part is represented by [8]:

$$F' = -(\text{œ} + |\text{œ}|)F/r - \alpha(E + 2M\alpha^{-2})G - \alpha VG,$$
$$G' = (\text{œ} - |\text{œ}|)G/r + \alpha(E - V)F. \quad (4)$$

Here α is the fine structure constant; œ is the Dirac angular quantum number; E is the state energy, F, G being the large and small radial components correspondingly. Substituting all expressions into (2), one may get the following general expression for imaginary part of the excited state energy of the three-quasi-particle system as a sum of the core proton and electron contributions [4]:

$$\mathrm{Im}E = \mathrm{Im}E_c + \mathrm{Im}E_p + \mathrm{Im}E_e,$$
$$\mathrm{Im}E_a = -Z_a^2/4\pi \sum_F \iint dr_{c_1} dr_{c_2} \iint dr_{p_1} dr_{p_2} \iint dr_{e_1} dr_{e_2} \Psi_I^*(1)\Psi_F^*(2)T_a(1,2)\Psi_F(1)\Psi_I(2), \quad (5)$$
$$T_a(1,2) = (\sin(w_{IF} r_{a_{12}})/r_{a_{12}}) \left(1/M\mu_a(\nabla_{r_{a_1}}, \nabla_{r_{a_2}}) + 1\right).$$

Here $r_{a_{12}} = |r_{a_1} - r_{a_2}$; w_{IF} is the transition full energy, which includes changing of the kinetic energy of the ion, i.e. the recoil energy; Ψ_c, Ψ_p, Ψ_e are the second quantized field operators of the core particles, of the protons and of the electrons respectively. The sum according to F gives the summation of the final states of the system.

In the second order of QED perturbation theory, the full width of a level is divided into the sum of the partial contributions, connected with the radiation decay into concrete final states of the system. These contributions are proportional to the probabilities of the corresponding transitions. The system of red (blue) satellites corresponds to the transitions with excitation (de-excitation) of the electron shell. The important quantity is the contribution of $\mathrm{Im}E_e$ to the relative intensity of satellite $k = P(pe)/P(p)$ (here $P(pe)$ is satellite intensity; $P(p)$ is the intensity of the nuclear transition). The intensity of the line is linked with $\mathrm{Im}E$ (5) as [3]:

$$P = 2\mathrm{Im}E/h. \quad (6)$$

Further it is convenient to separate the motion of the center of mass of the system, introducing the new variables:

$$R = \mu_c r_c + \mu_p r_p + \mu_e r_e, \qquad R_p = r_p - r_c, \qquad R_e = r_e - r_c.$$

In the zeroth order perturbation theory approximation a dependence of Ψ_I, Ψ_F from the variables R, R_p, R_e is factorized:

$$\Psi_A(R, R_p, R_e) = \Psi_A(R)\Psi_{Ap}(R_p)\Psi_{Ae}(R_e). \quad (7)$$

Here Ψ_A is plane waves, Ψ_{Ap} is function of state of the proton in potential $V(R_p)$, Ψ_{Ae} is Coulomb relativistic function.

The main effect of causing the electron satellites for nuclear transitions has kinematics nature, which is in shifting center of mass of the system under emission of γ-quanta relatively of the proton or electron orbital. In the concrete calculation one can use the standard expansion for operator $\mathbf{T}$ on the spherical functions, which generates the multiple expansion for the decay probability. The details of the calculation procedure, the definition of all contributions and the corresponding matrix elements are described in refs. ([4]–[8])

3 Results and conclusion

In this paper we have formulated a new advanced version of the relativistic energy approach to calculating parameters of electron-nuclear γ-transition spectra of nucleus in the atom. The intensities of the spectral satellites are defined in the relativistic version of the energy approach (S-matrix formalism) and gauge-invariant quantum-electrodynamical perturbation theory with the Dirac-Kohn-Sham density-functional zeroth approximation. In the calculational aspect using density-functional approximation significantly simplifies the computational procedure.

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