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## **OPTIMIZED RELATIVISTIC DIRAC-FOCK APPROACH TO CALCULATING THE HYPERFINE LINE SHIFT AND BROADENING FOR HEAVY ATOMS IN THE BUFFER GAS**

It is presented a new consistent relativistic approach to description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases, based on the atomic gauge-invariant relativistic perturbation theory with the optimized Dirac-Fock zeroth approximation with density functional correlation potential and the exchange perturbation theory for construction of the interatomic potential function. As illustration it is applied to calculating the interatomic potentials, hyperfine structure line collision shift and broadening for alkali and thallium atoms, in an atmosphere of the buffer inert gas. It is shown that an accurate accounting of relativistic and exchange-correlation provides physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases.

### **1. Introduction**

In Ref. [1-3] It has been presented a new consistent relativistic approach to hyperfine structure line collision shift and broadening for heavy atoms in an atmosphere of the buffer inert gas, based on the atomic gauge-invariant relativistic perturbation theory and the optimal construction of the interatomic potential function within exchange perturbation theory. As illustration it has been applied to calculating the interatomic potentials, hyperfine structure line collision shift for heavy atoms, namely, rubidium, cesium etc in an atmosphere of the buffer inert gas (He). It was shown that the consistent, accurate accounting the the relativistic and exchange-correlation, continuum pressure effects has to be done to get an adequate description of the energetic and spectral properties of the heavy atoms in an atmosphere of the heavy inert gases.

Let us remind that the broadening and shift of atomic spectral lines by collisions with neutral atoms has been studied extensively since the very beginning of atomic physics, physics of collisions etc [4–36]. These studied are of a great interest for modern atomic and molecular spectroscopy, quantum chemistry, laser physics and quantum electronics, astrophysics and metrology as well as for studying a role of weak interactions in atomic

optics and heavy-elements chemistry [37-48]. It is very important point that the computing the hyperfine structure line shift and broadening allows to check a quality of the orbitals basis and understand physical aspects of accounting the relativistic and correlation effects to the energetic and spectral characteristics of the two-center (multi-center) atomic systems. One of the known and widely used quantum methods to compute atomic parameters and spectral lines characteristics is the Dirac-Fock method. However, because of the known points connected with generation of non-optimized basis of wave functions and other ones (for example, the slow convergence of the corresponding PT series with the Dirac-Fock zeroth approximation, necessity of accurate accounting for the correlation effects etc) this method should be seriously improved. The most known improvement is in using the multiconfiguration Dirac-Fock approach.

In this paper we present a new consistent relativistic approach to description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases, based on the atomic gauge-invariant relativistic perturbation theory with the optimized Dirac-Fock zeroth approximation with density functional correlation potential and the exchange perturbation theory for construction of the interatomic potential function. As

illustration it is applied to calculating the, hyperfine structure line shift and broadening for alkali atoms in an atmosphere of the buffer inert gas. It is shown that an accurate accounting of relativistic and exchange-correlation provides physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases

## 2. Method

The basic expressions for the collision shift and broadening hyperfine structure spectral lines are taken from the kinetic theory of spectral lines [6,7,11,12]. In order to calculate a collision shift of the hyperfine structure spectral lines one can use the following expression known in the kinetic theory of spectral lines shape (see Refs. [1-7]):

$$f_p = \frac{D}{p} = \frac{4\pi w_0}{kT} \int_0^{\infty} [1 + g(R)] dw(R) \exp(-U(R)/kT) R^2 dR \quad (1)$$

$$g(R) = \begin{cases} \frac{2}{3\sqrt{\pi}} \left( -\frac{U(R)}{kT} \right)^{3/2}, & U < 0, \\ 0, & U > 0, \end{cases}$$

Here  $U(R)$  is an effective potential of interatomic interaction, which has the central symmetry in a case of the systems  $A-B$  (in our case, for example,  $A=Rb,Cs$ ;  $B=He$ );  $T$  is a temperature,  $w_0$  is a frequency of the hyperfine structure transition in an isolated active atom;  $dw(R)=Dw(R)/w_0$  is a relative local shift of the hyperfine structure line;  $(1+g(R))$  is a temperature form-factor.

The local shift is caused due to the disposition of the active atoms (say, the alkali atom and helium He) at the distance  $R$ . In order to calculate an effective potential of the interatomic interaction further we use the exchange perturbation theory formalism (the modified version EL-HAV) [4-6].

Since we are interested by the alkali (this atom can be treated as a one-quasiparticle systems, i.e. an atomic system with a single valence electron above a core of the closed shells) and the rare-earth atoms (here speech is about an one-, two- or even three-quasiparticle system), we use the clas-

sical model for their consideration. The interaction of alkali (A) atoms with a buffer (B) gas atom is treated in the adiabatic approximation and the approximation of the rigid cores. Here it is worth to remind very successful model potential simulations of the studied systems (see, for example, Refs. [13-26]).

In the hyperfine interaction Hamiltonian one should formally consider as a magnetic dipole interaction of moments of the electron and the nucleus of an active atom as an electric quadrupole interaction (however, let us remind that, as a rule, the moments of nuclei of the most (buffer) inert gas isotopes equal to zero).

The necessity of the strict treating relativistic effects causes using the following expression for a hyperfine interaction operator  $H_{\text{HF}}$  (see, eg., [3,5]):

$$H_{\text{HF}} = a \sum_{i=1}^N I \frac{\alpha_i \times r_i}{r_i^3}, \quad a = -2\mu \frac{e^2 h}{2m_p c}, \quad (2)$$

where  $I$  – the operator of the nuclear spin active atom,  $\alpha_i$  – Dirac matrices,  $m_p$  – proton mass,  $\mu$  – moment of the nucleus of the active atom, expressed in the nuclear Bohr magnetons. Of course, the summation in (2) is over all states of the electrons of the system, not belonging to the cores. The introduced model of consideration of the active atoms is important to describe an effective interatomic interaction potential (an active atom – an passive atom), which is centrally symmetric ( $J_A=1/2$ ) in our case (the interaction of an alkali atom with an inert gas atom). Let us underline that such an approximation is also acceptable in the case system “thallium atom – an inert gas atom” and some rare-earth atoms, in spite of the presence of p-electrons in the thallium (in the case of rare-earth atoms, the situation is more complicated). One of the most correct methods to describe heavy atoms in an atmosphere of inert gases is the relativistic Dirac-Fock one or the Dirac-Kohn-Sham method. It is obvious that more sophisticated relativistic many-body methods should be used for correct treating relativistic, exchange-correlation and even nuclear effects in heavy atoms (including the many-body correlation effects, intershell correlations, possibly the continuum pressure etc). In our calculation we

have used the relativistic functions, which are generated within the optimized Dirac-Fock zeroth approximation of the relativistic many body perturbation theory [38]. The potential of the interelectron interaction with accounting the retarding effect and magnetic interaction in the lowest order on parameter  $\alpha^2$  (the fine structure constant) is as follows:

$$V(r_i r_j) = \exp(i\omega_{ij} r_{ij}) \cdot \frac{(1 - \alpha_i \alpha_j)}{r_{ij}}, \quad (3)$$

where  $\omega_{ij}$  is the transition frequency;  $\alpha_i, \alpha_j$  are the Dirac matrices. The PT zeroth approximation is the optimized Dirac-Fock one (plus additional correlation potential [15]) with using the consistent relativistic energy approach in order to construct the optimal relativistic orbitals basis (for details see Refs. [37-49]). The optimization is reduced to minimization of the gauge dependent multielectron contribution  $Im\delta E_{minv}$  of the lowest relativistic perturbation theory corrections to the radiation widths of atomic levels. The minimization of the functional  $Im\delta E_{minv}$  leads to the Dirac-Fock-like equations for the electron density that are numerically solved. The further elaboration of the method can be reached by means of using the Dirac-Sturm approach [5]. To calculate an effective potential of the interatomic interaction we use a method of the exchange perturbation theory (in the modified version EL-HAV [2,5,6]). Within exactness to second order terms on potential of Coulomb interaction of the valent electrons and atomic cores a local shift can be written as:

$$\delta\omega(R) = \frac{S_0}{1 - S_0} + \Omega_1 + \Omega_2 - \sum_n \frac{C_n}{R^n}, \quad (4)$$

where values  $\Omega_1, \Omega_2$  are the non-exchange and exchange non-perturbation sums of the first order correspondingly, which express through the matrix elements of the hyperfine interaction operator. The other details are in Refs.[1-11].

### 3. Results and conclusion

Further we present some test results of our studying hyperfine line collisional shift for alkali atoms (rubidium and caesium) in the atmosphere

of the helium gas. In Table 1 and we present our theoretical results for the hyperfine line observed shift  $f_p$  (1/Torr) in a case of the Cs-He pairs. The experimental and alternative theoretical results by Batygin et al [5] for  $f_p$  are listed too. At present time there are no precise experimental data for a wide interval of temperatures in the literature. The theoretical data from Refs. [5] are obtained on the basis of calculation within the exchange perturbation theory with using the He wave functions in the Clementi-Rothaane approximation (column: Theory<sup>a</sup>), and in the Z-approximation (column: Theory<sup>b</sup>), and in the Löwdin approximation (column: Theory<sup>c</sup>).

Table 1

**The observed  $f_p$  ( $10^{-9}$  1/Torr) shifts for the systems of the Cs-He and corresponding theoretical data (see text)**

T, K	Exp	a	b	c	This
223	-	164	142	169	173
323	135	126	109	129	134
423	-	111	96	114	121
523	-	100	85	103	109
623	-	94	78	96	102
723	-	-	-	-	95
823	-	-	-	-	90

Note:<sup>a</sup> – calculation with the He wave functions in the Clementi-Rothaane approximation; <sup>b</sup> – the Z-approximation; <sup>c</sup> –Löwdin approximation [5];

In Tables 2 there are listed the values of the observed  $f_p$  ( $10^{-9}$  1/Torr) shifts for the systems of the pair: TI- He: C –our data, B- data by Mishchenko et al [7], A- data by Batygin-Sokolov [6]. In Table 3 there are listed the calculated adiabatic broadening values  $\Gamma_a/p$  (in Hz/Tor) for the thallium spectral lines for different temperatures and pairs TI- He, Kr, Xe.

Table 2

The observed  $f_p$  ( $10^{-9}$  1/Torr) shifts for the systems of the pair: **TI- He: C** –our data, **B-** data by Mischenko et al [7], **A-** data by Batygin-Sokolov [6].

T, K	A	B	C
700	155	137	133,1
800	151	134	130,2
900	147.5	131	128,0
1000	143	126	123,4

Note: Exp. Value (TI-He, T=700K):  $130 \pm 10$ ;

Table 3

Adiabatic broadening values  $\Gamma_a/p$  (in Hz/Tor) for the thallium spectral lines for different temperatures (pair: **TI- He, TI-Kr, TI-Xe**).

T, K	TI-He [4]	TI-He Our	TI-Kr Our	TI- Xe Our
700	2.83	2.49	6.79	17.27
800	2.86	2.52	5.88	14.58
900	2.90	2.56	5.24	12.87
1000	2.89	2.53	5.22	11.48

Our data confirm violation of the known Foli relationship between the observed  $f_p$  shift and the adiabatic broadening value ( $\Gamma_a/p \sim f_p$ ) in the standard theory of spectral lines, for spectral. One could see, that for example,  $(\Gamma_a/p)/f_p \sim 1/60$  for system of TI-He etc. Qualitatively similar, but quantitatively a little other estimates have been obtained in Refs. [3,4].

To conclude, let us underline that using the optimized relativistic orbitals basis (in our approach speech is about the optimized Dirac-Fock zeroth approximation with additional correlation potential) and consistent precise accounting for the exchange-correlation and other effects is prin-

cipally necessary for the physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases.

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#### **Summary**

It is presented a new consistent relativistic approach to description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases, based on the atomic gauge-invariant relativistic perturbation theory with the optimized Dirac-Fock zeroth approximation with density functional correlation potential and the exchange perturbation theory for construction of the interatomic potential. As illustration it is applied to calculating the hyperfine structure line collision shift and broadening for alkali and thallium atoms in an atmosphere of the buffer inert gas. It is shown that an accurate accounting of relativistic and exchange-correlation provides physically reasonable description of the energetic and spectral properties of the heavy atoms in an atmosphere of the inert gases.

**Keywords:** Relativistic many-body perturbation theory, Dirac-Fock approximation, hyperfine line collision shift

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### **НОВЫЙ РЕЛЯТИВИСТСКИЙ ПОДХОД К ОПРЕДЕЛЕНИЮ СДВИГА И УШИРЕНИЯ ЛИНИЙ СВЕРХТОНКОЙ СТРУКТУРЫ В ТЯЖЕЛЫХ АТОМАХ В БУФЕРНЫХ ГАЗАХ**

#### **Резюме**

Представлен новый релятивистский подход к определению сдвига и уширения линии сверхтонкой структуры тяжелых атомов в атмосфере буферных газов, который базируется на атомной калибровочно-инвариантной релятивистской теории возмущений с оптимизированным нулевым приближением Дирака-Фока с дополнительным корреляционным потенциалом и обменной теории возмущений для построения межатомного потенциала. В качестве иллюстрации приведены результаты расчета сдвига и уширения сверхтонких линий ряда тяжелых атомов, в частности, щелочных и атома таллия, в атмосфере буферных инертных газов. Показано, что аккуратный учет релятивистских, обменно-корреляционных эффектов обеспечивает адекватное описание энергетических и спектральных свойств тяжелых атомов в атмосфере тяжелых инертных газов.

**Ключевые слова:** релятивистская теория возмущений, приближение Дирака-Фока, столкновительный сдвиг линий сверхтонкой структуры



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## **НОВИЙ РЕЛЯТИВІСТСЬКИЙ ПІДХІД ДО ВІЗНАЧЕННЯ ЗСУВУ ТА УШИРЕННЯ ЛІНІЙ НАДТОНКОЇ СТРУКТУРИ У ВАЖКИХ АТОМАХ В БУФЕРНИХ ГАЗАХ**

### **Резюме**

Представлений новий релятивістський підхід до визначення зсуву і уширення лінії надтонкої структури важких атомів в атмосфері буферних газів, який базується на атомній калібрувально-інваріантній релятивістській теорії збурень з оптимізованим нульовим наближенням Дірака-Фока з додатковим кореляційним потенціалом і обмінній теорії збурень для побудови міжатомного потенціалу. Як ілюстрація, наведені результати розрахунку зсуву і уширення надтонких ліній ряду важких атомів, зокрема, лужних і атома талію, в атмосфері буферних інертних газів. Показано, що акуратне урахування релятивістських, обмінно-кореляційних ефектів забезпечує адекватний опис енергетичних і спектральних властивостей важких атомів в атмосфері важких інертних газів.

**Ключові слова:** релятивістська теорія збурень, наближення Дірака-Фока, зсув за рахунок зіткнень ліній надтонкої структури