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THEORETICAL STUDY OF RYDBERG ALKALI ATOMIC SYSTEMS IN A BLACK-BODY RADIATION FIELD: RELATIVISTIC APPROACH

We present the results of studying the characteristics of Rydberg alkali atomic systems in a black-body (BBR; thermal) radiation field, in particular, BBR induced Stark shift coefficient k. As theoretical approach the combined generalized relativistic energy approach and relativistic many-body perturbation theory (PT) with ab initio Dirac zeroth approximation is applied. Application of theory to computing the spectral parameters of studied atomic systems have demonstrated physically reasonable agreement between the theoretical and experimental data. carefully. It should be noted that our method takes carefully into account such important factors as the implementation of a gauge invariance principle when calculating the corresponding matrix elements, the correct degree of consideration of complex exchange-correlation effects (primarily, the effect of polarization of the core), and also generates a fairly optimal one-quasiparticle representation in within the limits of many-body relativistic PT with ab initio zeroth Dirac-Fock (Kohn-Sham) approximation. In any case, the formalism developed in this work, as it follows from the given results, can be used for precise calculations of the Stark shift coefficient k, the BBR shift parameter β, and other parameters.

1. Introduction

Modern theoretical photo-optics and spectroscopy of atomic systems, laser physics, photoelectronics and related physical fields are characterized by rapid development, connected, on the one hand, with the unprecedented progress of modern experimental methods and technologies due to the appearance of intense and super-intense sources of coherent laser radiation, pulses from several tens of femtoseconds to units of picoseconds and the ability to achieve peak intensities from 1019 W/cm2 to promising relativistic and higher ~10²⁴ W/cm² (we are primarily talking about modern types of free electron lasers such as TESLA, XFEL etc.), the active use of beam-foil spectroscopy methods, magneto-optical traps with the production of single Rydberg atoms, collider and accelerator technology, etc. [1-25].

Relatively new topic of the modern theory is connected with consistent treating the Rydberg atoms in a field of the Blackbody radiation (BBR). It should be noted that the BBR is one of the essential factors affecting the Rydberg states in atoms [1].

The account for the ac Stark shift, fast redistribution of the levels' population and photoionization provided by the environmental BBR became of a great importance for successfully handling atoms in their Rydberg states. The vast majority of existing papers on the description of Rydberg atoms in the thermal radiation field (c.g. [1-32]) are based on the Coulomb hydrogen-like approximation, different versions of the quantum defect method, classical and quasiclassical model approaches, the model and pseudo - potential methods. consider the problem of calculating the shift in the frequency of atomic transitions induced by BBR radiation, which is of fundamental importance for the operation of, for example, atomic clocks. It is well known that the main contribution to systematic frequency shifts is due to the Stark shift.

The so-called BBR shift is one of the most important contributions at room temperature for many frequency standards. A detailed overview of the problem is given, e.g. in works [3-11, 20,21] and numerous sources cited there.

It should be noted that at the present time, the sought-after research has been transformed into a separate highly intensive scientific field of research, and close attention is paid to theoretical developments, since the appropriate experimental measurements of BBR landslides are an extremely difficult academic task. In works [3-11,20], the current state of theoretical calculations of BBR shifts in various systems, which are of interest for the development of both microwave and optical frequency standards, is considered.

At the same time one should note that for heavy Rydberg atoms (both in the free state and in an external electromagnetic field) it is fundamentally important to accurately account for both relativistic and exchange-correlation effects. The quality and consistency of accounting for these effects also determine the accuracy of description of the energy and spectroscopic parameters of the heavy Rydberg atoms, including these atoms in a thermal radiation field. Naturally, the standard methods of the theoretical atomic physics, including the Hartree-Fock and Dirac-Fock approximations should be used in order to determine the thermal ionization characteristics of neutral and Rydberg atoms [1,2].

In this paper the results of studying the characteristics of Rydberg alkali atomic systems in a black-body (BBR; thermal) radiation field, in particular, BBR induced Stark shift coefficient k, on the basis of a new approach [20-22] are presented. As theoretical approach the combined generalized relativistic energy approach and relativistic many-body PT with ab initio Dirac zeroth approximation is applied (e.g.[23-33]).

2. Relativistic approach to atom in a Black-body radiation field

It is worth to remind that the electric field corresponding to thermal radiation according to Planck's law:

$$E^{2}(\omega)d\omega = \frac{8\alpha^{3}}{\pi} \frac{\omega^{3}d\omega}{\exp(\omega/k_{B}T) - 1},$$
(1)

leads to non-resonant perturbation of atomic transitions, the corresponding electric field

shift is then [7]:

$$\langle E^2 \rangle = (831.9 \text{ V/m})^2 \left(\frac{T(K)}{300} \right)^4.$$
 (2)

The shift in the atomic transition frequency due to the action of an electric field is known to be related to the static polarizability as:

$$\delta \nu = -\frac{1}{2} (831.9 \text{ V/m})^2 \left(\frac{T(K)}{300}\right)^4 \alpha_0 (1+\eta),$$

where η is an insignificant dynamic correction. It is not difficult to understand that the shift in the atomic transition frequency is actually the difference between the shifts of individual levels.

The key fundamental parameter is the β parameter of the relative BBR temperature-dependent atomic transition frequency shift, which is defined as [7,20]:

$$\frac{\delta\nu}{\nu_0} = \beta \left(\frac{T(K)}{T_0}\right)^4 \left(1 + \epsilon \left(\frac{T(K)}{T_0}\right)^2\right),\tag{4}$$

where, as usual, T_0 =300K. The parameter β can be calculated directly on the basis of data on the Stark coefficient k according to the expression:

$$\beta = \frac{k}{\nu_0} (831.9 \text{ V/m})^2.$$
 (5)

The fact is that the Stark coefficient is determined from the ratio for the frequency shift in a static electric field $\delta v = kE^2$. Accordingly, it can be related to the polarizability for the case of the initial and final states of the atomic system:

$$k = -\frac{1}{2} [\alpha_0(F) - \alpha_0(I)]. \tag{6}$$

It is also worth quoting formulas that define a scalar and tensor polarizability, namely, a scalar polarizability can be standardly defined as (see, for example, [1,2]):

$$\alpha_{JF}^{s}(\omega) = \alpha_{J}^{s}(\omega) = \frac{1}{2J+1} \sum_{m_{J}=-J}^{m_{J}=J} \alpha_{Jm_{J}}(\omega)$$

$$= \frac{1}{2} \frac{c^{3}}{a_{0}^{3}} \sum_{J'} \frac{2J_{u}+1}{2J_{d}+1} \frac{1}{(\omega_{J'J})^{2}} \frac{A_{J_{u}\to J_{d}}}{(\omega_{J'J})^{2}-\omega^{2}},$$

$$(7)$$

$$\omega_{J'J} = (E_{J'} - E_{J})/\hbar \qquad (8)$$

where I is the nuclear spin, J - total electronic

moment.

Further let us give characteristics of the used generalized energy approach [9-20] and relativistic perturbation theory with the zeroth approximation [21-32] to computing the atomic radiation and spectral parameters. Ac-

approximation [21-32] to computing the atomic radiation and spectral parameters. According to Ref. [11,22], the RMBPT zeroth order Hamiltonian of the Rydberg atomic system is as follows:

$$H_{0} = \sum_{i} \{ \alpha c p_{i} - \beta m c^{2} + [-Z/r_{i} + U_{MF}(r_{i} | b) + V_{XC}(r_{i})]$$
 (4)

where c is the velocity of light, α_i, α_j – the Dirac matrices, ω_{ij} –the transition frequency, Z is a charge of atomic nucleus. The general potential in (4) includes self-consistent Coulomb-like mean-field potential $U_{\rm MF}(r_i \vee b)$, ab ibitio one-particle exchange-correlation (relativistic generalized exchange Kohn-Sham potential plus generalized correlation potential) $V_{\rm XC}(r_i \vee b)$ with the gauge calibrated parameter b (it is determined within special relativistic procedure on the basis of relativistic energy approach (e.g. [1,2,21-26]).

The perturbation operator is as follows:

$$H^{PT} = \sum_{i>j} exp(i\omega_{ij}r_{ij}) \cdot \frac{(1-\alpha_i\alpha_j)}{r_{ij}} - \sum_{i} [U_{MF}(r_i) + V_{XC}(r_i \mid b)]$$
(5)

The multielectron interelectron exchange-correlation effects (the core polarization and screening effects, continuum pressure etc) are taken into consideration as the RMBPT second and higher orders contributions. The details of calculation of the corresponding matrix elements of the polarization and screening intere-

lectron interaction potentials are described in Refs. [9,22,33-38].

In order to calculate the values of A in (7) we use the known relativistic energy approach. Within it in the relativistic theory a radiation decay probability (ionization cross-section etc) is connected with the imaginary part of electron energy shift. The total energy shift of the state is usually presented in the form: $\Delta E = Re\Delta E + i \Gamma/2$, where Γ is interpreted as the level width, and a decay probability $P = \Gamma$. The imaginary part of electron energy shift is defined in the PT lowest order as:

Im
$$\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha > n > f \\ [\alpha < n \le f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}$$
 (6)

where $(\alpha > n > f)$ for electron and $(\alpha < n < f)$ for vacancy. The matrix element is determined as follows [23-25]:

$$V_{ijkl}^{|\omega|} = \iint dr_1 dr_2 \Psi_i^*(r_1) \Psi_j^*(r_2) \frac{\sin|\omega| r_{12}}{r_{12}} (1 - \alpha_1 \alpha_2) \Psi_k^*(r_2) \Psi_l^*(r_1)$$
(7)

Their detailed description of the matrix elements and procedure for their computing is presented in Refs. [20-25]. The relativistic wave functions are calculated by solution of the Dirac equation with the potential, which includes the Dirac-Fock consistent field potential and additionally polarization potential [1]. The detailed procedures of calculation of the radial and angular integrals (amplitudes) in the matrix elements are described in Refs. [1,2,23,24,29-38]. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

3. Results and conclusions

Until now, a considerable number of works have been used to calculate the Stark shift coefficient k (10^{-10} Hz/(V/m)²) and the BBR shift parameter β . Among the theoretical approaches used to calculate the specified parameters, various improved versions of the multi-particle relativistic PT method, taking

into account corrections up to higher PT orders, are repeatedly mentioned in this work. In table 1 there are presented the experimental and theoretical values of the Stark shift coefficient $k (10^{-10} \text{ Hz/(V/m)}^2)$ for transitions between components of the hyperfine structure of the ground state): Th1 – linearized coupled cluster method; Th2–the PT method with screened Coulomb interaction; Th3 is our RMBPT-DKS theory (see, e.g., [7,8,20]).

Table 1. The value of the Stark shift coefficient k (in 10⁻¹⁰ Hz/(V/m)²): Th1 – linearized curled-cluster method; Th2 –TK method (PTSCI); Th3 -our RMBPT-DKS theory (see text)

²³ Na	3s (F = 2)	Th1	-0.1285
	- F = 1	Th3	-0.126
		Exp	-0.124(3)
⁸⁷ Rb	5s (F = 2)	Th1	-1.272
	- F = 1	Th2	-1.240
		Th3	-1.226
		Exp	-1.23(3)
¹³³ Cs	6s (F = 2)	Th1	-2.271
	- F = 1	Th2	-2.260
		Th3	-2.245
		Exp1	-2.271(4)
		Exp2	-2.05(5)

The analysis of the presented data shows that, firstly, the theoretical results correlate reasonably well with each other. It is important to note that all theoretical calculations, as the most important component, include procedures for taking into account exchange-correlation corrections, although the classification of sought corrections and specific accounting schemes differ.

The method of connected clusters uses a standard methodology. It should be noted that in the PT method with screened Coulomb interaction (known as PTSCI), or the correlation potential method, the key approximation is the relativistic Hartree-Fock approximation using the correlation potential and random phase approximation. It should be noted that our method takes carefully into account such important factors as the implementation of a gauge invariance principle when calculating the corresponding matrix elements, the correct degree of consideration of complex exchange-correlation effects (primarily, the effect of polarization of the core). It is important to not too

that our method generates a fairly optimal onequasiparticle representation in within the limits of many-body relativistic PT with ab initio zeroth Dirac-Fock (Kohn-Sham) approximation.

In any case, the formalism developed in this work, as it follows from the given results, can be used for precise calculations of the Stark shift coefficient k, the BBR shift parameter β , and other parameters.

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Key words: Rydberg alkali atoms, relativistic theory, black-body radiation field.

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ТЕОРЕТИЧНЕ ДОСЛІДЖЕННЯ РІДБЕРГІВСЬКИХ ЛУЖНИХ АТОМНИХ СИСТЕМ У ПОЛІ ВИПРОМІНЮВАННЯ ЧОРНОГО ТІЛА: РЕЛЯТИВІСТСЬКИЙ ПІДХІД

Резюме. Наведено результати дослідження характеристик рідбергівських лужних атомних систем у полі чорнотільного (BBR; теплового) випромінювання, зокрема індукованого BBR коефіцієнта штарківського зсуву k. В якості теоретичного підходу застосовано комбінований узагальнений релятивістський енергетичний підхід і релятивістську багаточастинкову теорію збурень з ab initio нульовим наближенням Дірака. Застосування теорії для обчислення спектральних параметрів досліджуваних атомних систем продемонструвало фізично обгрунтовану узгодженість між теоретичними та експериментальними даними. Запропонований підхід ретельно враховує такі важливі чинники, як реалізація принципу калібрувальної інваріантності при розрахунку відповідних матричних елементів радіаційних переходів, атомних поляризованостей, врахування складних обмінно-кореляційних коректний ступінь (насамперед, ефекту поляризації атомного остову), а також генерує досить оптимальне одноквазічастинкове представлення в межах релятивістської багаточастинкової теорії збурень із оптимальним нульовим наближенням Дірака-Фока (Кона-Шема). Розвинутий метод може бути використаний для подальших обчислень індукованого BBR коефіцієнта штарківського зсуву, параметра зсуву BBR та інших характеристик атомів у BBR полі.

Ключові слова: рідбергівські лужні атоми, релятивістська теорія, чорнотільне теплове випромінювання.

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