Calculations of energies, matrix elements, polarizabilities and QED corrections for many-electron monovalent atoms and ions

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Introduction

In this study, we examine the applicability of the Dirac–Fock plus Core-Polarization (DFCP) method [1,2] to atomic characteristics calculations. We present results for static electric-dipole polarizability, the thermal Stark shift and the Bethe logarithm. The evaluation of these quantities requires summation over intermediate discrete states and integration over continuum states. While such summations can be carried out directly and with controlled convergence in exactly solvable systems (e.g., hydrogen-like atoms and ions), the situation becomes significantly more complex for many-electron atoms and ions due to the difficulty of reproducing the complete atomic spectrum.

The values of these quantities can be used in precision spectroscopy, in the development of atomic clocks, metrology, etc. The DFCP method is a semi-empirical approach based on the use of model potential (core polarization potential). We motivate the use of this method by the fact that it allows us to effectively combine the accuracy of calculations with the time required to calculate the characteristics of atoms.

In this paper, we present our version of this approach based on the use of a local version of the Dirac-Hartree-Fock potential [3]. Hereafter, we refer to such a method as LDFCP.

Method LDFCP

The stationary Dirac equation in the case of a central field $V(\mathbf{r})$ ($\hbar = c = 1$):

$$(-i\boldsymbol{\alpha}\cdot\nabla + \beta m + V(\mathbf{r}))\psi_n(\mathbf{r}) = \varepsilon_n\psi_n(\mathbf{r}). \tag{1}$$

Solution of equation:

$$\psi(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} g(r)\,\Omega_{\kappa m}(\mathbf{n}) \\ if(r)\,\Omega_{-\kappa m}(\mathbf{n}) \end{pmatrix}. \tag{2}$$

where $\kappa = l(l+1) - j(j+1) - \frac{1}{4}$.
The solution of the Dirac equation with a finite basis constructed with B splines [4] using the dual kinetic balance method, DKB [5]. Potential $V(r)$ is:

$$V(r) = V_{\rm LDF}(r) + V_{\rm CP}(r)\,, \tag{3}$$

where $V_{\rm LDF}(r)$ - the local version of the Dirac-Hartree-Fock potential [3]. $V_{\rm CP}(r)$ - the semi-empirical core polarization potential:

$$V_{\rm CP}(r) = -\frac{\alpha_c}{2\,r^4}\left(1 - e^{-r^6/\rho_\kappa^6}\right), \tag{4}$$

α_c - the static dipole polarizability of the core and ρ_κ - is the radial cutoff parameter, to be adjusted empirically (depends on l and j).

Li	Na	K	Rb	Cs	Fr
0.192486	0.9947	5.354	9.1	15.81	20.4

Table 1: Static core polarizability values used in this work, a.u. [6]

Polarizabilities

The polarizability of an atom can be considered as a measure of the response of the charge cloud to an external electric field.

Scalar polarizability:

$$\alpha_0 = \frac{2}{3(2j_a+1)}\sum_n \frac{|\langle a\|\mathbf{d}\|n\rangle|^2}{E_n - E_a} \tag{5}$$

Tensor polarizability:

$$\alpha_2 = 4\left(\frac{5j_a(2j_a-1)}{6(j_a+1)(2j_a+1)(2j_a+3)}\right)^{1/2}\sum_n (-1)^{j_a+j_n}\begin{Bmatrix} j_a & 1 & j_n \\ 1 & j_a & 2 \end{Bmatrix}\frac{|\langle a\|\mathbf{d}\|n\rangle|^2}{E_n - E_a} \tag{6}$$

Table 2: Scalar polarizability for alkali atoms, a.u. Blue values are from Ref. [6].

n	n^2S	$n^2P_{1/2}$	$n^2P_{3/2}$	$n^2D_{3/2}$	$n^2D_{5/2}$
			Li		
2	164.0	126.8	126.8		
	164.0	126.89	126.91		
3	4128.0	27466	27470	-14456	-14458
	4130.2	28239	28237	-14916	-14914
			Na		
3	161.6	360.5	362.1	6438.0	6413.0
	162.44	359.94	361.63	6419.7	6395.3
4	35336	262988	263020	4374090	4386700
	35281	27326	273230	4923700	4936000
			K		
3				1429	1415
				1422	1408
4	287.0	607.0	618.0	35897	35702
	290.25	602.1	612.7	35990	35810
			Rb		
4				586.0	553.0
				587.0	553.0
5	314.7	807.0	869.0	17806	17422
	318.28	805.0	868.0	18120	17740
			Cs		
5				-327.0	-423.0
				-328.0	-433.0
6	396.7	1307.0	1607.0	-7030	-9837
	399.57	1343	1655	-5620	-8330
			Fr		
6				-249.0	-584.0
				-259.0	-613.0
7	316.0	1173	2178	-1979	-9224
	316.3	1177	2213	-2500	-7420

Table 3: Tensor polarizability for alkali atoms, a.u. Blue values are from Ref. [6].

n	$n^2P_{3/2}$	$n^2D_{3/2}$	$n^2D_{5/2}$
		Li	
2	1.53		
	1.61		
3	-2087	11078	15828
	-2167	11400	16283
		Na	
3	-89.25	-3587	-5090
	-88.38	-3574.6	-5071.8
4	-174.8	-149169	-212575
	-167.7	-149260	-212740
		K	
3		-487.0	-678.0
		-484.0	-674.0
4	-111.7	-7775	-10908
	-108.7	-7810	-10960
		Rb	
4		-58.0	-35.0
		-59.0	-35.0
5	-169.1	-1205	-1086
	-166.6	-1310	-1240
		Cs	
5		346.0	649.0
		356.0	675.0
6	-260.0	9364	18425
	-262.0	8736	17290
		Fr	
6		235.0	863
		233.0	890
7	-454.0	4546	19882
	-453.9	4032	18480

Stark Shift of atomic level induced by Blackbody radiation

The effect of blackbody radiation field on an atom leads to a shift in the energy level (dynamic Stark effect) [7]:

$$\Delta E_a^{\rm BBR} = \frac{2}{3\pi\,(2j_a+1)}\sum_n \text{P.V.}\int_0^\infty d\omega n_\beta(\omega)\omega^3|\langle a|\boldsymbol{d}|n\rangle|^2\left[\frac{1}{E_n - E_a + \omega} + \frac{1}{E_n - E_a - \omega}\right] \tag{7}$$

where $n_\beta(\omega) = 1/[exp(\beta\omega) - 1]$ - Planck distribution, $\beta = 1/k_bT$ (k_b - Boltzmann constant, T - temperature), ω - the frequency of the thermal photon.

Table 4: Thermal Stark shifts at 300 K (Hz). , Blue values are from Ref. [7].

n	n^2S	$n^2P_{1/2}$	$n^2P_{3/2}$	$n^2D_{3/2}$	$n^2D_{5/2}$
			Li		
2	-1.41	-1.093	-1.094		
	-1.43	-1.145			
3	-38.1	46.56	46.57	-45.66	-45.64
	-38.62	50.80		-47.75	
			Na		
3	-1.388	-3.118	-3.133	-61.93	-61.95
	-1.389	-2.985	-2.998	-61.24	-61.25
4	-27.75	46.32	46.15	14.48	13.20
	-27.57	44.13	43.94	15.73	14.46
			K		
3				-13.03	-12.88
				-16.47	-16.30
4	-2.435	-5.251	-5.345	-160.5	-159.5
	-2.528	-5.370	-5.471	-171.9	-170.8
			Rb		
4				-5.088	-4.787
				-6.467	-6.975
5	-2.645	-7.004	-7.553	-166.5	-160.1
	-2.789	-7.511	-8.127	-188.7	-181.4
			Cs		
5				3.517	4.649
				5.497	5.315
6	-3.300	-11.98	-15.24	-65.64	-102.0
	-3.589	-14.85	-17.24	-70.41	-99.18
			Fr		
6				2.89	6.83
7	-2.558	-10.43	-21.51	-60.98	-144.3

The Bethe Logarithm

The contribution of intrinsic energy to the energy level shift can be estimated by calculating the Bethe logarithm for nonrelativistic systems. In the lowest order for a hydrogen-like atom in the s-state, the one-loop self-energy correction can be calculated using the following formula [8]:

$$\Delta E_a^{\rm SE} = \frac{4Z}{3}\alpha^3\left(\frac{19}{30} - 2\ln\alpha Z - \ln k_0\right)|\Psi(0)|^2 \tag{8}$$

$\ln k_0$ – the Bethe logarithm:

$$\ln k_0 = \frac{\sum_n |\langle a|\mathbf{d}|n\rangle|^2(E_n - E_a)^3\ln|E_n - E_a|}{\sum_n |\langle a|\mathbf{d}|n\rangle|^2(E_n - E_a)^3} \qquad \ln k_0 = \frac{\sum_n |\langle a|\mathbf{p}|n\rangle|^2(E_n - E_a)\ln|E_n - E_a|}{\sum_n |\langle a|\mathbf{p}|n\rangle|^2(E_n - E_a)} \tag{9}$$

in length and velocity guage respectively.

Table 5: Bethe logarithm for ground states atoms and ion

	Li (2s)	Be^+ (2s)	Na (3s)	K (4s)	Rb (5s)	Cs (6s)
			LDFCP (relativistic)			
	5.23	6.09	6.26	7.41	8.34	8.9
			LDF (non-relativistic)			
length	5.192	5.71	7.63321	8.65955	9.91856	10.6501
velocity	5.19211	5.70213	7.63317	8.65954	9.91856	10.6501
			local Kohn-Sham (non-relativistic)			
length	5.13128	5.673	7.6269	8.6596	9.91972	10.6516
velocity	5.13077	5.6693	7.62688	8.6595	9.91971	10.6516
			local CH (non-relativistic)			
length	5.187	5.72	7.64526	8.67203	9.92633	10.6562
velocity	5.18709	5.70948	7.64523	8.67202	9.92633	10.6562
	5.17817[9]	5.75167[10]	7.770[11]			

Conclusion and Discussion

- Method LDFCP provides us with a complete spectrum of the energies and wave functions of the effective one-particle Hamiltonian
- Calculated polarizabilities show good agreement with literature data
- It is assumed that our values of the thermal Stark shifts are more accurate
- The comparatively low computational and time costs of the LDFCP method
- The values of the Bethe logarithm within LDFCP cannot be considered reliable in relativistic calculations
- Applicable for precision atomic physics calculations

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