RELATIVISTIC CONFIGURATION-INTERACTION CALCULATION OF RELATIVISTIC RECOIL EFFECT FOR THE $^{2S+1}P_J - {}^1S_0$ TRANSITIONS IN LOW Z BERYLLIUMLIKE IONS

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Motivation and goals

- Test of QED in strong fields
- Study nuclear properties via electron structure of atom (ion)
- Astrophysical study of the fine-structure constant variation, isotopic abudance in the early Universe and astronimical objects, and so on

The main goal is to systematically study of the relativistic nuclear recoil effect for the $^{2S+1}P_J$ and $^1S_0$ states in 4 electron atomic systems

Method of calculation

- Relativistic recoil theory can be formulated only in the framework of QED [1]
- Within the Breit approximation MS Hamiltonian reads

$$\hat{H}_{\rm MS} = \hat{H}_{\rm NMS} + \hat{H}_{\rm RNMS} + \hat{H}_{\rm SMS} + \hat{H}_{\rm RSMS}$$

$$\hat{H}_{\rm NMS} = \frac{1}{2M}\sum_i \boldsymbol{p}_i^2 \qquad \hat{H}_{\rm SMS} = \frac{1}{2M}\sum_{i\neq j} \boldsymbol{p}_i\cdot\boldsymbol{p}_j$$

$$\hat{H}_{\rm RNMS} = -\frac{1}{2M}\sum_i \frac{\alpha Z}{r_i}\left[\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\right]\cdot\boldsymbol{p}_i$$

$$\hat{H}_{\rm RSMS} = -\frac{1}{2M}\sum_{i\neq j} \frac{\alpha Z}{r_i}\left[\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\right]\cdot\boldsymbol{p}_j$$

- Many-body perturbation theory combined with large-scale configuration interaction method in the basis of Dirac-Fock-Sturm orbitals (CI-DFS) [2]

$$\Psi = \sum_{n=1}^{\infty}\prod_{k=1}^{n} C_k a_k a_k^\dagger \Psi_{\rm DF}$$

- Extrapolation procedure in terms of $1/l^k$

Numerical details

The recoil correction of the first order in *m/M* is conveniently expressed in terms of the parameter *K*

$$\langle\Psi|\,\hat{H}_{\rm MS}\,|\Psi\rangle \equiv M/K$$

CI T+PT3 contribution to the K_{NMS}+ K_{RNMS} parameters for the ground state of Be-like Ne (Z = 10) in a.u. amu.

l_{max}	N = 10	N = 15	N = 20	N = 25	N → ∞
1	0.095970	0.096170	0.096201	0.096189	
2	0.093710	0.094187	0.094550	0.094787	
3	0.093429	0.094051	0.094467	0.094732	
4	0.093396	0.094032	0.094453	0.094721	
5	0.093384	0.094024	0.094448	0.094713	
∞	0.093373	0.094014(4)	0.094441(1)	0.094700(7)	0.09512(11)

Contributions to the $K_{\rm NMS}$+ $K_{\rm RNMS}$ parameters for the ground and singly excited states of Be-like Fe (Z = 26) in a.u. amu. In all 129 calculations.

$K_{\rm SMS}$ + $K_{\rm RSMS}$	$^1S_0$	$^3P_0$	$^3P_1$	$^3P_2$	$^1P_1$
PT2	5.51683(25)	–38.39854(22)	–38.47767(22)	–38.76400(23)	–38.54369(22)
PT3	–7.23167(78)	–0.09789(30)	–0.09613(30)	–0.09187(30)	–0.14727(21)
CI SD + PT3	3.0611(27)	0.00449(16)	0.00532(15)	0.00413(11)	0.01058(22)
CI SD	0.1383(19)	–0.00375(14)	–0.00352(11)	–0.00374(12)	–0.01015(72)
CI T + PT3	0.06403(3)	0.00041(1)	0.00047(3)	0.00038(3)	0.00329(7)
CI T	–0.0337(21)	0.00053(4)	0.00052(4)	0.00048(4)	0.00080(3)
CI Q + PT3	0.14302(6)	0.00002(0)	0.00002(2)	0.00001(1)	0.00005(1)
CI Q	–0.0578(9)	0.00000(1)	0.00001(1)	0.00001(1)	0.00005(3)
Total	1.2451(41)	–38.4947(4)	–38.5710(4)	–38.8546(4)	–38.6863(8)

Results

Energy (a.u.) and mass shift parameters (a.u. amu) for the ground state in the non-relativistic limit.

Z	E^{nr}	NMS^{nr}	$NMS - NMS^{nr}$	SMS^{nr}	$SMS - SMS^{nr}$
4	–14.66726(25)	14.66580(58)	–0.00199(82)	–0.46077(56)	0.00057(79)
	–14.66702 [3]	14.66671 [3]		–0.45991(40) [3]	
	–14.667356486 [4]			–0.460224(4) [7]	
6	–36.53489(13)	36.53589(32)	–0.00737(56)	–0.71431(66)	0.0034(10)
	–36.53458 [3]	36.53446 [3]		–0.71314(50) [3]	
	–36.534852338(35) [6]			–0.713671 [7]	
8	–68.41155(10)	68.41260(53)	–0.01788(70)	–0.9031(10)	0.0109(15)
	–68.41115 [3]	68.41085 [3]		–0.90194(50) [3]	
	–68.4115353 [7]			–0.902377 [7]	
10	–110.29064(9)	110.2920(7)	–0.03351(90)	–1.0290(14)	0.0269(17)
	–110.29018 [3]	110.2881 [3]		–1.0247(40) [3]	
	–110.2906495 [7]			–1.027164 [7]	

Mass shift parameter *K* for the $^{2S+1}P_J - {}^1S_0$ transitions energies in Be-like ions (Ghz amu).

Z	$^3P_0 - {}^1S_0$	$^3P_1 - {}^1S_0$	$^3P_2 - {}^1S_0$	$^1P_1 - {}^1S_0$
4	–1103(4)	–1103(5)	–1104(11)	–818(13)
6	–4348(6)	–4350(6)	–4352(8)	–4542(13)
	–4334 [8]	–4334 [8]	–4336 [8]	–4486 [8]
	–4313(7) [9]	–4314(7) [9]	–4314(7) [9]	–4451(80) [9]
8	–9634(6)	–9639(6)	–9646(6)	–10326(13)
	–9620 [8]	–9623 [8]	–9630 [8]	–10273 [8]
10	–16945(6)	–16957(6)	–16980(8)	–18138(13)
	–16929 [8]	–16939 [8]	–16962 [8]	–18079 [8]
12	–26289(14)	–26315(14)	–26372(14)	–27992(18)
	–26265 [8]	–26290 [8]	–26347 [8]	–27923 [8]
14	–37670(10)	–37723(10)	–37842(10)	–39904(14)
	–37638 [8]	–37689 [8]	–37808 [8]	–39823 [8]
16	–51102(11)	–51199(11)	–51421(12)	–53904(16)
	–51059 [8]	–51153 [8]	–51376 [8]	–53807 [8]
18	–66601(10)	–66761(10)	–67149(11)	–70019(15)
	–66543 [8]	–66700 [8]	–67087 [8]	–69904 [8]
20	–84183(12)	–84429(12)	–85062(13)	–88291(16)
	–84103 [8]	–84348 [8]	–84982 [8]	–88152 [8]
22	–103857(13)	–104215(13)	–105207(14)	–108757(17)
	–103753 [8]	–104110 [8]	–105104 [8]	–108590 [8]
24	–125627(15)	–126123(14)	–127619(15)	–131451(18)
	–125489 [8]	–125986 [8]	–127484 [8]	–131249 [8]
26	–149477(16)	–150138(16)	–152327(17)	–156402(19)
	–149297 [8]	–149959 [8]	–152156 [8]	–156135 [8]

Summary

- Systematic calculation of the recoil effect within the lowest relativistic correction for Be-like ions are performed. The basis set convergence and relativistic effects are studied.
- The most precise evaluations of the recoil effect within the Breit approximation have been performed for Be-like ions in the range 4 ≤ Z ≤ 26.
- The obtained non-relativistic values are in essential agreement with the most precise non-relativistic values, while we note some deviation with the relativistic data of work [8].

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