Relativistic Calculations of Higher-Order Electron-Correlation Corrections to the $2P_{1/2}$ — $2S_{1/2}$ Transition Energies for Lithium-Like Ions

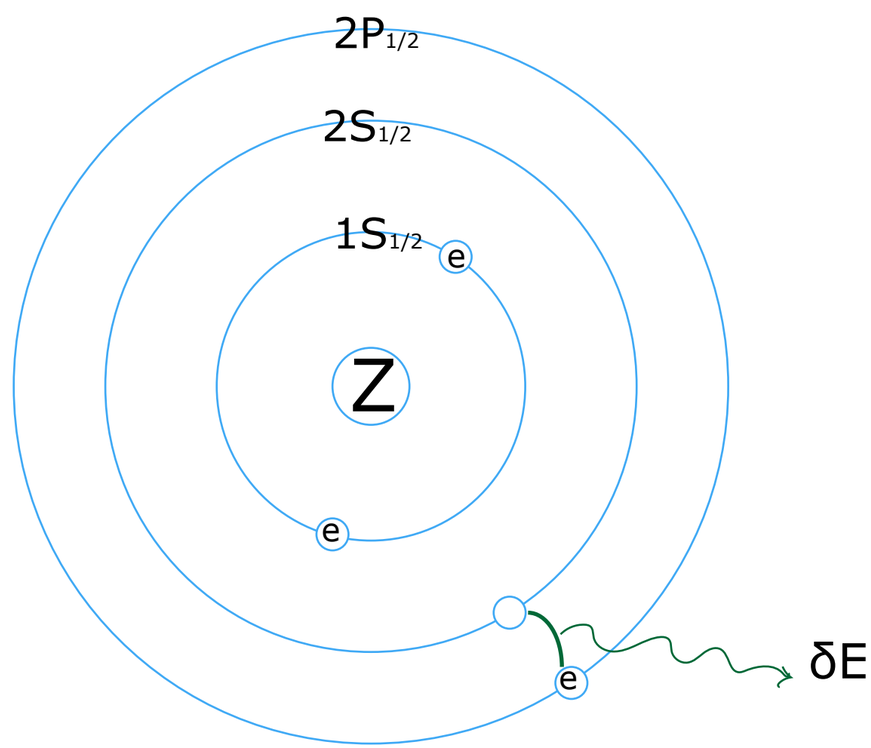
Mikhail Kaygorodov

st031727@student.spbu.ru

SPbU, 2017

Motivation

Consider Highly charged ion



Hydrogen-like problem was solved in 1925 by Schödinger

Several years after many-body quantum problem was studied

In 70's - 90's HCI studied experimentally (GSI, Darmstadt)

<u>Can be</u>
- produced for any Z
- stored for a long time
- measured with a high presicion

<u>Reasons</u>
- described theoretically
- test QED in the stronges fields

measure more precise than calculate

What is the main error in theoretical approach?

Breit Approximation

one photon exchange
from point of QED describes

$$I(w) = e^2 \alpha_1^\mu \alpha_2^\nu D_{\mu\nu}(\omega, \mathbf{r}_{12})$$

$$D_{\mu\nu}(\omega, \mathbf{r}_{12}) = -g_{\mu\nu} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\exp(i\mathbf{k}\cdot\mathbf{r}_{12})}{\omega^2 - \mathbf{k}^2 + i0}$$

Contribution to the E from diagrams can be calculated up to the second order rigorously but after no one still haven't managed how to calculate the diagrams

expand propagator in powers of ω and take limit $\omega \to 0$ one can derive a simplfied form of interaction and write it down as frequency independent Breit operator

$$\hat{H}^B = -\frac{1}{2} \sum_{i \neq j} \frac{2\boldsymbol{\alpha}_i \boldsymbol{\alpha}_j}{r_{ij}} + \left[\frac{(\boldsymbol{\alpha}_i \boldsymbol{r}_{ij}) \cdot (\boldsymbol{\alpha}_j \boldsymbol{r}_{ij})}{r_{ij}^3} - \frac{\boldsymbol{\alpha}_i \boldsymbol{\alpha}_j}{r_{ij}} \right]$$

it accounts retardation effects to the first order in αZ

Dirac-Coulomb-Breit Hamiltonian

$$\hat{H} = \hat{H}^D + \hat{H}^C + \hat{H}^B \tag{1}$$

$$\hat{H}^D = \sum_i \hat{h}_i^D \qquad \hat{h}^{\mathrm{D}} = c(\boldsymbol{\alpha} \cdot \boldsymbol{p}) + (\beta - 1)c^2 + V(\boldsymbol{r}) \tag{2}$$

$$\hat{H}^C = \frac{1}{2} \sum_{i \neq j} \frac{1}{|r_i - r_j|} \tag{3}$$

$$\hat{H}^B = -\frac{1}{2} \sum_{i \neq j} \frac{2\boldsymbol{\alpha}_i \boldsymbol{\alpha}_j}{r_{ij}} + \left[\frac{(\boldsymbol{\alpha}_i \boldsymbol{r}_{ij}) \cdot (\boldsymbol{\alpha}_j \boldsymbol{r}_{ij})}{r_{ij}^3} - \frac{\boldsymbol{\alpha}_i \boldsymbol{\alpha}_j}{r_{ij}} \right] \tag{4}$$

$$\hat{H}_{\mathrm{np}} = \Lambda_+ \hat{H} \Lambda_+ \tag{5}$$

Many-body wave function

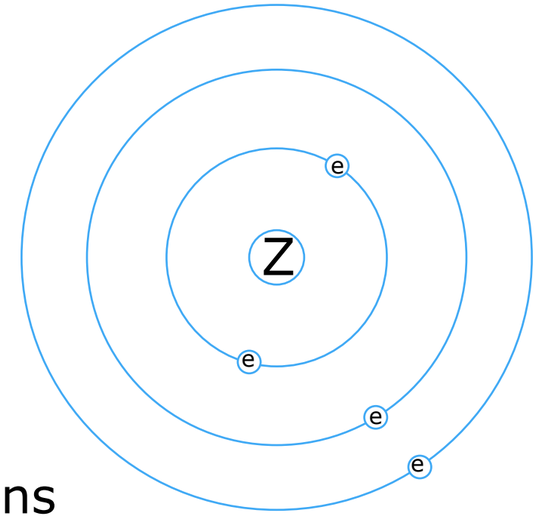
Wave function must be antisymmetric

We can solve problem for hydrogen atom (single electron)

obtain one particle wave functions φ_i

construct many-body wave function as Slater determinant

$$\Phi_{HF} = \det \varphi_i$$



but electrons in this approximation are not correlated

and we need to take into account a collective behaviour of electrons

We need to go beyond one-particle approximation

Configuration interaction(CI)

Let $\{\tilde{\varphi}_i\}_{i=1}^{M}$ be a set of virtual orbitals, where $M >> N_e$

$$\Psi_{\mathrm{CI}} = \Phi_{\mathrm{HF}} + \sum_{i,a} c_i^a \det\{\varphi_1, \varphi_2, \ldots, \underset{\text{i-th}}{\tilde{\varphi}_a}, \ldots, \varphi_N\} + \sum_{i,j,a,b} c_{i,j}^{a,b} \det\{\varphi_1, \ldots, \underset{\text{i-th}}{\tilde{\varphi}_a}, \ldots, \underset{\text{j-th}}{\tilde{\varphi}_b}, \ldots, \varphi_N\} + \ \ldots$$

single excitations(CIS) double excitations(CISD)

Applying variational principle we obtain a following matrix problem for coefficients c

$$\mathbf{HC} = E\mathbf{C},$$

where

$$H_{\alpha\beta} = < \alpha | \hat{H} | \beta >$$

Hamiltonian matrix has incredible size even in CI, but we cheated and built $\{\tilde{\varphi}_i\}$ with special properties which leads to sparce form of matrix H

But we do not need E! The problem was with higher-order corrections!

How to extract them?

Perturbation theory by interelectronic-interaction

Imbed parameter λ into $\hat{H}$ to separate terms of different orders in 1/Z

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda(\hat{H}^{\mathrm{D}} - \hat{H}_0) + \lambda \frac{1}{2} \sum_{i \neq j} u_{ij} \qquad \hat{H}(\lambda = 1) = \hat{H}$$

For small λ the total E can be expanded in powers of λ

$$E(\lambda) =< \Psi(\lambda)|\hat{H}(\lambda)|\Psi(\lambda) >= \sum_n \lambda^n \varepsilon^{(n)}$$

$$\varepsilon^{(n)} = \frac{1}{n!} \frac{d^n}{d\lambda^n} E(\lambda)\Big|_{\lambda=0}$$

Then the higher-order contribution is calculated as

$$\varepsilon^{3+} = E(\lambda = 1) - \varepsilon^{(0)} - \varepsilon^{(1)} - \varepsilon^{(2)}$$

$1s^2 2p_{1/2}$ — $1s^2 2s_{1/2}$ Transition energy for Z=30

L_{max}	δE, eV
SD, n = 15	
2	58.147183
3	-0.021012
4	-0.005176
5	-0.001857
6	-0.000850
7	-0.000434
8	-0.000220
9	-0.000094
≥ 10	-0.000077
SD, n = 20	
2	0.077651
3	-0.000056
4	-0.000029
5	-0.000010
≥ 6	-0.000010
T, n = 20	
2	-0.002139
3	-0.000070
≥ 4	-0.000050
SD, n = 25	
2	0.018681
3	-0.000012
4	-0.000007
SD, n = 30	
2	0.005029
SD, n $\to \infty$	
2	0.001355
SUM	58.2146
Kozhedub 2010	58.2135(3)(1)
Yerokhin 2007	58.2152

*include 1ph & 2ph QED

L_{max}	δE, eV
SD, n = 15	
2	-0.063396
3	0.003134
4	0.000926
5	0.000374
6	0.000184
7	0.000104
8	0.000060
9	0.000033
≥ 10	0.000027
SD, n = 20	
2	0.021714
3	-0.000004
4	-0.000003
5	0.000003
≥ 6	0.000001
T, n = 20	
2	-0.002139
3	-0.001310
≥ 4	-0.001128
SD, n = 25	
2	0.006682
3	-0.000002
4	0.000001
SD, n = 30	
2	0.005033
SD, n $\to \infty$	
2	0.000454
SUM	-0.0293
Kozhedub 2010	-0.0296(3)(1)
Yerokhin 2007	-0.0278

*3rd-order only

Thank you!