Model operator approach to calculations of the Lamb shifts in relativistic many-electron atoms

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in collaboration with

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Outline of the talk

- Introduction
- Perturbation theory for the QED calculations in the Furry picture
- Schrödinger-like equation for a relativistic atom in the framework of QED
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- Calculations with the model self-energy operator in many-electron systems
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Introduction

Quantum electrodynamics in the external field approximation
(Furry picture of QED)

High-Z few-electron ions

$$N \ll Z\,,$$

where Z is the nuclear charge number and N is the number of electrons.

To zeroth-order approximation:

$$(-i\,\vec{\alpha}\,\vec{\nabla} + m\beta + V_{\rm C}(r)\,)\,\psi\,(\vec{r}) = \varepsilon\,\psi\,(\vec{r})$$

Interelectronic-interaction and QED effects:

$$\frac{\text{Interelectronic interaction}}{\text{Binding energy}} \sim \frac{1}{Z}\,, \qquad \frac{\text{QED}}{\text{Binding energy}} \sim \alpha(\alpha Z)^2\,.$$

In uranium: $Z = 92$, $\alpha Z \approx 0.7$.

Introduction

Relativistic many-electron atoms and ions

The interelectronic interaction is not small and must be taken into account at the zero-order level:

$$V_{\rm C} \to V_{\rm eff} = V_{\rm C} + V_{\rm scr}\,,$$

where $V_{\rm scr}$ describes approximately the electron-electron interaction effects. Therefore, to zeroth order:

$$(-i\,\vec{\alpha}\,\vec{\nabla} + m\beta + V_{\rm eff}(r)\,)\,\psi\,(\vec{r}) = \varepsilon\,\psi\,(\vec{r})$$

In higher orders, besides the interelectronic-interaction and QED effects, one must add the interaction with $-V_{\rm scr}$.

Green function

Standard (2N-time) QED Green function for an N-electron atom:

$$G(x'_1,\ldots x'_N;x_1,\ldots x_N)=\langle 0|T\psi(x'_1)\cdots\psi(x'_N)\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle\,,$$

where $x=(t,\mathbf{x})$, $\psi(x)$ is the electron-positron field operator in the Heisenberg representation, and $\overline{\psi}(x)=\psi^\dagger\gamma^0$.
In the interaction representation:

$$G(x'_1,\ldots x'_N;x_1,\ldots x_N)$$
$$=\frac{\langle 0|T\psi_{\rm in}(x'_1)\cdots\psi_{\rm in}(x'_N)\overline{\psi}_{\rm in}(x_N)\cdots\overline{\psi}_{\rm in}(x_1)\exp\{-i\int d^4z\,\mathcal{H}_I(z)\}|0\rangle}{\langle 0|T\exp\{-i\int d^4z\,\mathcal{H}_I(z)\}|0\rangle}\,,$$

where

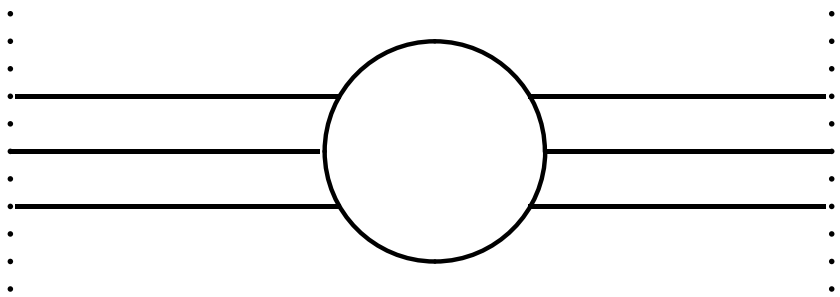
$$\mathcal{H}_I(x)=\frac{e}{2}\,[\overline{\psi}_{\rm in}(x)\gamma_\mu,\psi_{\rm in}(x)]A^\mu_{\rm in}(x)-\frac{\delta m}{2}\,[\overline{\psi}_{\rm in}(x),\psi_{\rm in}(x)]$$

is the interaction Hamiltonian.

Two-time Green function

We introduce the two-time Green function:

$$\widetilde{G}(t',t) \equiv G(t'_1 = t'_2 = \cdots t'_N \equiv t'; t_1 = t_2 = \cdots t_N \equiv t)$$



$t'_1 = t'_2 = \cdots = t'_N \equiv t'$ $\qquad$ $t_1 = t_2 = \cdots = t_N \equiv t$

The Fourier transform:

$$\mathcal{G}(E)\delta(E-E') = \frac{1}{2\pi i}\frac{1}{N!}\int_{-\infty}^{\infty} dt\, dt' \;\exp\left(iE't' - iEt\right)\widetilde{G}(t',t)\,.$$

Perturbation theory for quasidegenerate levels

We consider s degenerate or quasidegenerate states.
The projector on the unperturbed states:

$$P^{(0)} = \sum_{k=1}^{s} P_k^{(0)} = \sum_{k=1}^{s} u_k u_k^\dagger \, .$$

We project $\mathcal{G}(E)$ on the space $\Omega_s^{(0)}$ formed by the s unperturbed states:

$$g(E) = P^{(0)} \mathcal{G}(E) P^{(0)} \, .$$

We consider a contour Γ in the complex E plane:

Perturbation theory for quasidegenerate levels

We introduce operators K and P by

$$K \equiv \frac{1}{2\pi i} \oint_\Gamma dE\; E g(E)\,, \qquad P \equiv \frac{1}{2\pi i} \oint_\Gamma dE\; g(E)\,.$$

The energies and the wavefunctions are determined from the equations:

$$K v_k = E_k P v_k\,, \qquad v_{k'}^\dagger P v_k = \delta_{k'k}$$

The solvability condition yields:

$$\det\left(K - EP\right) = 0\,.$$

Schrödinger-like equation for a relativistic atom

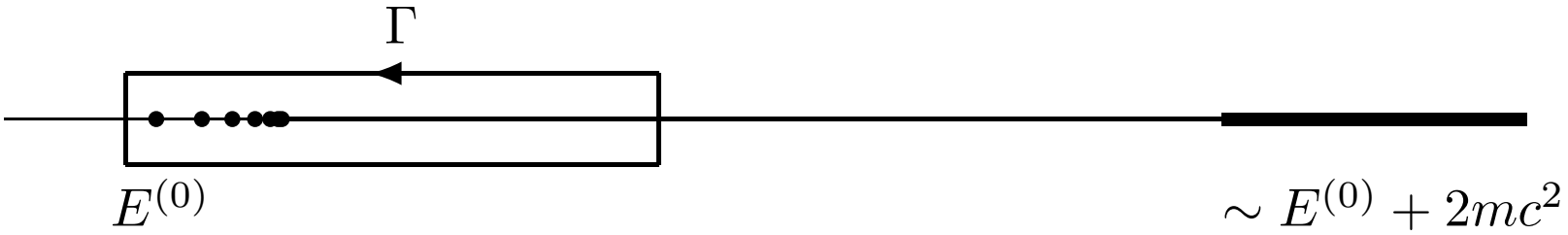
These equations can be transformed to the Schrödinger-like equation:

$$H\psi_k = E_k\psi_k\,, \qquad \psi_k^\dagger\psi_{k'} = \delta_{kk'}\,,$$

where $H \equiv P^{-\frac{1}{2}}\,K\,P^{-\frac{1}{2}}$ and $\psi_k \equiv P^{\frac{1}{2}}v_k$. The energy levels are determined from the equation:

$$\det(H - E) = 0\,.$$

The space of the quasidegenerate states can be extended to the space $\Omega_+^{(0)}$ that includes all positive-energy states whose energies are smaller than the pair-creation threashold:



In this picture the photon spectra are omitted.

Schrödinger-like equation for a relativistic atom

The operators K and P are constructed by perturbation theory:

$$\begin{aligned} K &= K^{(0)} + K^{(1)} + K^{(2)} + \cdots , \\ P &= P^{(0)} + P^{(1)} + P^{(2)} + \cdots . \end{aligned}$$

The operator H is

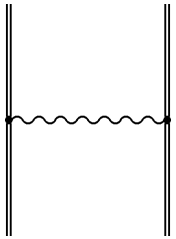
$$H = H^{(0)} + H^{(1)} + H^{(2)} + \cdots ,$$

where

$$\begin{aligned} H^{(0)} &= K^{(0)} , \\ H^{(1)} &= K^{(1)} - \frac{1}{2} P^{(1)} K^{(0)} - \frac{1}{2} K^{(0)} P^{(1)} , \\ H^{(2)} &= K^{(2)} - \frac{1}{2} P^{(2)} K^{(0)} - \frac{1}{2} K^{(0)} P^{(2)} - \frac{1}{2} P^{(1)} K^{(1)} - \frac{1}{2} K^{(1)} P^{(1)} \\ &\quad + \frac{3}{8} P^{(1)} P^{(1)} K^{(0)} + \frac{3}{8} K^{(0)} P^{(1)} P^{(1)} + \frac{1}{4} P^{(1)} K^{(0)} P^{(1)} . \end{aligned}$$

Interelectronic-interaction operator

One-photon exchange contribution to the Hamiltonian H:



In the space $\Omega_+^{(0)}$ we get

$$h^{\rm int} = \sum_{i\neq j,k\neq l}^{(\varepsilon_i,\varepsilon_j,\varepsilon_k,\varepsilon_l>0)} |\psi_i\psi_j\rangle\langle\psi_i\psi_j|\frac{1}{2}[I(\varepsilon_i-\varepsilon_k)+I(\varepsilon_j-\varepsilon_l)]|\psi_k\psi_l\rangle\langle\psi_k\psi_l|\,,$$

where

$$I(\omega) = e^2\alpha^\rho\alpha^\sigma D_{\rho\sigma}(\omega)\,,$$

$\alpha^\rho \equiv \gamma^0\gamma^\rho = (1,\boldsymbol{\alpha})$, $D_{\rho\sigma}(\omega)$ is the photon propagator, and ε_i is the one-electron Dirac energy.

Dirac-Coulomb-Breit Hamiltonian

Taking $h^{\rm int}$ in the Coulomb gauge at zero energy transfer ($\omega = \varepsilon_i - \varepsilon_k = 0$) and summing over atomic electrons leads to the Dirac-Coulomb-Breit Hamiltonian:

$$H = \Lambda^{(+)}\Big[\sum_i h_i^{\rm D} + \sum_{i<j}(V_{ij}^{\rm C} + V_{ij}^{\rm B})\Big]\Lambda^{(+)}\,,$$

where $\Lambda^{(+)}$ is the projector on the positive-energy states,

$$h_i^{\rm D} = \vec{\alpha}_i\cdot\vec{p}_i + m\beta_i + V_{\rm C}(r_i)\,, \quad V_{\rm C}(r) = -\frac{\alpha Z}{r}\,,$$

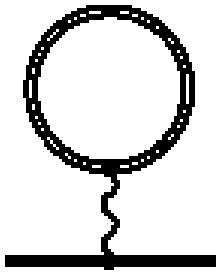
$$V_{ij}^{\rm C} = \frac{\alpha}{r_{ij}}\,, \qquad V_{ij}^{\rm B} = -\alpha\left[\frac{\vec{\alpha}_i\cdot\vec{\alpha}_j}{r_{ij}} + \frac{1}{2}(\vec{\nabla}_i\cdot\vec{\alpha}_i)(\vec{\nabla}_j\cdot\vec{\alpha}_j)r_{ij}\right].$$

To account for the nonzero energy transfer, one should simply replace $V_{ij}^{\rm C} + V_{ij}^{\rm B}$ by the interelectronic-interaction operator $h^{\rm int}$ derived above.

In the Feynman gauge, to get the Hamiltonian to the same accuracy, one has to account for the higher-order photon exchange diagrams.

Lamb shift operator for a relativistic atom

The QED contributions to the Hamiltonian H:



$$
\begin{aligned}
h^{\rm QED} &= h^{\rm SE} + h^{\rm VP} \\
&= \sum_{i,k}^{(\varepsilon_i,\varepsilon_k>0)} |\psi_i\rangle\langle\psi_i| \big[\frac{1}{2}(\Sigma^{\rm SE}(\varepsilon_i) + \Sigma^{\rm SE}(\varepsilon_k)) + V^{\rm VP}\big] |\psi_k\rangle\langle\psi_k| \,,
\end{aligned}
$$

where $\Sigma^{\rm SE}(\varepsilon_i)$ and $V^{\rm VP}$ are the renormalized self-energy (SE) and vacuum-polarization (VP) operators, respectively.

Details of the two-time Green function method and the derivation of these formulas can be found in *[V.M. Shabaev, Phys. Rep., 2002; JPB, 1993]*.

Lamb shift operator for a relativistic atom

The dominant part of the VP contribution is represented by the Uehling potential:

$$V_{\rm Uehl}(r) = -\alpha Z \frac{2\alpha\hbar^2}{3\pi} \int_0^\infty dr'\, 4\pi r' \rho(r') \int_1^\infty dt\, (1+\frac{1}{2t^2}) \frac{\sqrt{t^2-1}}{t^2} \times \frac{[\exp(-2m(c/\hbar)|r-r'|t) - \exp(-2m(c/\hbar)(r+r')t)]}{4mrt},$$

where α is the fine structure constant and $|e|Z\rho(r)$ is the density of the nuclear charge distribution ($\int \rho(r) d\mathbf{r} = 1$).

Evaluation of the remaining Wichmann-Kroll potential is a much more difficult problem *[G. Soff and P.J. Mohr, PRA, 1988; N.L. Manakov et al., JETP, 1989]*. To a good accuracy, it can be calculated with the help of the approximate formulas derived in *[A.G. Fainshten et al., JPB, 1991].*

Model self-energy operator for a relativistic atom

Let us now consider the SE operator:

$$h^{\rm SE} = \sum_{i,k}^{(\varepsilon_i,\varepsilon_k>0)} |\psi_i\rangle\langle\psi_i| \frac{1}{2}[\Sigma^{\rm SE}(\varepsilon_i) + \Sigma^{\rm SE}(\varepsilon_k)] |\psi_k\rangle\langle\psi_k| \,.$$

We represent $h^{\rm SE}$ as a sum of local and nonlocal parts. The local part is given by

$$V^{\rm SE}_{\rm loc} = \sum_\kappa A_\kappa \exp\left(-r/\lambda_{\rm C}\right) P_\kappa \,,$$

where P_κ is the projector on the states with the given value of $\kappa = (-1)^{j+l+1/2}(j+1/2)$, the constant A_κ is chosen to reproduce the SE shift for the lowest energy level at the given κ in the corresponding H-like ion, and $\lambda_{\rm C} = \hbar/(mc)$.

Model self-energy operator for a relativistic atom

We restrict the active space of the remaining SE operator, $h^{\rm SE} - V^{\rm SE}_{\rm loc}$, to to the basis functions $\{\phi_i(\mathbf{r})\}_{i=1}^n$ which, having the same angular parts as the H-like functions $\{\psi_i(\mathbf{r})\}_{i=1}^n$, are localized at smaller distances. With these functions, we approximate the one-electron SE operator as follows

$$h^{\rm SE} = V^{\rm SE}_{\rm loc} + \sum_{i,k=1}^{n} |\phi_i\rangle B_{ik} \langle\phi_k| \,,$$

where the matrix B_{ik} has to be determined to reproduce the diagonal and non-diagonal SE corrections with the H-like wave functions. This leads to the equations

$$\sum_{j,l=1}^{n} \langle\psi_i|\phi_j\rangle B_{jl} \langle\phi_l|\psi_k\rangle$$

$$= \langle\psi_i| \big[\frac{1}{2}(\Sigma(\varepsilon_i) + \Sigma(\varepsilon_k)) - V^{\rm SE}_{\rm loc}\big] |\psi_k\rangle \,.$$

Model self-energy operator for a relativistic atom

Now let us consider the choice of the functions $\{\phi_i(\mathbf{r})\}_{i=1}^{n}$. We construct them using the H-like wave functions multiplied with the factor

$$\rho_l(r) = \exp\left(-2\alpha Z(r/\lambda_{\rm C})/(1+l)\right),$$

where $l = |\kappa + 1/2| - 1/2$ is the orbital angular momentum of the state under consideration.
In what follows, we restrict the basis functions by ns, $np_{1/2}$, $np_{3/2}$, $nd_{3/2}$, and $nd_{5/2}$ states with the principal quantum number $n \leq 3$ for the s states and $n \leq 4$ for the p and d states, and put

$$\phi_i(\mathbf{r}) = \frac{1}{2}(I - (-1)^{s_i}\beta)\rho_{l_i}(r)\psi_i(\mathbf{r})\,,$$

where I is the identity matrix, β is the standard Dirac matrix, the index $s_i = n_i - l_i$ enumerates the positive energy states at the given κ, and n_i is the principal quantum number.

Model self-energy operator for a relativistic atom

Thus, the model SE operator is given by

$$
\begin{aligned}
h^{\rm SE} &= V^{\rm SE}_{\rm loc} + \frac{1}{4}\sum_{i,k}\sum_{j,l}(I-(-1)^{s_i}\beta)\rho_{l_i}(r)|\psi_i\rangle \\
&\quad\times((D^t)^{-1})_{ij}\langle\psi_j|\big[\frac{1}{2}(\Sigma(\varepsilon_j)+\Sigma(\varepsilon_l)) - V^{\rm SE}_{\rm loc}\big]|\psi_l\rangle \\
&\quad\times(D^{-1})_{lk}\langle\psi_k|\rho_{l_k}(r)(I-(-1)^{s_k}\beta),
\end{aligned}
$$

where the summations run over ns states with the principal quantum number $n \leq 3$ and over $np_{1/2}$, $np_{3/2}$, $nd_{3/2}$, and $nd_{5/2}$ states with $n \leq 4$,

$$
\begin{aligned}
\rho_{l_i}(r) &= \exp\left(-2\alpha Z(r/\lambda_{\rm C})/(1+l_i)\right), \\
D_{ik} &= \frac{1}{2}\langle\psi_i|(I-(-1)^{s_i}\beta)\rho_{l_i}(r)|\psi_k\rangle\,,
\end{aligned}
$$

and $s_i = n_i - l_i$.

Self-energy matrix elements with H-like wave functions

To complete the construction of the model SE operator, one needs to evaluate the matrix elements $\Sigma_{ik} \equiv \langle\psi_i|\frac{1}{2}(\Sigma(\varepsilon_i)+\Sigma(\varepsilon_k))|\psi_k\rangle$ with the H-like wave functions. To perform such calculations we used the method described in *[V.A. Yerokhin and V.M. Shabaev, PRA, 1999; V.A. Yerokhin, K. Pachucki, and V.M. Shabaev, PRA, 2005]*. The results of the calculations are conveniently expressed in terms of the function $F_{ik}(\alpha Z)$ defined by

$$\Sigma_{ik} \equiv \langle\psi_i|\frac{1}{2}[\Sigma(\varepsilon_i)+\Sigma(\varepsilon_k)]|\psi_k\rangle = \frac{\alpha}{\pi}\frac{(\alpha Z)^4}{(n_i n_k)^{3/2}}F_{ik}(\alpha Z)mc^2\,,$$

where n_i and n_k are the principal quantum numbers of the i and k states, respectively. For the diagonal matrix elements, these results are in a good agreement with the calculations performed in *[P.J. Mohr, PRA, 1992; P.J. Mohr and Y.-K. Kim, PRA, 1992; T. Beier, P.J. Mohr, H. Persson, and G. Soff, PRA, 1998]*.

Self-energy matrix elements with H-like wave functions

Self-energy matrix elements $F_{ik}(\alpha Z)$, defined by

$\Sigma_{ik} \equiv \langle\psi_i|\frac{1}{2}[\Sigma(\varepsilon_i)+\Sigma(\varepsilon_k)]|\psi_k\rangle = \frac{\alpha}{\pi}\frac{(\alpha Z)^4}{(n_i n_k)^{3/2}} F_{ik}(\alpha Z) mc^2$, with H-like wave functions for extended nuclei.

Z	$F_{1s\,1s}$	$F_{2s\,2s}$	$F_{3s\,3s}$	$F_{1s\,2s}$	$F_{1s\,3s}$	$F_{2s\,3s}$
10	4.6542	4.8944	4.9524	4.7961	4.8145	4.9325
30	2.5518	2.8386	2.8937	2.7084	2.7235	2.8748
60	1.6820	2.0923	2.1410	1.8795	1.8886	2.1242
90	1.4721	2.1431	2.1702	1.7615	1.7607	2.1625
120	1.7335	3.1256	3.0295	2.2753	2.2294	3.1125

Calculations with the model SE operator

To demonstrate the efficiency of the method, we applied it to calculations of the Lamb shifts in neutral alkali metals, Cu-like ions, superheavy atoms, and Li-like ions.

Ab initio calculations of the Lamb shift in alkali metals were performed *[J. Sapirstein and K.T. Cheng, PRA, 2002]* in the potential $U(r)$:

$$V(r) = -\frac{\alpha Z_{\rm eff}(r)}{r}\,,$$

where

$$Z_{\rm eff}(r) = Z_{\rm nuc}(r) - r\int_0^\infty dr'\,\frac{1}{r_>}\rho_{\rm t}(r') + x_\alpha\left[\frac{81}{32\pi^2}r\rho_{\rm t}\right]^{1/3}$$

and $\rho_{\rm t} = \rho_{\rm v} + \rho_{\rm c}$ is total (valence plus core) electron charge density. The choice $x_\alpha = 0$ corresponds to the Dirac-Hartree potential, $x_\alpha = 2/3$ gives the Kohn-Sham potential, and $x_\alpha = 1$ is the Dirac-Slater potential.

Self energy in neutral alkali metals

Self-energy function $F(\alpha Z)$, defined by $\Delta E^{\rm SE} = \frac{\alpha}{\pi}\frac{(\alpha Z)^4}{n^3}F(\alpha Z)mc^2$, for neutral alkali metals in different potentials.

Atom	Method	$x_\alpha = 0$	$x_\alpha = 1/3$	$x_\alpha = 2/3$	$x_\alpha = 1$
Na $3s_{1/2}$	$\langle v\|V_{\rm loc}^{\rm SE}\|v\rangle$	0.166	0.163	0.176	0.214
	$\langle v\|H^{\rm SE}\|v\rangle$	0.170	0.168	0.183	0.224
	Exact[a]	0.169	0.167	0.181	0.223
Rb $5s_{1/2}$	$\langle v\|V_{\rm loc}^{\rm SE}\|v\rangle$	0.0187	0.0193	0.0230	0.0320
	$\langle v\|H^{\rm SE}\|v\rangle$	0.0229	0.0237	0.0284	0.0397
	Exact[a]	0.0228	0.0236	0.0283	0.0396
Fr $7s_{1/2}$	$\langle v\|V_{\rm loc}^{\rm SE}\|v\rangle$	0.0047	0.0052	0.0067	0.0102
	$\langle v\|H^{\rm SE}\|v\rangle$	0.0069	0.0076	0.0099	0.0151
	Exact[a]	0.0068	0.0075	0.0098	0.0150

[a] *J. Sapirstein and K.T. Cheng, PRA, 2002.*

Self energy in Cu-like ions

Self-energy contribution to the $4s - 4p_{1/2}$ and $4s - 4p_{3/2}$ transition energies in Cu-like ions, in eV.

Ion	Transition	Model SE operator	Exact[a]
Yb^{41+}	$4s - 4p_{1/2}$	-1.29	-1.28
	$4s - 4p_{3/2}$	-1.21	-1.21
	$4p_{1/2} - 4d_{3/2}$	-0.10	-0.11
	$4p_{3/2} - 4d_{3/2}$	-0.18	-0.18
	$4p_{3/2} - 4d_{5/2}$	-0.14	-0.14
U^{63+}	$4s - 4p_{1/2}$	-4.24	-4.24
	$4s - 4p_{3/2}$	-4.32	-4.33
	$4p_{1/2} - 4d_{3/2}$	-0.87	-0.88
	$4p_{3/2} - 4d_{3/2}$	-0.79	-0.79
	$4p_{3/2} - 4d_{5/2}$	-0.63	-0.65

[a] *J. Sapirstein and K.T. Cheng, PRA, 2002.*

Self energy in superheavy atoms

Self-energy contribution to the binding energy of the valence electrons in Rg and Cn, in eV. In this work, the perturbation theory (PT) value is obtained by averaging the model SE potential with the Dirac-Fock wave function of the valence electron, while the DF value is obtained by including this potential into the DF equations.

Atom	Valence electron	Method	This work	*I. Goidenko, EPJD, 2009*	Other works
Rg	$7s$	PT	-0.088	-0.089	-0.087[a]
		DF	-0.105	-0.102	
		Welton meth.			-0.084[b]
		Local SE pot.			-0.089[c]
Cn	$7s$	PT	-0.101	-0.103	
		DF	-0.105	-0.110	

[a] *L. Labzowsky et al., PRA, 1999;* [b] *P. Indelicato et al., EPJD, 2007;*

[c] *C. Thierfelder and P. Schwerdtfeger, PRA, 2010.*

Screened self energy in Li-like ions

Screened self energy for the $2s$, $2p_{1/2}$, and $2p_{3/2}$ states of Li-like ions, in eV. The Kohn-Sham (KS) and Dirac-Fock (DF) results are obtained using the model SE potential approach.

Z	State	KS	DF	PT[a]	PT[b]
20	$2s$	-0.047	-0.045	-0.044	-0.046
	$2p_{1/2}$	-0.009	-0.008	-0.008	-0.008
	$2p_{3/2}$	-0.012	-0.011	-0.013	-0.013
50	$2s$	-0.50	-0.49	-0.48	
	$2p_{1/2}$	-0.13	-0.12	-0.12	
	$2p_{3/2}$	-0.14	-0.14	-0.16	
83	$2s$	-2.35	-2.25	-2.32	-2.26
	$2p_{1/2}$	-0.97	-0.98	-1.07	-1.07
	$2p_{3/2}$	-0.65	-0.61	-0.75	-0.76

[a] *Y.S. Kozhedub et al., PRA, 2010;* [b] *J. Sapirstein and K.T. Cheng, PRA, 2011.*

Conclusion

- Schrödinger-like equation for a relativistic many-electron atom can be derived from the first principles of QED by the two-time Green function method.
- The QED contribution can be approximated by a model operator, which provides a very simple and efficient tool for evaluation of the Lamb shifts in many-electron atoms and ions [V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, Phys. Rev. A 88, 012513 (2013)].