Flambaum-Ginges Radiative Potential method

Radiative QED corrections can be included into the atomic wavefunctions using the Flambdaum-Ginges radiative potential method developed in Ref. [1]; we also include the (small) finite nuclear size corrections [2, 3]. In this method, an effective potential, $V_{\rm rad}$, is added to the Hamiltonian before the equations are solved. The potential can be written as the sum of the Uehling (vacuum polarisation) and self-energy potentials, see Fig. 1. The self-energy potential itself is written as the sum of the high- and low-frequency electric contributions, and the magnetic contribution:

$$V_{\rm rad}(\boldsymbol{r}) = V_{\rm Ueh}(r) + V^h_{\rm SE}(r) + V^l_{\rm SE}(r) + V^{\rm mag}_{\rm SE}(\boldsymbol{r}). \tag{1}$$

The sign convention here for $V_{\rm rad}$ (i.e., with $\hat{H} \to \hat{H} - V_{\rm rad}$) is from Ref. [1].

Including this potential into the Hartree-Fock equations (instead of adding it as a subsequent perturbation) gives an important contribution (core relaxation), especially for states with $l > 0$. The first three (electric) terms on the RHS of Eq. (1),

$$V^{\rm el}(r) = V_{\rm Ueh}(r) + V^h_{\rm SE}(r) + V^l_{\rm SE}(r), \tag{2}$$

are simple scalar terms, and can be included into the calculations simply (e.g., by adding them to the nuclear potential). The final (magnetic) term, which can be expressed as [3]

$$V^{\rm mag}_{\rm SE}(\boldsymbol{r}) = i(\boldsymbol{\gamma}\cdot\boldsymbol{n})H^{\rm mag}(r), \tag{3}$$

leads to off-diagonal terms in the Hamiltonian.

Inclusion into Dirac equation

Using atomic units[1], the single-electron Dirac equation is

$$(h_D - \varepsilon)\,\phi(\boldsymbol{r}) = 0, \tag{4}$$

where h_D is the Dirac Hamiltonian (see, e.g., Ref. [4]):

$$h_D = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + c^2(\beta - 1) + \hat{V}, \tag{5}$$

and $\boldsymbol{\alpha} = \gamma^0\boldsymbol{\gamma}$ and $\beta = \gamma^0$ are Dirac matrices. Here, $\hat{V}$ is the atomic potential (including nuclear and electronic potentials). Note that we have subtracted the electron rest energy, so the total relativistic energy is $E = \varepsilon + c^2$. The single-particle orbitals can be written in the form

$$\phi_{n\kappa m}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} f_{n\kappa}(r)\,\Omega_{\kappa m}(\boldsymbol{n}) \\ i g_{n\kappa}(r)\,\Omega_{-\kappa,m}(\boldsymbol{n})\end{pmatrix}, \tag{6}$$

where n is the principle quantum number, $\kappa = (l-j)(2j+1)$ is the Dirac quantum number, $m = j_z$ is the projection of $\boldsymbol{j} = \boldsymbol{l}+\boldsymbol{s}$ (total electron angular momentum) onto the quantisation axis, and Ω is a (two-component) spherical spinor,

$$\Omega_{\kappa m} \equiv \sum_{s_z=\pm 1/2} \langle l, m-s_z,\, 1/2, s_z | j, m\rangle\, Y_{l,m-s_z}(\boldsymbol{n})\,\chi_{s_z}, \tag{7}$$

with $\langle j_1 m_1 j_2 m_2 | JM\rangle$ a Clebsch-Gordon coefficient, Y_{lm} a spherical harmonic, $\boldsymbol{n} = \boldsymbol{r}/r$, and χ_{s_z} is a spin eigenstate ($s_z = \pm 1/2$). The terms in ϕ are orthonormal as:

$$\int (f_{n\kappa}f_{n'\kappa} + g_{n\kappa}g_{n'\kappa})\,{\rm d}r = \delta_{n'n} \tag{8}$$

$$\int \left(\Omega^\dagger_{\kappa m}\Omega_{\kappa' m'}\right){\rm d}\Omega = \delta_{\kappa'\kappa}\delta_{m'm}. \tag{9}$$

[1] $\hbar = m_e = e = |e| = 1$, $c = 1/\alpha \approx 137$ (note: $e > 0$ here)

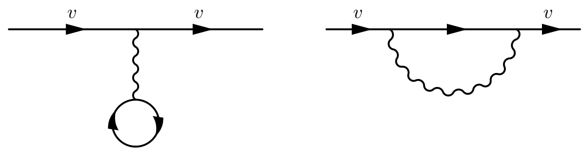

Figure 1: Vacuum polarisation (left) and self-energy (right) diagrams. In the radiative potential method, the self-energy diagram is replaced with an effective local potential [1].

Then, we can define the radial Dirac equation in the form:

$$(h_r - \varepsilon)\,F_{n\kappa} = 0, \tag{10}$$

where we defined the *radial spinor*,

$$F_{n\kappa} = \begin{pmatrix} f_{n\kappa}(r) \\ g_{n\kappa}(r)\end{pmatrix}, \tag{11}$$

and *radial Hamiltonian*,

$$h_r = \begin{pmatrix} \hat{V} & c(\frac{\kappa}{r} - \partial_r) \\ c(\frac{\kappa}{r} + \partial_r) & \hat{V} - 2c^2 \end{pmatrix}. \tag{12}$$

The QED radiative potential can be included via additions to the radial derivative as:

$$\partial_r F = \alpha \begin{pmatrix} (-c\kappa/r + H^{\rm mag}) & (\varepsilon - \hat{V} + V^{\rm el} + 2c^2) \\ -(\varepsilon - \hat{V} + V^{\rm el}) & (c\kappa/r - H^{\rm mag}) \end{pmatrix} F. \tag{13}$$

Explicit form of radiative potential

Detailed expressions for the individual contributions to $V_{\rm rad}$ are given in Refs. [1–3][2] – they involve some rather nasty integrals that must be evaluated carefully. For the Uehling potential (with $\rho = r/\lambda\!\!\!^{-}_c$ and $\rho_n = r_N/\lambda\!\!\!^{-}_c$)[3] we have:

$$V_{\rm Ueh}(r) = \frac{Z\alpha}{3\pi\, r}\int_1^\infty {\rm d}t\,\frac{\sqrt{t^2-1}}{t^4}\left(2t^2+1\right)\, e^{-2t\rho}\,G_{\rm Ueh}(r,t), \tag{14}$$

where r_N is the nuclear radius ($r_N = \sqrt{5/3}\,r_{\rm rms}$) and

$$G_{\rm Ueh}(r,t) = \begin{cases} 3\,(2t\rho_n)^{-3}\left[(2t\rho_n)\cosh(2t\rho_n) - \sinh(2t\rho_n)\right] & r \geq r_n \\ 3\,(2t\rho_n)^{-3}\,e^{2t\rho}\left[2t\rho - e^{-2t\rho_n}(1+2t\rho_n)\sinh(2t\rho)\right] & r < r_n. \end{cases} \tag{15}$$

Note that $G_{\rm Ueh} \to 1$ as $r_N \to 0$.

For the electric self-energy potential, we have

$$V^l_{\rm SE}(r) = -B_l(Z)Z^4\alpha^3F^l_{\rm SE}(r) \tag{16}$$

where, with $\xi(x) \equiv (x+1)e^{-x}$,

$$F^l_{\rm SE}(r) = \frac{3}{2rr_N^3Z^2}\int_0^{r_N} r'\left[\xi(Z|r-r'|) - \xi(Z(r+r'))\right]{\rm d}r'. \tag{17}$$

Note that $F^l_{\rm SE}(r) = e^{-Zr/a_B}$ as $r_N \to 0$. And:

$$V^h_{\rm SE}(r) = -A_l(Z)\frac{Z\alpha}{\pi r}\int_1^\infty {\rm d}t\, I_1(t,Z) \times \left[e^{-2t\rho}G_{\rm Ueh}(r,t) - I_2(r,t,Z)\right], \tag{18}$$

[2] Note: there is a small typo in Eq. (14) of Ref. [3] ($V^{\rm step}_{\rm high}$); the $r \leq r_N$ and $r > r_N$ terms should be swapped.

[3] $\lambda\!\!\!^{-}_c$ is electron (reduced) Compton wavelength. Atomic units: $\lambda\!\!\!^{-}_c = \alpha$.

where $G_{\rm Ueh}$ is the same as from the Uehling potential,

$$I_1(r,t,Z) = \frac{1}{\sqrt{t^2-1}}\Bigg\{\frac{1}{t^2} - \frac{3}{2} + \left(1-\frac{1}{2t^2}\right)\left[\ln(t^2-1) + 4\ln\left((Z\alpha)^{-1}+\frac{1}{2}\right)\right]\Bigg\}, \quad (19)$$

and

$$I_2(r,t,Z) = \frac{3r_A}{2r_N^3}\int_0^{r_N} r'\Big[E_1\left([|r-r'|+r_A]2t/\lambda\!\!\!^{-}_c\right) - E_1\left([r+r'+r_A]2t/\lambda\!\!\!^{-}_c\right)\Big]{\rm d}r', \quad (20)$$

E_1 is the exponential integral, and $r_A \equiv 0.07Z^2\alpha^3$. Here, A_l and B_l are order-1 fitting factors, taken from Ref. [3]. Note that $I_2 \to e^{-2t\rho}r_A/[r/a_B + r_A]$ as $r_N \to 0$.

Finally for the magnetic form factor:

$$H^{\rm mag}(r) = \frac{Z\alpha^2}{4\pi r^2}\int_1^\infty {\rm d}t \frac{1}{t^2\sqrt{t^2-1}} \times \left[(1+2t\eta)e^{-2t\rho}G_{\rm mag}(r,t) - (\chi/\rho_n)^3\right], \quad (21)$$

where $\eta = \max(\rho,\rho_n)$, $\chi = \min(\rho,\rho_n)$, and

$$G_{\rm mag} = \frac{3}{(2t\rho_n)^3}\left(e^{2t(\rho-\eta)}\left[2t\chi\cosh(2t\chi) - \sinh(2t\chi)\right]\right). \quad (22)$$

Note that $G_{\rm mag} \to 1$ as $R_n \to 0$.

References

[1] V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **72**, 052115 (2005).

[2] J. S. M. Ginges and J. C. Berengut, J. Phys. B **49**, 095001 (2016).

[3] J. S. M. Ginges and J. C. Berengut, Phys. Rev. A **93**, 052509 (2016).

[4] H. A. Bethe and E. E. Salpeter, *Quantum mechanics of one-and two-electron atoms* (Plenum Publishing Corporation, New York, 1977).