

# Helium fine structure

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The leading contributions to the helium fine structure beyond the first-order relativistic contribution were first derived by Araki [1] and Sucher [2], starting from the Bethe-Salpeter equation [3] and including the non-relativistic as well as the relativistic momentum regions. Following particularly the approach of Sucher, Douglas and Kroll [4] have derived all terms of order  $\alpha^4$  H(artree), where no contributions in the relativistic region were found. The same approach was later used by Zhang [5, 6] to derive corrections of order  $\alpha^5 \log \alpha$  H and of order  $\alpha^5$  H in the non-relativistic region and recoil corrections to order  $\alpha^4 m/M$  H (see also Ref. [7]). Later some additional effects of order  $\alpha^5$  H due to relativistic momenta were found by Zhang and Drake [8]. The radiative parts are treated more rigorously by Zhang in a separate paper [9]. Using a different approach, Pachuchi and Sapirstein [10] have derived all contributions of order  $\alpha^5$  H and report some disagreement with the early results of Zhang [5].

The approach of Sucher – that is followed by Douglas and Kroll and Zhang – is based directly on the BS equation and then makes it easy to identify the contributions in terms of Feynman diagrams and therefore convenient to use for us in identifying terms that can be evaluated numerically. The approach of Pachuchi is more difficult to use in this respect.

Here, I shall follow mainly the presentation of Douglas and Kroll (DK), which is quite detailed and easy to follow. It is largely based upon the thesis of Sucher (S) [2]. I will also give some comments about the work of Zhang (Z) [5]. S, DK and Z work mainly in the momentum representation, but I shall entirely use the coordinate representation.

## The Bethe-Salpeter equation

The two-particle, two-times Green's function satisfies the Dyson equation (DK 2.2) (see Fetter and Walecka [11], Ch. 3&4)

$$G(x'_1 x'_2; x_{10} x_{20}) = G_0(x'_1 x'_2; x_{10} x_{20}) + \iiint \int d^4 x_1 d^4 x_2 d^4 x_3 d^4 x_4 G_0(x'_1 x'_2; x_3 x_4) \kappa(x_3 x_4; x_1 x_2) G(x_1 x_2; x_{10} x_{20}) \quad (1)$$

which is illustrated in Fig. 1.

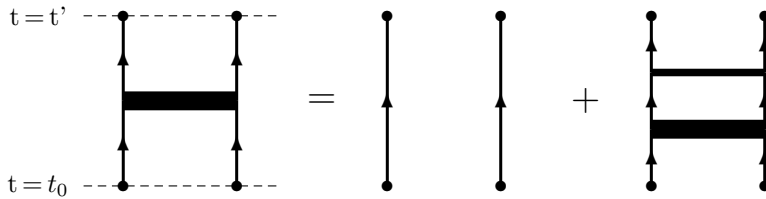


Figure 1:

The very thick horizontal line represents all interactions between the electrons, and the thinner line represents the kernel  $\kappa$  of all *non-separable* interactions, i.e., interactions that cannot be separated into several diagrams of the same kind by cutting the diagram along a horizontal line.

$G_0$  is the zeroth-order Green's function

$$G_0(x'_1 x'_2; x_{10} x_{20}) = S_1(x'_1; x_{10}) S_2(x'_2; x_{20}) \quad (2)$$

where  $S$  is the electron propagator or zeroth-order single-particle Green's function

$$\begin{aligned} S(x', x_0) &= \int \frac{d\omega}{2\pi} S(\omega) e^{-i\omega\tau} \quad \tau = t' - t_0 \\ S(\omega) &= \frac{|r\rangle\langle r|}{\omega - \varepsilon_r + i\eta_r} = \frac{\Lambda_+}{\omega - h + i\eta} + \frac{\Lambda_-}{\omega - h - i\eta} \end{aligned} \quad (3)$$

Here,  $h$  is the single-electron Dirac Hamiltonian in the field of the nucleus and  $\Lambda_{\pm}$  are projection operators for positive and negative-energy single-particle states.

In operator form the Dyson equation (1) becomes

$$G = G_0 + G_0 \kappa G \quad (4)$$

which can be expressed

$$(\mathcal{F} - \kappa) G = 1 \quad (5)$$

with  $\mathcal{F} = G_0^{-1}$ . The homogeneous part represents the equation for the corresponding wave function (DK 2.5, 2.26; Z 1)

$$\boxed{(\mathcal{F} - \kappa) \Psi = 0} \quad (6)$$

This is one form of the **Bethe-Salpeter equation**. (My  $\kappa$  corresponds to  $\mathcal{G}$  in S and DK and to  $g$  in Z.)

[Compare the Green's-function equation for the Schrödinger wave function  $\Psi_S$  (see Lindgren-Morrison (LM) [12] Sect.9.3)

$$(E - H + i\eta) G^+ = 1 \quad (7)$$

corresponding to the Schrödinger equation

$$H \Phi = E \Phi \quad (8)$$

Formally this holds only for a *time-independent* Hamiltonian but since the interactions are *physically* time-independent, this might be justified.]

The kernel can be separated into non-radiative (exchange) and radiative parts (DK 2.37, Fig. 3)

$$\kappa = \kappa_I + \kappa^{rad} \quad (9)$$

DK separates  $\kappa_I$  furthermore into (DK 3.5, Fig. 5)

$$\kappa_I = I_c + \kappa_T + \kappa_{T \times c} + \kappa_{T \times c^2} + \kappa_{T \times T} + \dots \quad (10)$$

where  $I_c$  is the Coulomb interaction  $I_c = 1/r_{12}$ ,  $\kappa_T$  interaction with a single transverse photon,  $\kappa_{T \times c}$  a transverse photon + one Coulomb etc.

For the perturbative expansion it is convenient to separate the kernel into a Coulomb interaction and a remainder (S 1.28, DK 3.4, Z 10)

$$\kappa = I_c + \kappa_{\Delta} \quad (11)$$

where

$$\kappa_{\Delta} = \kappa_T + \kappa_{T \times c} + \kappa_{T \times c^2} + \kappa_{T \times T} + \dots + \kappa^{rad} \quad (12)$$

The BS equation (6) can now be expressed

$$(\mathcal{F} - \kappa_{\Delta}) \Psi = I_c \Psi \quad (13)$$

or (S 1.30, DK 3.6)

$$\Psi = (\mathcal{F} - \kappa_{\Delta})^{-1} I_c \Psi \quad (14)$$

Using the identity (S 1.35, DK 3.11)

$$(A - B)^{-1} \equiv A^{-1} + A^{-1}B(A - B)^{-1} \quad (15)$$

this equation becomes (DK 3.12)

$$\Psi = [G_0 + G_0\kappa_\Delta(\mathcal{F} - \kappa_\Delta)^{-1}]I_c\Psi \quad (16)$$

with  $\mathcal{F} = G_0^{-1}$ .

The fourier transform of the zeroth-order Green's function (2) with respect to  $\tau = t' - t_0$  is (DK 3.21)

$$\begin{aligned} G_0(\epsilon; \mathbf{x}'_1, \mathbf{x}'_2; \mathbf{x}_{10}, \mathbf{x}_{20}) &= \int \frac{d\tau}{2\pi} e^{i\epsilon\tau} G_0(\tau; \mathbf{x}'_1, \mathbf{x}'_2; \mathbf{x}_{10}, \mathbf{x}_{20}) \\ &= \int \frac{d\omega}{2\pi} \frac{|r\rangle\langle r|}{\omega - \epsilon_r + i\eta_r} \frac{|s\rangle\langle s|}{\epsilon - \omega - \epsilon_s + i\eta_s} \end{aligned} \quad (17)$$

where  $r, s$  run over positive- and negative-energy states. With the two-electron projection operators  $\Lambda_{++}$  etc, this becomes (DK 3.24)

$$iG_0(\epsilon) = \frac{|rs\rangle\langle rs|}{\epsilon - \epsilon_r - \epsilon_s} (\Lambda_{++} - \Lambda_{--}) = \frac{1}{\epsilon - H_0} (\Lambda_{++} - \Lambda_{--}) \quad (18)$$

with  $H_0 = h_1 + h_2$ .

We can assume that the exact wave function has the time dependence

$$\Psi(t, \mathbf{x}_1, \mathbf{x}_2) = e^{-iEt} \Phi(\mathbf{x}_1, \mathbf{x}_2) \quad (19)$$

where  $E$  is the energy of the system and  $\Phi$  is the time-independent wave function that is a solution to the time-independent Schrödinger equation (8) The fourier transform of the wave function then leads to

$$\Psi(\epsilon, \mathbf{x}_1, \mathbf{x}_2) = \int \frac{dt}{2\pi} e^{i\epsilon t} \Psi(t, \mathbf{x}_1, \mathbf{x}_2) = \delta(E - \epsilon) \Phi(\mathbf{x}_1, \mathbf{x}_2) \quad (20)$$

and the integration over the parameter  $\epsilon$  that DK (3.7) and Z (14) perform simply generates the time-independent wave function  $\Phi$ , and we can replace  $\epsilon$  by  $E$  in the zeroth-order Green's function (18).

By fourier transforming the entire BS (16) and integrating over  $\epsilon$ , the result becomes (the factors of  $i$  do not seem correct)

$$\boxed{\left[ H_0 + (\Lambda_{++} - \Lambda_{--})I_c + i \int \frac{d\epsilon}{2\pi} DG_0\kappa_\Delta(\mathcal{F} - \kappa_\Delta)^{-1}I_c \right] \Psi(E) = E\Psi(E)} \quad (21)$$

with  $D = E - H_0$ . This is the form of the **Bethe-Salpater equation**, derived by Sucher (S 1.47) and rederived by Douglas and Kroll (DK 3.26) and by Zhang (Z 15).

The operator on the lhs can be written in the form  $H_c + H_\Delta$ , where (S 2.2, DK 3.28)

$$H_c = H_0 + \Lambda_{++}I_c\Lambda_{++} \quad (22)$$

is the Hamiltonian of the *no-(virtual-) pair Dirac-Coulomb equation* (Z 16)

$$H_c \Psi_c = E_c \Psi_c \quad (23)$$

and (S 2.3)

$$H_\Delta = \Lambda_{++}I_c(1 - \Lambda_{++}) - \Lambda_{--}I_c + \left[ i \int \frac{d\epsilon}{2\pi} DG_0\kappa_\Delta(\mathcal{F} - \kappa_\Delta)^{-1}I_c \right] = H_{\Delta 1} + H_{\Delta 2} \quad (24)$$

is the *remaining "QED part"* (DK 3.29, Z 17). The first part  $H_{\Delta 1}$  represents virtual pairs due to the Coulomb interaction and the second part effects of relativity and transverse photons.

In order to include electron self energy and vacuum polarizations, the electron propagators (2) are replaced by propagators with self-energy insertions  $\Sigma(\epsilon)$ , properly renormalized (DK 2.10)

$$S'(\epsilon) = \frac{|r\rangle\langle r|}{\epsilon - \epsilon_r - \Sigma(\epsilon) + i\eta_r} \quad (25)$$

Also renormalized photon self energies have to be inserted into the photon lines.

By including also the instantaneous Breit interaction in  $I_c$ , the no-pair Hamiltonian (22) becomes the standard *Dirac-Coulomb-Breit Hamiltonian* of the *No-Virtual-Pair Approximation* (NVPA) and the remainder (24) would be what we refer to as "*QED effects*".

## Perturbation expansion of the BS equation

The effect of the QED Hamiltonian (24) can be expanded perturbatively, using the Brillouin-Wigner perturbation theory (LM 9.39, DK 3.36)

$$\Delta E = \langle \Psi_0 | V + VT_E V + VT_E VT_E V + \dots | \Psi_0 \rangle = \langle \Psi_0 | \frac{V}{1 - T_E V} | \Psi_0 \rangle \quad (26)$$

where  $T_E$  is the BW resolvent (LM 9.16, DK 3.38)

$$T_E = \Gamma_Q = \frac{Q}{E - H_0} \quad (27)$$

The unperturbed wave function is in our case one solution of the no-pair Dirac-Coulomb equation (23),  $\Psi_c$ , and we can assume that the perturbation is expanded in other eigenfunctions of  $H_c$ .  $Q$  is the projection operator that excludes the state  $\Psi_c$  (assuming no degeneracy) and then

$$\Gamma_Q = \frac{Q}{E - H_c} \quad (28)$$

This leads to the expansion (S 2.13, DK 3.43, Z 28)

$$\Delta E^{(1)} = \langle \Psi_c | H_{\Delta} | \Psi_c \rangle \quad (29a)$$

$$\Delta E^{(2)} = \langle \Psi_c | H_{\Delta} \Gamma_Q H_{\Delta} | \Psi_c \rangle \quad (29b)$$

$$\Delta E^{(3)} = \langle \Psi_c | H_{\Delta} \Gamma_Q H_{\Delta} \Gamma_Q H_{\Delta} | \Psi_c \rangle \quad (29c)$$

etc.

Since  $\Lambda_{++}|\Psi_c\rangle = |\Psi_c\rangle$  and  $\Lambda_{--}|\Psi_c\rangle = 0$ , it follows that  $\langle \Psi_c | H_{\Delta 1} | \Psi_c \rangle \equiv 0$ , and the first-order correction becomes (DK 3.44)

$$\Delta E^{(1)} = \langle \Psi_c | H_{\Delta 2} | \Psi_c \rangle = \langle \Psi_c | i \int \frac{d\epsilon}{2\pi} D G_0 J G_0 I_c | \Psi_c \rangle \quad (30)$$

with  $\mathcal{F}^{-1} = G_0$  and (DK 3.45)

$$J = \kappa_{\Delta} (1 - G_0 \kappa_{\Delta})^{-1} \quad (31)$$

The second-order corrections are (DK 3.46, Z 30)

$$\Delta E_a^{(2)} = \langle \Psi_c | H_{\Delta 1} \Gamma_Q H_{\Delta 1} | \Psi_c \rangle = -\langle \Psi_c | I_c \Lambda_{--} \Gamma_Q \Lambda_{--} I_c | \Psi_c \rangle \quad (32a)$$

$$\Delta E_b^{(2)} = \langle \Psi_c | H_{\Delta 1} \Gamma_Q H_{\Delta 2} | \Psi_c \rangle = \langle \Psi_c | I_c \Lambda_{--} \Gamma_Q i \int \frac{d\epsilon}{2\pi} D G_0 J G_0 I_c | \Psi_c \rangle \quad (32b)$$

(Note that the two  $I_c$  are missing from the DK equation.)

$$\Delta E_c^{(2)} = \langle \Psi_c | H_{\Delta 2} \Gamma_Q H_{\Delta 1} | \Psi_c \rangle = \langle \Psi_c | i \int \frac{d\epsilon}{2\pi} D G_0 J G_0 I_c \Gamma_Q \Lambda_{--} I_c | \Psi_c \rangle \quad (32c)$$

(This agrees with Z 30 but not with DK 3.46 – the factor  $I_c \mathcal{L}_{++}$  should be removed.)

$$\Delta E_d^{(2)} = \langle \Psi_c | H_{\Delta 2} \Gamma_Q H_{\Delta 2} | \Psi_c \rangle = \langle \Psi_c | i \int \frac{d\epsilon}{2\pi} D G_0 J G_0 I_c \Gamma_Q i \int \frac{d\epsilon}{2\pi} D G_0 J G_0 I_c | \Psi_c \rangle \quad (32d)$$

Since  $\Gamma_Q D \approx Q$  and  $\Lambda_{--} Q = \Lambda_{--}$ ,  $\Gamma_Q$  can in the first three equations be replaced by  $D^{-1}$ . Then the results agree – apart from the misprints mentioned above – with the results of DK and Z.

According to DK  $\Delta E_a^{(2)}$ ,  $\Delta E_c^{(2)}$  and  $\Delta E^{(3)}$  do not contribute to the fs in order  $\alpha^4$  (Hartrees). This holds also in the next order according to Zhang, but  $\Delta E^{(3)}$  will contribute to the singlet energy in that order. (I do not see the reason why  $\Delta E_b^{(2)}$  contributes, while  $\Delta E_c^{(2)}$  does not, as they seem to be quite equivalent.) In the relativistic momentum region the second-order part  $\Delta E_a^{(2)}$  contributes to the energy already in order  $\alpha^3 H$  and to the fine structure in order  $\alpha^5 H$  [5, p.1256].

The zeroth-order Green's function (2) can be reformulated in the following way (DK 3.48)

$$G_0 = S_1 S_2 \equiv (S_1 + S_2)(S_1^{-1} + S_2^{-1})^{-1} = \frac{S_1 + S_2}{E - H_0} = D^{-1}(S_1 + S_2) \quad (33)$$

With  $E = E_c + \Delta E$  and

$$D_c = E_c - H_0 = D - \Delta E \quad (34)$$

we have (DK 3.50a, note misprint)

$$D^{-1} = \frac{1}{D_c} - \frac{\Delta E}{D_c D} \quad (35)$$

The first-order contribution can then be expressed (DK 3.49, Z 29)

$$\begin{aligned} \Delta E^{(1)} &= \langle \Psi_c | D^{-1} i \int \frac{d\epsilon}{2\pi} (S_1 + S_2) J (S_1 + S_2) | \Psi_c \rangle \\ &= \langle \Psi_c | D_c^{-1} (1 - \Delta E/D) i \int \frac{d\epsilon}{2\pi} (S_1 + S_2) J (S_1 + S_2) | \Psi_c \rangle \end{aligned} \quad (36)$$

Using the relation (34), we have  $E_c - H_c = D_c - \Lambda_{++} C \Lambda_{++}$ , and the no-pair equation (23) can be written (DK 3.51)

$$(D_c - \Lambda_{++} I_c) \Psi_c = 0 \quad (37)$$

Then the second-order correction  $\Delta E_b^{(2)}$  (32b) can be expressed

$$\Delta E_b^{(2)} = \langle \Psi_c | (I_c - D_c) i \int \frac{d\epsilon}{2\pi} G_0 J G_0 I_c | \Psi_c \rangle \quad (38)$$

This is consistent with (Z 30). This can be combined with the first-order correction  $\Delta E^{(1)}$  (30), yielding (DK 3.52,54, Z 37)

$$\langle \Psi_c | (I_c + \Delta E) i \int \frac{d\epsilon}{2\pi} G_0 J G_0 I_c | \Psi_c \rangle \quad (39)$$

**Both DK and Z have the  $\Delta E$  term with the opposite sign.**

We make the expansion (DK 3.45, Z 32)

$$J = \kappa_\Delta(1 - G_0\kappa_\Delta)^{-1} = \kappa_\Delta + \kappa_\Delta G_0\kappa_\Delta + \dots \quad (40)$$

where diagrams from the second and higher terms in this expansion are *separable* (reducible). Making the replacement (DK 3.53, Z 12)

$$\kappa_\Delta = \kappa_T + \Delta\kappa \quad (41)$$

where  $\kappa_T$  represents the interaction of a single transverse photon, the expression (39) becomes (DK 3.54)

$$\langle \Psi_c | I_c \text{ i } \int \frac{d\epsilon}{2\pi} G_0 [\kappa_T + \kappa_T G_0 \kappa_T + \Delta\kappa + \dots] G_0 I_c | \Psi_c \rangle \quad (42)$$

The expression for  $\Delta E_d^{(2)}$  (32d) becomes similarly in lowest order

$$\langle \Psi_c | \text{i} \int \frac{d\epsilon}{2\pi} D G_0 \kappa_T G_0 I_c \Gamma_Q \text{i} \int \frac{d\epsilon}{2\pi} D G_0 \kappa_T G_0 I_c | \Psi_c \rangle \quad (43)$$

The only additional term that contributes to the fs in this order is then the second part of  $\Delta E^{(1)}$  (36)

$$\Delta E \langle \Psi_c | I_c \text{ i} \int \frac{d\epsilon}{2\pi} G_0 \kappa_T G_0 I_c | \Psi_c \rangle \quad (44)$$

As noted, the last term differs in sign from DK 3.54.

The complete contribution to the fs to order  $\alpha^4$  then becomes

$$\begin{aligned} & \langle \Psi_c | I_c \text{ i} \int \frac{d\epsilon}{2\pi} G_0 [\kappa_T + \kappa_T G_0 \kappa_T + \Delta\kappa] G_0 I_c | \Psi_c \rangle \\ + & \langle \Psi_c | \text{i} \int \frac{d\epsilon}{2\pi} D G_0 \kappa_T G_0 I_c \Gamma_Q \text{i} \int \frac{d\epsilon}{2\pi} D G_0 \kappa_T G_0 I_c | \Psi_c \rangle \\ + & \Delta E \langle \Psi_c | I_c \text{ i} \int \frac{d\epsilon}{2\pi} G_0 \kappa_T G_0 I_c | \Psi_c \rangle \end{aligned} \quad (45)$$

with

$$\Delta\kappa = \kappa_{T \times c} + \kappa_{T \times c^2} + \kappa_{T \times T} + \kappa^{rad} \quad (46)$$

Zhang (Z 37) gives the following expression for the energy correction (transferred to our notations), valid to order  $\alpha^5$  H, which is consistent with DK

$$\begin{aligned} \Delta E &= \left\langle \Psi_c \left| \text{i} \int \frac{d\epsilon}{2\pi} I_c G_0 J G_0 I_c - \Delta E \text{i} \int \frac{d\epsilon}{2\pi} (S_{1+} + S_{2+}) J (S_1 + S_2) D_c^2 I_c \right. \right. \\ &+ \left. \left. \text{i} \int \frac{d\epsilon}{2\pi} D G_0 J G_0 I_c \Gamma_Q \text{i} \int \frac{d\epsilon'}{2\pi} D G_0 J G_0 I_c \right| \Psi \right\rangle \end{aligned} \quad (47)$$

In addition, there is a contribution in the relativistic momentum region from Coulomb interactions to this order. In this order it is necessary to consider the Coulomb crossings to all orders in the one- and two-transverse-photon exchange

## Comparison with our numerical approach

Douglas and Kroll discuss in Chapter 4 (9 pages!) the Coulomb ladder diagrams, leading to the terms  $\Delta W_c^6(i)$ ,  $i = 1 - 5$  (DK 4.36). These effects will be dealt with in our relativistic pair program. In Chapter 5 (11 pages!) DK discuss diagrams with a single transverse photon, leading to the terms  $\Delta W_T^6(i)$ ,  $i = 1 - 8$  (DK 5.35). All these effects will in our approach also be evaluated numerically.

In Chapter 6 DK discuss the diagrams with two transverse photons, i.e., the effects of  $\kappa_{T \times T}$  and  $\kappa_T G_0 \kappa_T$ , referred to as  $\Delta E^{T \times T}$  and  $\Delta E^{T \cdot T}$ , respectively. The latter represents a separable diagram and can be evaluated numerically by iterating the one-photon process (instantaneous Breit and retarded photon). The effect of  $T \times T$  with no pairs is found to be of order  $\alpha^5 + \alpha^5 \log \alpha$  H, and the effect of double pairs is also found to give no contribution to the fs in order  $\alpha^4$  H. The pair effect with Coulomb interactions is also found to vanish in this order. That leaves only the term  $\Delta E^{T \times T}$  with a single pair to be evaluated analytically.

In Chapter 7 DK discuss radiative corrections in a phenomenological way, based upon the anomalous magnetic moment of the electron. The numerical results of DK are given in Ref. [13].

Zhang deals with a single transverse photon in his section III (14 pages and 93 equations!) and the Coulomb ladder in section V. The Coulomb crossings to all orders, needed in this order, can be done numerically with our approach. There is also a contribution from the Coulomb interactions to order  $\alpha^5$  H, which can also be evaluated numerically. This leaves also here only the two-photon crossing  $\Delta E^{T \times T}$  (with Coulomb crossings) to be estimated analytically. Zhang treats also the radiative corrections more rigorously than DK, particularly in Ref. [9]. The phenomenological approach of DK is confirmed to be justified to order  $\alpha^4$  H, but is not sufficient in the next order.

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