

# The helium fine-structure controversy

Ingvar Lindgren

Physics Department, University of Gothenburg, Göteborg, Sweden

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## Abstract

There is presently disagreement between theory and experiment as well as between different theoretical calculations concerning the fine-structure splitting of the lowest  $P$  state of the neutral helium atom. We believe that we have found a minor error in the formulas used by Drake *et al.* (Can. J. Phys. 80, 1195 (2002)) in their calculations, and we may have an explanation how the error has occurred. To what extent this might resolve (part of) the discrepancy is not known at present.

## 1 Introduction

The fine structure of the lowest  $P$  state of neutral helium is of great principal interest, since a comparison between theory and experiment might yield an accurate and independent determination of the fine-structure constant,  $\alpha$ . Unfortunately, various theoretical calculations disagree, and there is also a significant discrepancy between theory and experiment, when using an accurate value of  $\alpha$ , determined in other ways, primarily from the  $g$ -factor of the free electron. Even with  $\alpha$  as a free-running parameter, it is not possible to match theory and experiment for the two fine-structure separations.

The most accurate experimental results are obtained by Gabrielse *et al.* [1] and by Inguscio *et al.* [2]. The theoretical calculations have been performed by Drake and coworkers [3] as well as by Pachucki and Sapirstein [4].

The calculations of Drake *et al.* are based upon the works of Sucher [5] and of Douglas and Kroll [6]. We have now discovered that there is most likely a minor error in the formulas of Douglas and Kroll and the corresponding formulas of Zhang [7] on which the works of Drake *et al.* are based. This is estimated to lead to a correction of order  $\alpha^5$  Ry, which is beyond the accuracy of Douglas and Kroll but might be relevant for the works of Drake and Zhang. We do not know at present the magnitude of the effect and to what extent this might resolve some of the discrepancies, but this is certainly worth investigating. Below we shall review the analyses of Douglas-Kroll (DK) and Zhang (Z), which are based on the early work of Sucher (S) [5], and point out where we believe the mistake has been made.

## 2 The analysis of Sucher, Douglas and Kroll

In his thesis Sucher performed a perturbation expansion of the Bethe-Salpeter equation (BSE) [8], which with somewhat different notations can be expressed

$$\begin{aligned} \Psi(x, x') &= \iiint d^4 x_1 d^4 x_2 d^4 x'_1 d^4 x'_2 \\ &\times G'_0(x, x'; x_2, x'_2) (-i)\Sigma^*(x_2, x'_2; x_1, x'_1) \Psi(x_1, x'_1) \end{aligned} \quad (1)$$

$G'_0$  is the zeroth-order two-particle Green's function, dressed with all kinds of single-particle self-energy insertions, and  $\Sigma^*$  is the irreducible or proper two-particle self energy. The function  $G'_0$  is a product of two single-particle Green's functions, satisfying the relation

$$\left(i\frac{\partial}{\partial t} - h_1\right)G(x, x_0) = i\delta^4(x - x_0) \quad (2)$$

which leads to (S 1.6, DK 2.19)

$$\left(i\frac{\partial}{\partial t} - h_1\right)\left(i\frac{\partial}{\partial t'} - h_2\right)\Psi(x, x') = i\iint d^4 x_1 d^4 x'_1 \Sigma^*(x, x'; x_1, x'_1) \Psi(x_1, x'_1) \quad (3)$$

where  $h_{1,2}$  are the Dirac single-particle Hamiltonians.

With the wave function being of the form

$$\Psi(x, x') = \Psi(T, \tau, \mathbf{x}, \mathbf{x}') = e^{-iET} \Psi(\tau, \mathbf{x}, \mathbf{x}') \quad (4)$$

where  $T = (t + t')/2$  is the average time and  $\tau = t - t'$  is the relative time, the BSE can after a Fourier transform be expressed in operator form (S 1.12, DK 2.26, Z 1)

$$\mathcal{F}\Psi(\epsilon) = g\Psi(\epsilon) \quad (5)$$

Here,

$$\mathcal{F} = \left(E/2 + \epsilon - h_1\right)\left(E/2 - \epsilon - h_2\right) \quad (6)$$

and

$$g\Psi(\epsilon) = \frac{i}{2\pi} \Sigma^*(\epsilon) \Phi \quad (7)$$

where (S 1.31, DK 3.7, Z 14)

$$\Phi = \int d\epsilon \Psi(\epsilon) \quad (8)$$

is the "equal-time" function.

The interaction  $g$  can be separated into a Coulomb part and a "remainder"

$$g = g_c + g_\Delta \quad (9)$$

leading to

$$\Psi(\epsilon) = (\mathcal{F} - g_\Delta)^{-1} g_c \Psi(\epsilon) \quad (10)$$

From Eq. (7) it follows that (S 1.32), (DK 3.8)

$$g_c \Psi(\epsilon) = \frac{i}{2\pi} I_c \Phi \quad (11)$$

where  $I_c$  is the Coulomb interaction.

Integrating Eq. (11) over the relative energy  $\epsilon$ , leads to (S 1.34, DK 3.10)

$$\Phi = i \int \frac{d\epsilon}{2\pi} (\mathcal{F} - g_\Delta)^{-1} I_c \Phi \quad (12)$$

The inverse of the operator  $\mathcal{F}$  is essentially a product of two electron propagators, yielding

$$i \int \frac{d\epsilon}{2\pi} \mathcal{F}^{-1} = -G_0(E) = \frac{1}{E - h_1 - h_2} (\Lambda_{++} - \Lambda_{--}) \quad (13)$$

where  $\Lambda_{++}$ ,  $\Lambda_{--}$  are two-particle projection operators for doubly positive and negative states, respectively. This leads to the equation (S 1.47), (DK 3.26)

$$\boxed{\left[ h_1 + h_2 + (\Lambda_{++} - \Lambda_{--}) I_c + i \int \frac{d\epsilon}{2\pi} D \mathcal{F}^{-1} g_\Delta (\mathcal{F} - g_\Delta)^{-1} I_c \right] \Phi = E \Phi} \quad (14)$$

where

$$D = E - h_1 - h_2 \quad (15)$$

This is the starting point for the further analysis.

### 3 Perturbation expansion of the BS equation

The operator on the left-hand side of Eq. (14) can be separated into a *no-pair Coulomb operator*

$$H_c = h_1 + h_2 + \Lambda_{++} I_c \Lambda_{++} \quad (16a)$$

a *Coulomb virtual-pair operator*

$$H_{\Delta 1} = \Lambda_{++} I_c (1 - \Lambda_{++}) - \Lambda_{--} I_c \quad (16b)$$

and a *relativity and transverse photon operator*

$$H_{\Delta 2} = i \int \frac{d\epsilon}{2\pi} D \mathcal{F}^{-1} g_\Delta (\mathcal{F} - g_\Delta)^{-1} I_c \quad (16c)$$

Starting from the no-pair approximation

$$H_c \Psi_c = E_c \Psi_c \quad (17)$$

the Brillouin-Wigner expansion yields the energy contribution

$$\Delta E = E - E_c = \langle \Psi_c | V + V \Gamma V + V \Gamma V \Gamma V + \dots | \Psi_c \rangle \quad (18)$$

where

$$\Gamma = \Gamma_Q(E) = \frac{Q}{E - H_c} \quad (19)$$

is the resolvent. This leads to the expansion terms (S 2.19-21, DK 3.43, Z 28)

$$\Delta E^{(1)} = \langle \Psi_c | H_{\Delta 1} | \Psi_c \rangle \quad (20a)$$

$$\Delta E^{(2)} = \langle \Psi_c | H_{\Delta} \Gamma H_{\Delta} | \Psi_c \rangle \quad (20b)$$

$$\Delta E^{(3)} = \langle \Psi_c | H_{\Delta} \Gamma H_{\Delta} \Gamma H_{\Delta} | \Psi_c \rangle \quad (20c)$$

etc.

It can be shown that there is no first-order contribution from  $H_{\Delta 1}$ , and the first-order energy contribution then becomes (DK 3.44)

$$\Delta E^{(1)} = \langle \Psi_c | H_{\Delta 2} | \Psi_c \rangle = \langle \Psi_c | i \int \frac{d\epsilon}{2\pi} D \mathcal{F}^{-1} J \mathcal{F}^{-1} I_c | \Psi_c \rangle \quad (21)$$

where

$$J = g_{\Delta} (1 - \mathcal{F}^{-1} g_{\Delta})^{-1} \quad (22)$$

Of special interest here is one of the second-order contributions (DK 3.46, note some misprints)

$$\Delta E_b^{(2)} = \langle \Psi_c | H_{\Delta 1} \Gamma H_{\Delta 2} | \Psi_c \rangle = \langle \Psi_c | I_c \Lambda_{--} \Gamma i \int \frac{d\epsilon}{2\pi} D \mathcal{F}^{-1} J \mathcal{F}^{-1} I_c | \Psi_c \rangle \quad (23)$$

It can easily be shown that  $\Lambda_{--} \Gamma D = \Lambda_{--}$  (DK 3.41). Using the relation (16a) and with  $D_c = E - c - h_1 - h_2$ , we have  $E_c - H_c = D_c - \Lambda_{++} D_c \Lambda_{++}$ , and the no-pair equation (17) can be written (DK 3.51)

$$(D_c - \Lambda_{++} I_c) \Psi_c = 0 \quad (24)$$

Then the second-order correction  $\Delta E_b^{(2)}$  (23) can be expressed

$$\Delta E_b^{(2)} = \langle \Psi_c | (I_c - D_c) i \int \frac{d\epsilon}{2\pi} \mathcal{F}^{-1} J \mathcal{F}^{-1} I_c | \Psi_c \rangle \quad (25)$$

This can be combined with the first-order correction  $\Delta E^{(1)}$  (21), yielding

$$\langle \Psi_c | (D + I_c - D_c) i \int \frac{d\epsilon}{2\pi} \mathcal{F}^{-1} J \mathcal{F}^{-1} I_c | \Psi_c \rangle = \langle \Psi_c | (I_c + \Delta E) i \int \frac{d\epsilon}{2\pi} \mathcal{F}^{-1} J \mathcal{F}^{-1} I_c | \Psi_c \rangle \quad (26)$$

Here, the  $\Delta E$  term differs in sign from (DK 3.54) and (Z 37).

The reason for the discrepancy between our result here and those of Douglas and Kroll and of Zhang seems to be that the latter use the relation

$$\mathcal{F}^{-1} = S_1 S_2 \equiv (S_1 + S_2) (S_1^{-1} + S_2^{-1})^{-1} = D^{-1} (S_1 + S_2) \quad (27)$$

where  $S_{1,2}$  are electron propagators, and the identity (DK 3.50a, note misprint)

$$D^{-1} = \frac{1}{D_c} - \frac{\Delta E}{D_c D} \quad (28)$$

to transform the first-order equation (21) to

$$\Delta E^{(1)} = \langle \Psi_c | D_c^{-1} (1 - \Delta E/D) i \int \frac{d\epsilon}{2\pi} (S_1 + S_2) J (S_1 + S_2) I_c | \Psi_c \rangle \quad (29)$$

and the second-order correction (25) to

$$\Delta E_b^{(2)} = \langle \Psi_c | (I_c - D_c) D^{-2} i \int \frac{d\epsilon}{2\pi} (S_1 + S_2) J (S_1 + S_2) I_c | \Psi_c \rangle \quad (30)$$

Then they cancel  $D_c^{-1}$  in the first equation against  $D_c D^{-2}$  in the second. Zhang approximates  $D$  by  $D_c$  in all  $\Delta E^{(1)}$  and  $\Delta E^{(2)}$  expressions, which leads to the same cancellation. According to Eq. (28), this leads to an error of  $2\Delta E/(D_c D)$ , which explains the difference.

The difference is of the form  $2\Delta E \times \Delta E^{(1)}$ , which is of order  $\alpha^5$  Ry. The correction  $\Delta E$  represents the difference between the full energy and the Dirac-Coulomb energy, which contains the instantaneous Breit interaction and therefore of order  $\alpha^2$  Ry. This interaction does not contribute to the fine-structure splitting, and therefore  $\Delta E^{(1)}$  is order  $\alpha^3$  Ry, making the correction of order  $\alpha^5$  Ry. This does not affect the work of Douglas and Kroll, who study corrections up to  $\alpha^4$  Ry, while it is of relevance for Zhang and Drake who go one step further.

## 4 Equal-time approximation

Another possible source of the discrepancy between theory and experiment might be the fact that the calculations – following Sucher – are based upon the so-called *equal-time approximation*, where the particles are assumed to have the same time. This is in contrast to the covariant Bethe-Salpeter equation, where the particles have individual times. It is hard to tell what size an effect of this kind might have on the results and to what extent it can be visible at the present level of accuracy. Most likely, however, this will be the case at some level.

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