Appendix: C

C.1 Derivation of the Effective Atomic EDM Operator

Let us start from the total atomic EDM expression obtained within the relativistic framework, in Chapter 3, Section §3.1.1 which is re-written below [cf. see Eq. (3.21)]:

\[
\langle D \rangle = d_e \left\{ \langle \phi_m^{(0)} | \beta \sigma | \phi_m^{(0)} \rangle - \sum_{n \neq m} \frac{\langle \phi_m^{(0)} | \beta \sigma \cdot E_{\text{int}} | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | e z | \phi_m^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right. \\
- \left. \sum_{n \neq m} \frac{\langle \phi_n^{(0)} | e z | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | \beta \sigma \cdot E_{\text{int}} | \phi_n^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right\}. 
\]

(C.1)

Let us decompose \( \langle D \rangle \) as the following:

\[
\langle D \rangle = \langle D^0 \rangle + \langle D^1 \rangle .
\]

(C.2)

where, \( \langle D^0 \rangle = d_e \langle \phi_m^{(0)} | \beta \sigma | \phi_m^{(0)} \rangle \),

(C.3)

and \( \langle D^1 \rangle = -d_e \left\{ \sum_{n \neq m} \frac{\langle \phi_m^{(0)} | \beta \sigma \cdot E_{\text{int}} | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | e z | \phi_m^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right. \\
+ \left. \sum_{n \neq m} \frac{\langle \phi_n^{(0)} | e z | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | \beta \sigma \cdot E_{\text{int}} | \phi_n^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right\} .
\]

(C.4)

The total atomic Hamiltonian in the presence of the electron EDM as a perturbation is given by,

\[
H = H_0 + d_e H'.
\]

From Eq. (3.11 and C.1), it is clear that the effective perturbed Hamiltonian due to intrinsic electron EDM is \(^1\),

\[
H' = -\beta \sigma \cdot E_{\text{int}}.
\]

(C.5)

Therefore,

\[
H = \{ c \alpha \cdot p + \beta m c^2 + V(r) \} - d_e \beta \sigma \cdot E_{\text{int}}.
\]

(C.6)

\(^1\)The summation over the individual electrons is dropped for the time being.
Let us work out the following commutator, the reason for which will be evident later on.

\[
[\beta \sigma \cdot \nabla, H_0] = \left[\beta \sigma \cdot \nabla, (c\alpha \cdot p + \beta mc^2 + V(r))\right],
\]
\[
= c[\beta \sigma \cdot \nabla, \alpha \cdot p] + mc^2[\beta \sigma \cdot \nabla, \beta] + [\beta \sigma \cdot \nabla, V(r)]. \tag{C.7}
\]

Let us consider each of the three terms in Eq. (C.7) separately and solve them one by one, as below.

(a) The first commutator in Eq. (C.7), \([\beta \sigma \cdot \nabla, \alpha \cdot p]\).

\[
[\beta \sigma \cdot \nabla, c\alpha \cdot p] = \frac{ic}{\hbar}[\beta \sigma \cdot p, \alpha \cdot p],
\]
\[
= \frac{ic}{\hbar} \sum_{kl} p_k p_l \{[\beta \sigma_k, \alpha_l] \},
\]
\[
= \frac{ic}{\hbar} \left\{ \sum_k \gamma_k^2 [\beta \sigma_k, \alpha_k] + \sum_{k \neq l} p_k p_l \{[\beta \sigma_k, \alpha_l] \} \right\}. \tag{C.8}
\]

From the algebra of Dirac matrices, we know the following results (The notations are adopted from J. J. Sakurai’s *Advanced Quantum Mechanics* textbook):

- \(\gamma_k = \begin{pmatrix} 0 & -i \sigma_k^P \\ i \sigma_k^P & 0 \end{pmatrix} \); \(\gamma_5 = -\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \); \(\beta \equiv \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \); \(\sigma_k = \sigma_k^P \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \).

where \(\sigma_k^P\) are the Pauli spin matrices, \(I\) is the Identity Matrix and \(k \equiv \{x, y, z\}\).

- \(\alpha_k\alpha_l + \alpha_l\alpha_k = 0\) and \(\alpha_k\beta + \beta\alpha_k = 0\), i.e., the Dirac matrices \(\alpha_k\) and \(\beta\) anti-commute with each other.

- \(\alpha_k = i\beta \gamma_k \Rightarrow \alpha_k = -\gamma_5 \sigma_k = -\sigma_k \gamma_5\); Also, \(\sigma_k = -\gamma_5 \alpha_k\), where \(\gamma_5 = \gamma_x \gamma_y \gamma_z \beta\).

- \(\alpha_k^2 = \beta^2 = I\); \(\gamma_3^2 = 1\) and \(\gamma_5 = \gamma_5^4\).

- \(\gamma_5 \gamma_k + \gamma_k \gamma_5 = 0\) and \(\gamma_5 \beta + \beta \gamma_5 = 0\); whereas, \(\gamma_5 \alpha_k = \alpha_k \gamma_5\).
Now consider,

\[
[\beta \sigma_k, \alpha_l] = \beta \sigma_k \alpha_l - \alpha_l \beta \sigma_k \\
= \beta \sigma_k \alpha_l + \alpha_l \sigma_k \\
= \beta (\sigma_k \alpha_l + \alpha_l \sigma_k) \\
= \beta (-\gamma_5 \alpha_k \alpha_l - \alpha_l \gamma_5 \alpha_k) \\
= -\beta \gamma_5 (\alpha_k \alpha_l + \alpha_l \alpha_k) \\
= 0 \quad \text{(C.9)}
\]

\[
[\beta \sigma_k, \alpha_k] = \beta \sigma_k \alpha_k - \alpha_k \beta \sigma_k \\
= -\beta \gamma_5 \alpha_k^2 + \alpha_k \beta \gamma_5 \alpha_k \\
= -\beta \gamma_5 - \beta \gamma_5 \\
= -2\beta \gamma_5 \quad \text{(C.10)}
\]

\[
\Rightarrow [\beta \sigma \cdot \nabla, c\alpha \cdot \mathbf{p}] = -\frac{2i c}{\hbar} \beta \gamma_5 \mathbf{p}^2. \quad \text{(C.11)}
\]

(b) The second commutator in Eq. (C.7), \([\beta \sigma \cdot \nabla, \beta]\).

\[
[\beta \sigma \cdot \nabla, \beta] = \frac{i mc}{\hbar} [\sigma \cdot \mathbf{p}, \beta], \\
= \frac{i mc}{\hbar} \sum_k p_k [\sigma_k, \beta]. \quad \text{(C.12)}
\]

\[
[\sigma_k, \beta] = [-\gamma_5 \alpha_k, \beta], \\
= -\gamma_5 \alpha_k \beta + \beta \gamma_5 \alpha_k, \\
= -\gamma_5 \alpha_k \beta - \gamma_5 \beta \alpha_k, \\
= -\gamma_5 [\alpha_k, \beta] \\
= 0. \quad \text{(C.13)}
\]

\[
\Rightarrow [\beta \sigma \cdot \nabla, \beta] = 0. \quad \text{(C.14)}
\]

(c) The third commutator in Eq. (C.7), \([\beta \sigma \cdot \nabla, V(r)]\).
Let us take the scalar potential to be, \( V(r) = e v. \)

\[
[\sigma \cdot \nabla, V(r)] = \left[ \sigma_x \frac{\partial}{\partial x}, V \right] + \left[ \sigma_y \frac{\partial}{\partial y}, V \right] + \left[ \sigma_z \frac{\partial}{\partial z}, V \right],
\]

\[
= e \sigma_x \left[ \frac{\partial}{\partial x}, v \right] + e \sigma_y \left[ \frac{\partial}{\partial y}, v \right] + e \sigma_z \left[ \frac{\partial}{\partial z}, v \right],
\]

\[
= - \frac{e \sigma_x}{i \hbar} [p_x, v] - \frac{e \sigma_y}{i \hbar} [p_y, v] - \frac{e \sigma_z}{i \hbar} [p_z, v],
\]

\[
= \frac{e \sigma_x}{i \hbar} [v, p_x] + \frac{e \sigma_y}{i \hbar} [v, p_y] + \frac{e \sigma_z}{i \hbar} [v, p_z].
\] (C.15)

We have the following relation,

\[
[F(q), p] = i \hbar \frac{\partial}{\partial q} F, \quad \text{where} \quad [q, p] = i \hbar.
\] (C.16)

using which the Eq. (C.15) reduces to,

\[
[\sigma \cdot \nabla, V(r)] = \frac{e \sigma_x}{i \hbar} \left( i \hbar \frac{\partial v}{\partial x} \right) + \frac{e \sigma_y}{i \hbar} \left( i \hbar \frac{\partial v}{\partial y} \right) + \frac{e \sigma_z}{i \hbar} \left( i \hbar \frac{\partial v}{\partial z} \right),
\]

\[
= - e \sigma_x E_x - e \sigma_y E_y - e \sigma_z E_z,
\] (C.17)

\[\Rightarrow [\beta \sigma \cdot \nabla, V(r)] = -e \beta \sigma \cdot E_{\text{int}}.\] (C.18)

On assembling back the results of the three commutators obtained in Eqns. (C.11, C.14 and C.18), the Eq. (C.7) becomes,

\[
[\beta \sigma \cdot \nabla, H_0] = - \frac{2i c}{\hbar} \beta \gamma_5 p^2 - e \beta \sigma \cdot E_{\text{int}},
\] (C.19)

or, in other words,

\[-e \beta \sigma \cdot E_{\text{int}} = [\beta \sigma \cdot \nabla, H_0] + \frac{2i c}{\hbar} \beta \gamma_5 p^2.\] (C.20)

On inserting the above result in Eq. (C.4) for \( \langle D^1 \rangle \) we get,

\[
\langle D^1 \rangle = d_e \left\{ \sum_{n \neq m} \frac{\langle \phi_m^{(0)} | (\beta \sigma \cdot \nabla, H_0) + \frac{2i c}{\hbar} \beta \gamma_5 p^2 | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right\} \left\{ \sum_{nm} \frac{\langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | (\beta \sigma \cdot \nabla, H_0) + \frac{2i c}{\hbar} \beta \gamma_5 p^2 | \phi_n^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right\}. \] (C.21)
Let us consider the following for the sake of simplifying it further,

\[ \langle D^1 \rangle = \langle D^{1.1} \rangle + \langle D^{1.2} \rangle \]  

where, \( \langle D^{1.1} \rangle = d \epsilon \left\{ \sum_{n \neq m} \frac{\langle \phi_m^{(0)} | [\beta \sigma \cdot \nabla, H_0] | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} + \sum_{n \neq m} \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | [\beta \sigma \cdot \nabla, H_0] | \phi_n^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right\} \).  

And \( \langle D^{1.2} \rangle = \left( \frac{2 \epsilon d \epsilon}{h} \right) \left\{ \sum_{n \neq m} \frac{\langle \phi_m^{(0)} | (i \beta \gamma_5 \mathbf{p}^2) | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} + \sum_{n \neq m} \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | (i \beta \gamma_5 \mathbf{p}^2) | \phi_n^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \right\} \).  

The commutator in \( \langle D^{1.1} \rangle \) can be simplified further, as below:

\[ \langle \phi_m^{(0)} | [\beta \sigma \cdot \nabla, H_0] | \phi_n^{(0)} \rangle = \langle \phi_m^{(0)} | (\beta \sigma \cdot \nabla) H_0 | \phi_n^{(0)} \rangle - \langle \phi_m^{(0)} | H_0 (\beta \sigma \cdot \nabla) | \phi_n^{(0)} \rangle, \]

\[ = E_m^{(0)} \langle \phi_m^{(0)} | \beta \sigma \cdot \nabla | \phi_n^{(0)} \rangle - E_n^{(0)} \langle \phi_n^{(0)} | \beta \sigma \cdot \nabla | \phi_m^{(0)} \rangle, \]

\[ = \left( E_m^{(0)} - E_n^{(0)} \right) \langle \phi_m^{(0)} | \beta \sigma \cdot \nabla | \phi_n^{(0)} \rangle. \]  

We have the completeness theorem given by,

\[ \sum_{n \neq m} |\phi_n^{(0)} \rangle \langle \phi_n^{(0)} | = 1 - |\phi_m^{(0)} \rangle \langle \phi_m^{(0)} |. \]  

Now, using Eqns. (C.25 and C.26), we can write,

\[ \sum_{n \neq m} \frac{\langle \phi_m^{(0)} | [\beta \sigma \cdot \nabla, H_0] | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} = - \langle \phi_m^{(0)} | (\beta \sigma \cdot \nabla) | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | z | \phi_m^{(0)} \rangle, \]

\[ = - \langle \phi_m^{(0)} | (\beta \sigma \cdot \nabla) z | \phi_m^{(0)} \rangle + \langle \phi_m^{(0)} | (\beta \sigma \cdot \nabla) | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | z | \phi_m^{(0)} \rangle. \]  

By using Eq. (C.27), one can simplify Eq. (C.23) as the following,

\[ \langle D^{1.1} \rangle = d \epsilon \langle \phi_n^{(0)} | [z, (\beta \sigma \cdot \nabla)] | \phi_n^{(0)} \rangle. \]
Now consider the following commutator,
\[ [z, (\beta \sigma \cdot \nabla)] = \beta \sigma_x \left[ z, \frac{\partial}{\partial x} \right] + \beta \sigma_y \left[ z, \frac{\partial}{\partial y} \right] + \beta \sigma_z \left[ z, \frac{\partial}{\partial z} \right], \]
\[ = \frac{i \beta \sigma_z}{\hbar} [z, p_z] + \frac{i \beta \sigma_y}{\hbar} [z, p_y] + \frac{i \beta \sigma_x}{\hbar} [z, p_x], \]
\[ = \frac{i \beta \sigma_x}{\hbar} \left( i \hbar \right) \frac{dz}{dz}, \]
\[ = -\beta \sigma_z. \quad (C.29) \]

\[ \Rightarrow \langle D^{1,1} \rangle = -d_e \langle \phi^{(0)}_n | \beta \sigma | \phi^{(0)}_n \rangle. \quad (C.30) \]

Now consider the term \( \langle D^{1,2} \rangle \) given in Eq. (C.24),
\[ \langle D^{1,2} \rangle = \left( \frac{2 c d_e}{\hbar} \right) \left\{ \sum_{n \neq m} \left( \frac{\phi^{(0)}_m | (i \beta \gamma_5 \mathbf{p}^2) | \phi^{(0)}_n \rangle (\phi^{(0)}_n | z | \phi^{(0)}_m)\rangle}{E^{(0)}_m - E^{(0)}_n} \right) + \sum_{n \neq m} \left( \frac{\phi^{(0)}_m | z | \phi^{(0)}_n \rangle (\phi^{(0)}_n | (i \beta \gamma_5 \mathbf{p}^2) | \phi^{(0)}_m \rangle)}{E^{(0)}_m - E^{(0)}_n} \right) \right\}. \quad (C.31) \]

Since \( z \) is real and hence \( z^\dagger = z \). Using the commutation relations of \( \beta \) and \( \gamma_5 \) we can show that, \( (i \beta \gamma_5 \mathbf{p}^2)^\dagger = (i \beta \gamma_5 \mathbf{p}^2) \). Hence, one can write the second term of Eq. (C.31) as the hermitian conjugate (h.c.) of the first term.

Therefore, \( \langle D^{1,2} \rangle = \left( \frac{2 c d_e}{\hbar} \right) \sum_{n \neq m} \left( \frac{\phi^{(0)}_m | (i \beta \gamma_5 \mathbf{p}^2) | \phi^{(0)}_n \rangle (\phi^{(0)}_n | z | \phi^{(0)}_m)\rangle}{E^{(0)}_m - E^{(0)}_n} \right) + h.c. \quad (C.32) \]

Using Eqns. (C.30 and C.32) in Eq. (C.22), we write,
\[ \langle D \rangle = -d_e \langle \phi^{(0)}_n | \beta \sigma | \phi^{(0)}_n \rangle + \left( \frac{2 c d_e}{\hbar} \right) \sum_{n \neq m} \left( \frac{\phi^{(0)}_m | (i \beta \gamma_5 \mathbf{p}^2) | \phi^{(0)}_n \rangle (\phi^{(0)}_n | z | \phi^{(0)}_m)\rangle}{E^{(0)}_m - E^{(0)}_n} \right) + h.c. \quad (C.33) \]

From Eq. (C.2), the total atomic EDM \( \langle D \rangle \) becomes,
\[ \langle D \rangle = \langle D^{0} \rangle + \langle D^{1} \rangle, \]
\[ = \left\{ d_e (\phi^{(0)}_n | \beta \sigma | \phi^{(0)}_n) - d_e (\phi^{(0)}_n | \beta \sigma | \phi^{(0)}_n) \right\} + \left( \frac{2 c d_e}{\hbar} \right) \sum_{n \neq m} \left( \frac{\phi^{(0)}_m | (i \beta \gamma_5 \mathbf{p}^2) | \phi^{(0)}_n \rangle (\phi^{(0)}_n | z | \phi^{(0)}_m)\rangle}{E^{(0)}_m - E^{(0)}_n} \right) + h.c., \]
\[ = \left( \frac{2 c d_e}{\hbar} \right) \sum_{n \neq m} \left( \frac{\phi^{(0)}_m | (i \beta \gamma_5 \mathbf{p}^2) | \phi^{(0)}_n \rangle (\phi^{(0)}_n | z | \phi^{(0)}_m)\rangle}{E^{(0)}_m - E^{(0)}_n} \right) + h.c. \quad (C.34) \]
Thus, the effective atomic EDM operator in the relativistic framework is given by

\[
\langle D \rangle = \left( \frac{2ie\alpha}{c\hbar} \right) \sum_{n\neq m} \frac{\langle \phi_m^{(0)} | \sum_i (\beta \gamma_5 \mathbf{p}^2_i | \phi_n^{(0)} \rangle \langle \phi_n^{(0)} | \sum_i e z_i | \phi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} + h.c. \quad (C.35)
\]

Here, we have shown that the EDM of an atom turns out to be non-zero when the electron is assumed to have intrinsic EDM and when it is treated relativistically.

One can also prove that, despite one considers the relativistic form of \( H_0 \), the total atomic EDM effectively vanishes by the similar cancellation of its different terms unless one considers the relativistic form of the interaction Hamiltonian, \( H_{EDM} \).

The important role of \( \beta \) in the interaction Hamiltonian has been pointed out by Salpeter (1958) who argued that the interaction of the EDM with the electromagnetic field has to be included into the Dirac equation in a Lorentz covariant manner. Later on, Sandars (1968) also emphasized the fact that the presence of \( \beta \) is the reason why Schiff's general theorem on the absence of effects linear in EDMs does not apply in the relativistic case.

\(^2\text{Note that, the summation over the individual electrons is re-introduced.}\)