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Gauge dependence of interelectronic potentials

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Abstract. It has been demonstrated by Gorceix and Indelicato and others that the effective potentials for the interaction between the electrons, derived in the Feynman and Coulomb gauges, respectively, lead to different results, when applied in a many-body procedure, even when the orbitals are generated in a local potential. This apparent gauge dependence is due to the fact that the standard many-body procedures include only the reducible part of the multiphoton exchange, while the irreducible part does contribute to leading relativistic order in the Feynman gauge but not in the Coulomb gauge. It is shown explicitly that when the irreducible part of the two-photon exchange (crossing photons) is taken into account, this gauge dependence is removed to leading relativistic order. The situation is expected to be the same in higher orders.

1. Introduction

There is now an increasing interest in relativistic many-body calculations, where combined relativistic and correlation effects are considered. For this purpose it is desirable to express the problem by means of a Schrödinger-like equation with an effective Hamiltonian. If such a Hamiltonian is available—to the desired degree of approximation—then it would be possible to apply the highly developed techniques of non-relativistic many-body theory, such as multiconfiguration Hartree-Fock (MCHF), many-body perturbation theory (MBPT) or coupled-cluster approach (CCA) also in the relativistic case.

In principle, an effective Hamiltonian expressed in terms of effective interaction potentials can be derived from QED, and several attempts have been made along this line. The potentials obtained in such a procedure, however, depend upon the particular gauge employed, and questions have been raised in the literature how this gauge dependence should be handled in a many-body context. Gorceix *et al* (1987) and Gorceix and Indelicato (1988) have found that the potentials derived in the Coulomb and Feynman gauges, respectively, lead to significantly different numerical results in a MCDF calculation. They conclude that the ambiguity is not entirely related to the use of SCF wavefunctions but is partly more fundamental in origin. It has been pointed out by Sucher (1988, 1989) that the iterative use of the first-order Feynman gauge potential leads to an error already in the leading relativistic order, $O(\alpha^2$ Hartree) (where using the atomic Hartree unit; 1 Hartree $= \alpha^2 mc^2$). Recently, Lindroth and Mårtensson-Pendrill (1989) have examined the gauge dependence further and found that the discrepancy remains, even if one goes beyond the no (-virtual)-pair approximation. As a curiosity they have noted that the discrepancy can be removed in leading order, if single-virtual-pair excitations are evaluated in the low-frequency limit, which is not valid for such excitations.

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Potentials derived from physical scattering processes should be gauge independent, provided *all* diagrams of a certain order are considered, as emphasised by Feinberg and Sucher (1988) in a comprehensive study of the two-photon problem. In a standard MBPT treatment, however, only the so-called *reducible* part of the multi-photon exchange diagrams is included, which leads to an apparent gauge dependence. In the present note an analysis is made of the complete two-photon exchange between the electrons (omitting self-energy and other radiative effects), and it is shown explicitly that the ladder part (non-crossing photons) is reproduced correctly to leading order in either gauge by using the standard potentials in second-order perturbation theory. The key point is, however, that also the crossed diagram (crossing photons) contributes to this order in non-Coulomb gauges. This part is *irreducible* in the sense that it is not included in a procedure, where the single-photon potential is used repeatedly in a perturbation scheme. It is found that this irreducible part corresponds exactly to the discrepancy found in the analyses of Gorceix and Indelicato and of Lindroth and Mårtensson-Pendrill. This part can be expressed by means of a 'correction' potential, or irreducible two-photon potential, which has *the same form* as the potential contribution due to a single virtual pair, although it lies entirely within the NVP approximation. This is the underlying reason for the strange-looking result of Lindroth and Mårtensson-Pendrill, mentioned above. In the Coulomb gauge the correct electron–electron interaction is reproduced in leading order *without* any correction potential, and is from that point of view more convenient to use in a many-body treatment. In order to go beyond the leading order, however, irreducible two-, three-photon potentials are needed in any gauge, and a more detailed analysis is needed in order to find out which approach is most convenient on that level of sophistication.

In the present analysis we consider only effects of $O(\alpha^2$ Hartree). In non-Coulomb gauges there are also spurious contributions of $O(\alpha$ Hartree), which are known to cancel, when crossed photons are considered (Love 1978, Lindgren 1988, p 384).

2. Single-photon exchange

As an introduction we consider the exchange of a single virtual photon between the electrons, which will reproduce the well known fact that the first-order energy contribution is gauge independent.

The exchange of a single virtual photon between two bound-state electrons, represented by the Feynman diagram in figure 1(a) can be expressed by means of the second-order S matrix ($\hbar = 1$)

$$S^{(2)} = -\tfrac{1}{2}\int\int \mathrm{d}^4x_1\, \mathrm{d}^4x_2\; T[\mathscr{H}_{\mathrm{int}}(x_1)\mathscr{H}_{\mathrm{int}}(x_2)]\exp(-\delta_1|t_1| - \delta_2|t_2|) \qquad (2.1)$$

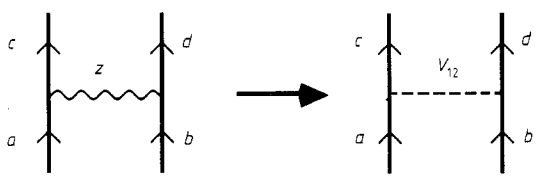

Figure 1. The Feynman representation of the exchange of a single, virtual photon between two electrons (a) is compared with an effective-potential interaction (b). The heavy lines represent electronic states in the bound-interaction picture.

where T is the time-ordering symbol and

$$\mathscr{H}_{\rm int}(x) = -e\bar{\Psi}(x)\gamma^{\mu}A_{\mu}(x)\Psi(x) = -e\Psi^{\dagger}(x)\alpha^{\mu}A_{\mu}(x)\Psi(x). \tag{2.2}$$

The Dirac fields are given in the bound-interaction picture by

$$\Psi(x) = \sum_j c_j\phi_j(x) = \sum_j c_j\phi_j(\boldsymbol{x})\exp(-i\varepsilon_j t)$$

$$\bar{\Psi}(x) = \Psi^{\dagger}(x)\gamma^0 \qquad \Psi^{\dagger}(x) = \sum_j c_j^{\dagger}\phi_j^{\dagger}(x) = \sum_j c_j^{\dagger}\phi_j^{\dagger}(\boldsymbol{x})\exp(i\varepsilon_j t) \tag{2.3}$$

where the orbitals $\{\phi_j\}$ are generated by the Dirac Hamiltonian with the nuclear potential and an external-field potential U

$$h_0\phi_j = \varepsilon_j\phi_j \qquad h_0 = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 - Z\,e^2/4\pi\varepsilon_0 r + U \tag{2.4}$$

and $c_j/c_j^{\dagger}$ are the corresponding annihilation/creation operators. The gamma matrices are here represented by

$$\gamma^{\mu} = \gamma^0\alpha^{\mu} \qquad \alpha^{\mu} = (1, \boldsymbol{\alpha}) \qquad \gamma^0 = \beta$$

where $\boldsymbol{\alpha}, \beta$ are the standard Dirac matrices. δ_1, δ_2 are damping coefficients, which eventually go to zero in the adiabatic approximation (Gell-Mann and Low 1951, Sucher 1957, 1989, Mohr 1989).

The scattering amplitude for the process in figure 1(a) is

$$\langle cd|S^{(2)}|ab\rangle = -\frac{ie^2}{c}\sum_j\int\int d^4x_1\,d^4x_2\,\phi_d^{\dagger}(x_2)\alpha^{\nu}\phi_b(x_2)\phi_c^{\dagger}(x_1)\alpha^{\mu}\phi_a(x_1)D_{F\nu\mu}(x_2-x_1) \tag{2.5}$$

where the Feynman photon propagator, $D_{F\nu\mu}(x_2-x_1)$, is defined by

$$\langle 0|T[A_{\nu}(x_2)A_{\mu}(x_1)|0\rangle = \frac{i}{c}D_{F\nu\mu}(x_2-x_1) \tag{2.6}$$

After performing the time integrations, this becomes

$$\langle cd|S^{(2)}|ab\rangle = -2\pi i\,e^2 c\int_{-\infty}^{\infty} dz\,\delta(\varepsilon_c-\varepsilon_a+z)\delta(\varepsilon_d-\varepsilon_b-z)$$

$$\times\int\int d^3x_1\,d^3x_2\,\phi_d^{\dagger}(\boldsymbol{x}_2)\alpha^{\nu}\phi_b(\boldsymbol{x}_2)\phi_c^{\dagger}(\boldsymbol{x}_1)\alpha^{\mu}\phi_a(\boldsymbol{x}_1)D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1;\,z) \tag{2.7}$$

where $D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1;\,z)$ is the Fourier transform of the photon propagator with respect to time

$$D_{F\nu\mu}(x_2-x_1) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dz\,\exp[-iz(t_2-t_1)]D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1;\,z) \tag{2.8}$$

Performing the z integration yields

$$\langle cd|S^{(2)}|ab\rangle = -2\pi i\,e^2 c\delta(\varepsilon_a+\varepsilon_b-\varepsilon_c-\varepsilon_d)\langle cd|\alpha_1^{\mu}\alpha_2^{\nu}D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1;\,cq)|ab\rangle \tag{2.9}$$

where $cq = \varepsilon_a - \varepsilon_c = \varepsilon_d - \varepsilon_b$.

Formally, the S-matrix element (2.9) is the same as that of potential scattering (figure 1(b))

$$\langle cd|S^{(1)}|ab\rangle = -2\pi i\delta(\varepsilon_a+\varepsilon_b-\varepsilon_c-\varepsilon_d)\langle cd|V_{12}|ab\rangle \tag{2.10}$$

with the potential given by

$$V_{12} = V_{12}(cq) = e^2 c\alpha_1^{\mu}\alpha_2^{\nu}D_{F\mu\nu}(\boldsymbol{x}_2-\boldsymbol{x}_1;\,cq). \tag{2.11}$$

This gives

$$V_{12}^{F}(cq) = \frac{e^2}{4\pi\varepsilon_0}(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\frac{\exp(i|q|r_{12})}{r_{12}} \tag{2.12a}$$

$$V_{12}^{C}(cq) = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_{12}} - \boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2\frac{\exp(i|q|r_{12})}{r_{12}} + \left[\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1, \left(\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2, \frac{\exp(i|q|r_{12})-1}{q^2 r_{12}}\right)\right]\right) \tag{2.12b}$$

in the Feynman and the Coulomb gauges, respectively. By means of the Gellman-Low-Sucher procedure it can be shown that such a potential leads to the correct first-order shift

$$\Delta^{(1)}E = \langle\Phi|V_{12}(cq)|\Phi\rangle = \langle ab|V_{12}(cq)|ab\rangle - \langle ba|V_{12}(cq)|ab\rangle \tag{2.13}$$

where Φ is the *antisymmetrised*, unperturbed state $|\{ab\}\rangle$

In the limit $q \Rightarrow 0$ the potentials (2.12) reduce to

$$V_{12}^{F}(0) = \frac{e^2}{4\pi\varepsilon_0}(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)/r_{12} \tag{2.14a}$$

$$V_{12}^{C}(cq) = \frac{e^2}{4\pi\varepsilon_0}\{1-\tfrac{1}{2}[\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1\cdot\boldsymbol{r}_{12})(\boldsymbol{\alpha}_2\cdot\boldsymbol{r}_{12})/r_{12}^2]\}/r_{12} \tag{2.14b}$$

known as the Coulomb-Gaunt and the Coulomb-Breit interactions, respectively.

If the orbitals are generated in a *local* external potential (2.4), then the commutators in (2.12*b*) can be replaced by

$$-\frac{1}{c^2q^2}[h_0(1),[h_0(2),A]] \qquad A = \frac{\exp(i|q|r_{12})-1}{r_{12}} \tag{2.15}$$

and the difference between the potentials becomes

$$\langle cd|V_{12}^{F} - V_{12}^{C}|ab\rangle = \frac{e^2}{4\pi\varepsilon_0}\left(1+\frac{(\varepsilon_c-\varepsilon_a)(\varepsilon_d-\varepsilon_b)}{c^2q_{ca}^2}\right)\langle cd|A|ab\rangle \tag{2.16}$$

which vanishes in the case of energy conservation. This reproduces the well known fact that the two potentials give exactly the same first-order energy shift in the case of a local potential.

3. Two-photon exchange

In second order there are two Feynman diagrams contributing to the interelectronic interaction, the 'ladder' and the 'crossed' diagrams, shown in figure 2, omitting self-energy and other radiative effects. Performing the time integrations as before, the

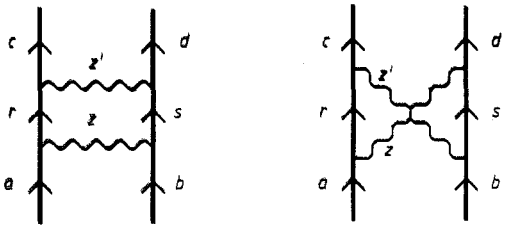

Figure 2. The two-photon exchange between the electrons is represented by two Feynman diagrams, the 'ladder' and the 'crossed-photon' diagram.

S-matrix element for the ladder diagram can be expressed

$$\begin{aligned}\langle cd|S_{\mathrm{L}}^{(4)}|ab\rangle &= \delta(\varepsilon_a+\varepsilon_b-\varepsilon_c-\varepsilon_d)\\ &\times \mathrm{e}^4c^2\int\int\int\int \mathrm{d}^3x_1\ldots\mathrm{d}^3x_4\,\phi_d^\dagger(x_4)\alpha^\tau S_{\mathrm{F}}(x_4,x_2;\varepsilon_b+z)\alpha^\nu\phi_b(x_2)\\ &\times\phi_c(x_3)\alpha^\sigma S_{\mathrm{F}}(x_3,x_1;\varepsilon_a-z)\alpha^\mu\phi_a(x_1)\\ &\times D_{\mathrm{F}\tau\sigma}(x_4-x_3;\varepsilon_a-\varepsilon_c-z)D_{\mathrm{F}\nu\mu}(x_2-x_1;z)\end{aligned}\tag{3.1}$$

where $S_{\mathrm{F}}(x',x;z)$ is the Fourier transform of the *Feynman electron propagator*

$$\begin{aligned}S_{\mathrm{F}}(x',x) &= -\mathrm{i}\langle 0|T[\Psi(x')\Psi^\dagger(x)|0\rangle = \frac{1}{2\pi}\int \mathrm{d}z\,\exp[-\mathrm{i}z(t'-t)]S_{\mathrm{F}}(x',x;z)\\ S_{\mathrm{F}}(x',x;z) &= \sum_i \frac{\phi(x')\phi^\dagger(x)}{z-\varepsilon_i+\mathrm{i}\eta\varepsilon_i}.\end{aligned}\tag{3.2}$$

(Note that in this formalism energy is conserved at each vertex, using the energy parameters of the propagators.) With the potential (2.11) the corresponding two-photon potential can in any gauge be expressed

$$\langle cd|V_{\mathrm{L}}^{(2)}|ab\rangle = -\frac{1}{2\pi\mathrm{i}}\sum_{rs}\int \mathrm{d}z\,\frac{\langle c_3d_4|V_{34}(\varepsilon_a-\varepsilon_c-z)|r_3s_4\rangle\langle r_1s_2|V_{12}(z)|a_1b_2\rangle}{(\varepsilon_a-\varepsilon_r-z+\mathrm{i}\eta\varepsilon_r)(\varepsilon_b-\varepsilon_s+z+\mathrm{i}\eta\varepsilon_s)}\tag{3.3}$$

and similarly for the crossed diagram

$$\langle cd|V_{\mathrm{X}}^{(2)}|ab\rangle = -\frac{1}{2\pi\mathrm{i}}\sum_{rs}\int \mathrm{d}z\,\frac{\langle c_3s_4|V_{34}(\varepsilon_a-\varepsilon_c-z)|r_3b_4\rangle\langle r_1d_2|V_{12}(z)|a_1s_2\rangle}{(\varepsilon_a-\varepsilon_r-z+\mathrm{i}\eta\varepsilon_r)(\varepsilon_d-\varepsilon_s-z+\mathrm{i}\eta\varepsilon_s)}.\tag{3.4}$$

In the present study we are not concerned with terms beyond the leading relativistic order $\mathrm{O}(\alpha^2$ Hartree). (We also omit terms of $\mathrm{O}(\alpha$ Hartree), which, as mentioned in the introduction, are known to cancel.) Therefore, we need not consider virtual-pair excitations, which means that all intermediate states will have *positive* energy. In the Coulomb gauge we can then use the unretarded potential (2.14*b*), which is correct to that order also off the energy shell. In the Feynman gauge, on the other hand, we must include the leading part of the retardation. Since the imaginary part of the potential does not enter in this order (Lindgren 1989, p 383), we can here use the form

$$V^{\mathrm{F}}(cq) = (1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\cos(qr_{12})/r_{12} = (1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)(\mathrm{e}^{\mathrm{i}qr_{12}}+\mathrm{e}^{-\mathrm{i}qr_{12}})/2r_{12}\tag{3.5}$$

leaving out the factor $\mathrm{e}^2/4\pi\varepsilon_0$. Only one of the interactions can be retarded in the order we consider, and standard complex integration technique then gives in either gauge

$$\begin{aligned}\langle cd|V_{\mathrm{L}}^{(2)}|ab\rangle &= \tfrac{1}{2}\sum_{rs}\{\langle cd|r_{12}^{-1}|rs\rangle\langle rs|V(a-r)+V(b-s)|ab\rangle\\ &\quad+\langle cd|V(c-r)+V(d-s)|rs\rangle\langle rs|r_{12}^{-1}|ab\rangle\}/(\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s)\\ &= \sum_{rs}\{\langle cd|r_{12}^{-1}|rs\rangle\langle rs|V^{\mathrm{BM}}|ab\rangle\\ &\quad+\langle cd|V^{\mathrm{BM}}|rs\rangle\langle rs|r_{12}^{-1}|ab\rangle\}/(\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s).\end{aligned}\tag{3.6}$$

Here, $V(i-j)=V(\varepsilon_i-\varepsilon_j)$ and V^{BM} is the generalised potential of Brown (1952) and Mittleman (1972)

$$\langle rs|V^{\mathrm{BM}}|ab\rangle = \tfrac{1}{2}\langle rs|V(a-r)+V(b-s)|ab\rangle.\tag{3.7}$$

To leading order the ladder potential (3.6) can be expressed

$$\langle cd|V_{\mathrm{L}}^{(2)}|ab\rangle = \sum_{rs} \langle cd|V^{\mathrm{BM}}|rs\rangle\langle rs|V^{\mathrm{BM}}|ab\rangle/(\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s) \tag{3.8}$$

which represents the *reducible* part of the two-photon interaction, since it can be expressed by means of repeated use of a single-photon potential. The Brown-Mittleman potential is in the Coulomb gauge identical to leading relativistic order to the unretarded Coulomb-Breit potential (2.14*b*), which means that the ladder diagram is correctly reproduced to that order by iterating the latter potential.

For the crossed diagram we get in an analogous way

$$\begin{aligned}\langle cd|V_X^{(2)}|ab\rangle &= -\tfrac{1}{2}\sum_{rs}\{\langle cs|r_{12}^{-1}|rb\rangle\langle rd|V(a-r)-V(d-s)|as\rangle \\ &\quad +\langle cs|V(c-r)-V(b-s)|rb\rangle\langle rd|r_{12}^{-1}|as\rangle\}/(\varepsilon_a+\varepsilon_s-\varepsilon_d-\varepsilon_r) \qquad (3.9)\\ &= -\sum_{rs}\{\langle cd|r_{12}^{-1}|rs\rangle\langle rs|V^{\mathrm{diff}}|ab\rangle \\ &\quad +\langle cd|V^{\mathrm{diff}}|rs\rangle\langle rs|r_{12}^{-1}|ab\rangle\}/(\varepsilon_a+\varepsilon_s-\varepsilon_d-\varepsilon_r)\end{aligned}$$

where V^{diff} is the 'difference' potential

$$\langle rs|V^{\mathrm{diff}}|ab\rangle = \tfrac{1}{2}\langle rs|V(a-r) \quad V(b-s)|ab\rangle. \tag{3.10}$$

Only retardation contributes to the latter potential, and therefore the leading relativistic part vanishes in the Coulomb gauge, but not in the Feynman gauge.

The results given above can also be obtained from the more general two-photon potentials (Lindgren 1989)

$$\begin{aligned}\langle cd|V_L^{(2)}|ab\rangle &= \tfrac{1}{2}\sum_{rs}\{\mathrm{sgn}(\varepsilon_r)\langle cd|V(c-r)|rs\rangle\langle rs|V(a-r)|ab\rangle \\ &\quad +\mathrm{sgn}(\varepsilon_s)\langle cd|V(d-s)|rs\rangle\langle rs|V(b-s)|ab\rangle\}/(\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s) \qquad (3.11a)\\ \langle cd|V_X^{(2)}|ab\rangle &= \tfrac{1}{2}\sum_{rs}\{-\mathrm{sgn}(\varepsilon_r)\langle cs|V(c-r)|rb\rangle\langle rd|V(a-r)|as\rangle \\ &\quad +\mathrm{sgn}(\varepsilon_s)\langle cs|V(b-s)|rb\rangle\langle rd|V(d-s)|as\rangle\}/(\varepsilon_a+\varepsilon_s-\varepsilon_r-\varepsilon_d) \qquad (3.11b)\end{aligned}$$

by considering the leading relativistic contribution.

The potential of the crossed diagram (3.9) is *irreducible*, since it cannot be expressed in terms of single-photon potentials in a perturbative way. Formally, however, we can express this as a second-order perturbation expression applied to the particle-hole diagram (figure 3(*b*)), where one of the interactions is the Brown-Mittleman potential

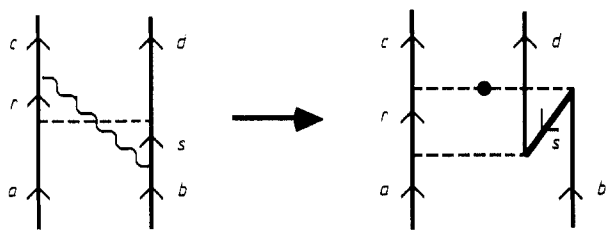

Figure 3. The structure of the crossed-photon diagram (*a*) is similar to the standard MBPT diagram with a single particle-hole (*b*), although it contributes also in the no-virtual-pair approximation. One of the interactions is here of the average type (3.6) and the other is the difference potential (3.9).

(3.7) and the other is the difference potential (3.9). The fact that the leading relativistic part of the latter vanishes in the Coulomb gauge, but not in the Feynman gauge is the source of the apparent gauge dependence, which will be further analysed in the following section.

4. Comparison between the two-photon contributions

It follows from the treatment above that in the Coulomb gauge the standard Coulomb + (energy-independent) Breit potential applied in second-order perturbation theory within the no-virtual-pair approximation reproduces correctly the leading relativistic contribution of $O(\alpha^2$ Hartree) to the two-photon interaction between the electrons. This implies that using that gauge the irreducible part of the two-photon interaction enters first in higher orders in α. The situation is different in the Feynman gauge, where not even the energy-dependent form of the one-photon potential is sufficient to yield the leading order correctly. Here, also the irreducible part, corresponding to crossed-photon exchange, enters already in $O(\alpha^2$ Hartree). We shall now show explicitly that when this irreducible part is taken into account, the two gauges give the same two-photon contribution to that order.

4.1. Ladder diagram

We shall first compare the ladder part of the two-photon contribution (3.6). We express the single-photon potentials, $V(i-j)$, as a Coulomb–Gaunt part and a remainder

$$V(i-j) = (1-\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) r_{12}^{-1} + R_{ij} \tag{4.1}$$

where in the leading order

$$\begin{aligned} &R_{ij}^{\mathrm{F}} = q_{ij}^2 F_0 \qquad F_0 = -\tfrac{1}{2} r_{12} \\ &R_{ij}^{\mathrm{C}} = R^{\mathrm{C}} = -c^{-2}[h_0(1), [h_0(2), F_0]] \end{aligned} \tag{4.2}$$

in the Feynman and Coulomb gauges, respectively. The difference between the ladder contributions in the two gauges now becomes

$$\begin{aligned} \langle cd|\delta V_{\mathrm{L}}^{(2)}|ab\rangle &= \tfrac{1}{2}\sum_{rs} \{\langle cd|r_{12}^{-1}|rs\rangle\langle rs|R_{ar}^{\mathrm{F}} + R_{bs}^{\mathrm{F}} - 2R^{\mathrm{C}}|ab\rangle \\ &\quad + \langle cd|R_{cr}^{\mathrm{F}} + R_{ds}^{\mathrm{F}} - 2R^{\mathrm{C}}|rs\rangle\langle rs|r_{12}^{-1}|ab\rangle\}/(\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s) \\ &= \tfrac{1}{2}\sum_{rs} \{\langle cd|r_{12}^{-1}|rs\rangle\langle rs|(q_{ar} + q_{bs})^2 F_0|ab\rangle \\ &\quad + \langle cd|(q_{cr} + q_{ds})^2 F_0|rs\rangle\langle rs|r_{12}^{-1}|ab\rangle\}/(\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s) \end{aligned} \tag{4.3}$$

where $q_{ij} = (\varepsilon_i - \varepsilon_j)/c$. But $q_{cr} + q_{ds} = q_{ar} + q_{bs} = (\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s)/c$, so one factor cancels the energy denominator, as observed by Lindroth and Mårtensson-Pendrill (1989). Expressing the other factor in terms of commutators, we get

$$\begin{aligned} \langle cd|\delta V_L^{(2)}|ab\rangle &= \frac{1}{2c^2}\sum_{rs} \{\langle cd|r_{12}^{-1}|rs\rangle\langle rs|[F_0, h_0(1) + h_0(2)]|ab\rangle \\ &\quad + \langle cd|[h_0(1) + h_0(2), F_0]|rs\rangle\langle rs|r_{12}^{-1}|ab\rangle\} \\ &= \frac{1}{2c^2}\langle cd|[h_0(1) + h_0(2), F_0]\Lambda_{++} r_{12}^{-1} + r_{12}^{-1}\Lambda_{++}[F_0, h_0(1) + h_0(2)]|ab\rangle \end{aligned} \tag{4.4}$$

where Λ_{++} is the projection operator for the positive-energy virtual states. This is the discrepancy between the two gauges found by Gorceix and Indelicato (1988) and by Lindroth and Mårtensson-Pendrill (1989). However, these authors considered only the *reducible* part of the two-photon interaction, and we shall see below that this discrepancy is removed when also the *irreducible* part, due to *crossed photons* in the Feynman gauge, is taken into account.

4.2. Crossed diagram

From the two-photon expression for the crossed photons (3.8) we get

$$\begin{aligned}\langle cd|\delta V_X^{(2)}|ab\rangle &= -\tfrac{1}{2}\sum_{rs}\{\langle cs|r_{12}^{-1}|rb\rangle\langle rd|R_{ar}^F - R_{ds}^F|as\rangle \\ &\quad + \langle cs|R_{cr}^F - R_{bs}^F|rb\rangle\langle rd|r_{12}^{-1}|as\rangle\}/(\varepsilon_a+\varepsilon_s-\varepsilon_d-\varepsilon_r) \\ &= -\tfrac{1}{2}\sum_{rs}\{\langle cs|(q_{cr}^2 - q_{sb}^2)F_0|rb\rangle\langle rd|r_{12}^{-1}|as\rangle \\ &\quad + \langle cs|r_{12}^{-1}|rb\rangle\langle rd|(q_{ra}^2 - q_{ds}^2)F_0|as\rangle\}/(\varepsilon_a+\varepsilon_s-\varepsilon_d-\varepsilon_r). \qquad (4.5)\end{aligned}$$

Also here one factor cancels the energy denominator, and the result can be expressed

$$\begin{aligned}\langle cd|\delta V_X^{(2)}|ab\rangle &= -\frac{1}{2c^2}\sum_{rs}\{(\varepsilon_a+\varepsilon_d-\varepsilon_r-\varepsilon_s)\langle cs|r_{12}^{-1}|rb\rangle\langle rd|F_0|as\rangle \\ &\quad + (\varepsilon_c+\varepsilon_b-\varepsilon_r-\varepsilon_s)\langle cs|F_0|rb\rangle\langle rd|r_{12}^{-1}|as\rangle\}. \qquad (4.6)\end{aligned}$$

Exchanging the second orbital between the bras and the kets, gives

$$\langle cd|\delta V_X^{(2)}|ab\rangle = -\frac{1}{2c^2}\langle cb^*|[h_0(1)+h_0(2), F_0]\Lambda_{++}r_{12}^{-1} + r_{12}^{-1}\Lambda_{++}[F_0, h_0(1)+h_0(2)]|ad^*\rangle. \qquad (4.7)$$

We can here exchange the second orbital once more, and then we see that *this irreducible contribution exactly cancels the discrepancy (4.4) found in the reducible, ladder contribution between the gauges.*

5. Conclusions

By using a single-photon potential in a many-body calculation within the no-virtual-pair (NVP) approximation the *reducible* part of the two-photon interaction between a pair of electrons is properly taken into account to $O(\alpha^2$ Hartree). In the Coulomb gauge this represents the entire interaction to this order, while in the Feynman gauge also the *irreducible* part due to *crossing photons*—still within the NVP approximation—is of the same order. When this part is taken into account, the two gauges yield the same energy shift to that order. The virtual-pair excitations do not contribute in this order. There will be contributions to leading order in the Feynman gauge also from the exchange of more than two photons, and this will be analysed in a forthcoming paper.

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