Erratum: "Perspectives of relativistic quantum chemistry: The negative energy cat smiles" [Phys. Chem. Chem. Phys. 14, 35 (2012)]

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Received XX, Accepted XX
First published on the web Xth XXXXXXXXXX 200X
DOI: XX

To reveal the contribution of negative energy states to correlation, a complete derivation of the first and second order (nonradiative) QED energies for instantaneously interacting electrons is presented based on the simple rules for algebraically evaluating the Feynman diagrams. The previous equations that hold only for the special case of two electrons are hence corrected.

Although claimed for a many electron system, some of the (nonradiative and nonretarded) QED energy expressions (i.e., Eqs. (92), (95), and (107)) in Ref.[1] are found to hold only for the special case of two electrons. In particular, except for the diagrams considered before (see Figs. (3a) to (3h)), the so-called three-electron-two-photon diagram[2] shown in Fig. (3i) should also be included for the second order energy $E^{(2)}$ of a many-electron system. Since the QED energy expressions for more than three electrons have not yet been documented in the literature, it is worthwhile to make a complete derivation here. For this purpose, some simple rules are first provided in Appendix A so as to directly write down the algebraic equations for the Feynman diagrams. Further combined with the integral identities in Appendix B, the elements of the S-matrix and hence the energy shifts can readily be evaluated. It is further shown that the disconnected but linked diagrams shown in Fig. (4) should also be considered to precisely cancel the singular terms arising from Fig. (3), a point that is rarely mentioned in the QED literature. The final two-body terms of $E^{(2)}$ include Eqs. (30), (31), (42), and (76), while the one-body terms include Eqs. (97) and (99). Consequently, Eqs. (95) and (107) in Ref.[1] should be replaced with the present Eqs. (42) and (99), respectively. Although formerly the same, Eq. (92) in Ref.[1] (actually the first term of the present Eq. (32)) should be understood as the present Eq. (72) arising from Fig. (3i). Notwithstanding these corrections for the equations, which are only necessary for more generality, none of the statements in the original context needs to be revised. In particular, the '*(time-independent) potential-independent no-pair approximation + (time-dependent) perturbative QED*' approach advocated therein for high-precision structure calculations is not altered. This approach not only gets rid of the intrinsic $O(Z\alpha)^3$ uncertainty of the no-pair DC/DCB equation, but also paves a seamless bridge between relativistic quantum chemistry and QED that used to be two mutually exclusive subfields.

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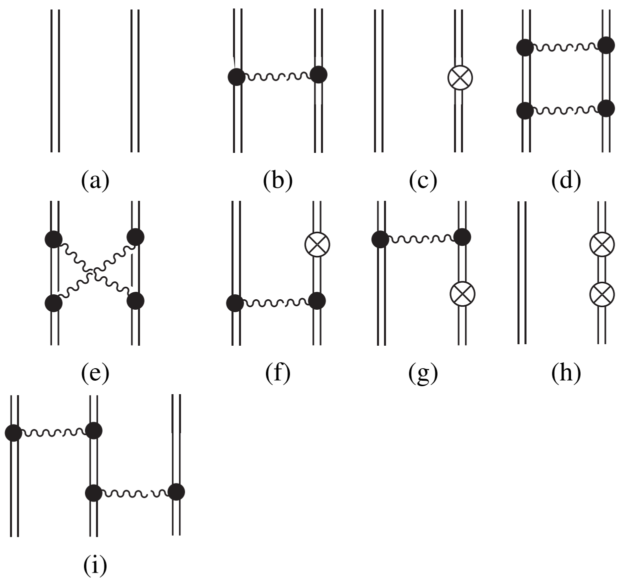
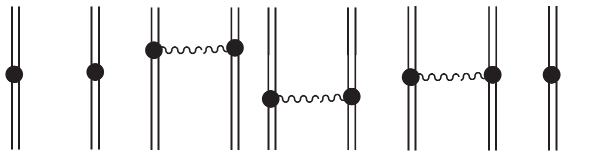
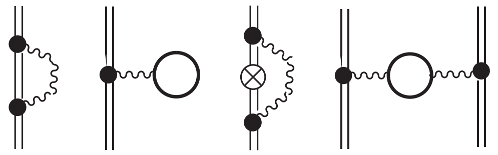


Fig. 3 Feynman diagrams associated with the zeroth (a), first (b, c), and second (d-i) order energies



(a) (b) (c)

Fig. 4 Disconnected but linked Feynman diagrams



(a) (b) (c) (d)

Fig. 5 Feynman diagrams for (a) electron self-energy, (b) vacuum polarization, (c) vertex correction, and (d) photon self-energy

Acknowledgments

The author is grateful to Prof. J. Sapirstein for drawing his attention to the three-electron-two-photon diagram and Dr. Y. Xiao for carefully checking the equations. The research of this work is supported by the National Natural Science Foundation of China (Project No. 21033001).

A The S-matrix

According to the S-matrix formulation of QED, we need to consider the diagrams in Figs. (3) to calculate the first and second order energies due to the perturbing potentials (cf. Eqs. (85) and (86) in Ref.[1]) by means of the following formulae

$$E^{(1)} = \lim_{\gamma\to 0}\frac{i\gamma}{2}\{\langle\alpha|S^{(1)}|\alpha\rangle+[2\langle\alpha|S^{(2)}|\alpha\rangle -\langle\alpha|S^{(1)}|\alpha\rangle^2]\}, \quad (1)$$

$$E^{(2)} = \lim_{\gamma\to 0}\frac{i\gamma}{2}\{[3\langle\alpha|S^{(3)}|\alpha\rangle-3\langle\alpha|S^{(1)}|\alpha\rangle\langle\alpha|S^{(2)}|\alpha\rangle] +[4\langle\alpha|S^{(4)}|\alpha\rangle-2\langle\alpha|S^{(2)}|\alpha\rangle^2]\}, \quad (2)$$

where $|\alpha\rangle$ represents the unperturbed electronic state. It will be shown later on that the disconnected but linked diagrams in Fig. (4) are also needed to fully cancel the singular terms arising from Fig. (3), a point that is rarely mentioned in the QED literature. The n-th order S-matrix defined as

$$S^{(n)} = \frac{(-i)^n}{n!}\int dx_1^4\cdots\int dx_n^4 T[\mathscr{H}(x_1)\cdots\mathscr{H}(x_n)] \times e^{-\gamma(|t_1|+\cdots|t_n|)}, \quad (3)$$

$$\mathscr{H}(x) = -e\phi^\dagger(x)c\alpha^\mu A_\mu(x)\phi(x) \quad (4)$$

can be rewritten in second-quantized form

$$S^{(n)}=\frac{n_d}{n!}(S^{(n)})^{q_1q_2\cdots q_m}_{p_1p_2\cdots p_m}\{a^{p_1p_2\cdots p_m}_{q_1q_2\cdots q_m}\}_n, \quad (5)$$

where $\{p_1,p_2,\cdots,p_m\}$ and $\{q_1,q_2,\cdots,q_m\}$ denote the respective outgoing and incoming free orbital lines of a Feynman diagram, while n_d represents the degeneracy of the diagram. The weight factor n_d can be counted as follows: Each of the possible assignments of the electron propagators

$$S_F(x_i,x_j) = \int\frac{d\omega}{2\pi}S_F(\omega;\vec{r}_i,\vec{r}_j)e^{-i\omega(t_i-t_j)}, \quad i\le j, \quad (6)$$

$$S_F(\omega;\vec{r}_i,\vec{r}_j) = \frac{\varphi_p(\vec{r}_i)\varphi_p^\dagger(\vec{r}_j)}{\omega-\varepsilon_p(1-i\eta)} \quad (7)$$

contributes a factor of two if $i<j$ or a factor of one if $i=j$. The numbers of such electron propagators are denoted as n_{F2} and n_{F1}, respectively. In contrast, each of the possible assignments (n_P) of *all* the photon interactions $I(z;\vec{r}_i,\vec{r}_j)$ contributes a factor of one independently of the ordering of the vertices i and j, i.e., $I(z;\vec{r}_j,\vec{r}_i)=I(z;\vec{r}_i,\vec{r}_j)$. Therefore, $n_d=max(1,n_{F1}+2n_{F2})\times max(1,n_P)$. Specific examples are given in Table 2. The integral $(S^{(n)})^{q_1q_2\cdots q_m}_{p_1p_2\cdots p_m}$ in Eq. (5) reads

$$\begin{aligned}(S^{(n)})^{q_1q_2\cdots q_m}_{p_1p_2\cdots p_m} &= (-1)^{n_l}\int\frac{z_1}{2\pi}\int\frac{z_2}{2\pi}\cdots\int\frac{\omega_1}{2\pi}\int\frac{\omega_2}{2\pi}\cdots\\ &\times \langle p_1p_2\cdots p_m|\\ &\times (-i)I(z_1;\vec{r}_{i_1},\vec{r}_{i_2})(-i)I(z_2;\vec{r}_{i_3},\vec{r}_{i_4})\cdots\\ &\times iS_F(\omega_1;\vec{r}_{j_1},\vec{r}_{j_2})iS_F(\omega_2;\vec{r}_{j_3},\vec{r}_{j_4})\cdots\\ &\times |q_1q_2\cdots q_m\rangle\\ &\times 2\pi\Delta_\gamma(E_1)2\pi\Delta_\gamma(E_2)\cdots2\pi\Delta_\gamma(E_n). \quad (8)\end{aligned}$$

That is, there is a factor $\int\frac{d\omega}{2\pi}iS_F(\omega;\vec{r}_i,\vec{r}_j)$ for each contracted pair of electron fields and a factor $\int\frac{dz}{2\pi}(-i)I(z;\vec{r}_k,\vec{r}_l)$ for each photon interaction. In the Coulomb gauge, the instantaneous Coulomb/Breit interaction $I(z;\vec{r}_k,\vec{r}_l)$ is simply the $g(k,l)$ operator defined in Eq. (5) in Ref.[1]. Note that there is no z-integration for the counter potential $-U(\vec{r})$, see Eq. (86) in Ref.[1]. Furthermore, there is a factor $2\pi\Delta_\gamma(E_i)$ for each vertex arising from the time integration (see Eq. (104)). The argument E_i is just the difference between the incoming and outgoing orbital energies/photon frequencies through the vertex. Finally, there is a global factor $(-1)^{n_l}$, with n_l being the number of loops. These rules of thumb for evaluating the Feynman diagrams have been documented in the recent book by Lindgren[3]. However, they are only complete when combined with the present rules for counting the degeneracy n_d of the diagrams. The integral identities in Sec. B can further be employed to facilitate the evaluation of $(S^{(n)})^{q_1q_2\cdots q_m}_{p_1p_2\cdots p_m}$ (8). The following identity is also very useful for evaluating the expectation value of the excitation operator $\{a^{p_1p_2\cdots p_m}_{q_1q_2\cdots q_m}\}_n$ (normal ordered with respect to the NES) over the unperturbed state

$|\alpha\rangle$:

$$
\begin{aligned}
\langle\alpha|a^{p_1p_2\cdots p_{m-1}p_m}_{q_1q_2\cdots q_{m-1}q_m}|\alpha\rangle = \langle\alpha| \quad & \delta^{p_m}_{q_m} a^{p_1p_2\cdots p_{m-2}p_{m-1}}_{q_1q_2\cdots q_{m-2}q_{m-1}} \\
- \quad & \delta^{p_m}_{q_{m-1}} a^{p_1p_2\cdots p_{m-2}p_{m-1}}_{q_1q_2\cdots q_{m-2}q_m} \\
- \quad & \delta^{p_m}_{q_{m-2}} a^{p_1p_2\cdots p_{m-2}p_{m-1}}_{q_1q_2\cdots q_m q_{m-1}} \\
- \quad & \cdots \\
- \quad & \delta^{p_m}_{q_2} a^{p_1p_2\cdots p_{m-2}p_{m-1}}_{q_1q_m\cdots q_{m-2}q_{m-1}} \\
- \quad & \delta^{p_m}_{q_1} a^{p_1p_2\cdots p_{m-2}p_{m-1}}_{q_mq_2\cdots q_{m-2}q_{m-1}}|\alpha\rangle \\
\times \quad & n_{p_1}n_{p_2}\cdots n_{p_m}, \qquad (9)
\end{aligned}
$$

where $\{n_{p_i}\}$ are the occupation numbers (0 or 1) in $|\alpha\rangle$. The repeated use of Eq. (9) will lead to the final fully contracted result.

Table 2 Degeneracy (n_d) of low-order Feynman diagrams. n_{F2}: number of electron-field contractions between two different vertices enumerated in an ascending order; n_{F1}: number of electron-field contractions within the same vertex; n_P: number of possible assignments of *all* the photon interactions; $n_d = max(1, n_{F1} + 2n_{F2}) \times max(1, n_P)$.

Diagram	n_{F2}	n_{F1}	n_P	n_d	$n_d/n!$
Fig. 3(b)	0	0	1	1	1/2
Fig. 3(c)	0	0	1	1	1
Fig. 3(d)	$\frac{1}{2}C_4^2+\frac{1}{2}C_4^2$	0	1	12	1/2
Fig. 3(e)	$\frac{1}{2}C_4^2+\frac{1}{2}C_4^2$	0	1	12	1/2
Fig. 3(f)	C_3^2	0	1	6	1
Fig. 3(g)	C_3^2	0	1	6	1
Fig. 3(h)	C_2^2	0	0	2	1
Fig. 3(i)	C_4^2	0	2	24	1
Fig. 4(a)	0	0	0	1	1/2
Fig. 4(b)	0	0	$\frac{1}{2}C_4^2$	3	1/8
Fig. 4(c)	0	0	C_3^2	3	1/2
Fig. 5(a)	C_2^2	0	1	2	1
Fig. 5(b)	0	C_2^1	1	2	1
Fig. 5(c)	C_3^2	0	1	6	1
Fig. 5(d)	C_4^2	0	2	24	1

With the above rules and the integral identities, the $S^{(n)}$ operators (5) can readily be constructed for the diagrams in Figs. (3) and (4). Although the enumeration of the vertices $x_i = \vec{r}_i t$, the 'direction' of the virtual photons z_i, as well as the designation of the free orbital lines are completely arbitrary, the following expressions follow the convention that, for a given diagram, the vertices are enumerated in a clockwise and ascending order, the virtual photons are directed from the left to right, while the outgoing (incoming) free orbital lines are denoted as $p, q, \cdots$ $(r, s, \cdots)$ from the left to right. In addition, the frequency ω_i in the electron propagator goes always upwards. These 'directions' are necessary just for calculating the arguments $E_i = E_{in} - E_{out}$ of the vertex $2\pi\Delta(E_i)$ functions.

Fig. (3b):

$$S^{(2)} = \frac{1}{2}(S^{(2)})^{rs}_{pq}\{a^{pq}_{rs}\}_n, \qquad (10)$$

$$
\begin{aligned}
(S^{(2)})^{rs}_{pq} = \quad & \int \frac{dz}{2\pi}\langle pq|(-i)I(z;\vec{r}_2,\vec{r}_1)|rs\rangle \\
\times \quad & 2\pi\Delta_\gamma(\varepsilon_r - \varepsilon_p - z)2\pi\Delta_\gamma(\varepsilon_s - \varepsilon_q + z) \quad (11) \\
\to \quad & -ig^{rs}_{pq}2\pi\Delta_\gamma(\varepsilon_r + \varepsilon_s - \varepsilon_p - \varepsilon_q). \quad (12)
\end{aligned}
$$

Note that Eq. (11) holds for the full instantaneous and retarded interactions, whereas Eq. (12), as indicated by the arrow, is confined only for the instantaneous interaction $g(1,2)$ (cf. Eq. (5) in Ref.[1]). This assumption is adopted throughout. The expectation value of $S^{(2)}$ over the unperturbed electronic state $|\alpha\rangle$ reads

$$\langle\alpha|S^{(2)}|\alpha\rangle = \frac{\bar{g}^{ij}_{ij}}{2i\gamma}, \qquad (13)$$

which contributes to the first order energy (cf. Eq. (1)) as

$$E^{(1)}_{3b} = \frac{i\gamma}{2}[2\langle\alpha|S^{(2)}|\alpha\rangle] = \frac{1}{2}(V_{HF})^i_i. \qquad (14)$$

Fig. (3c):

$$
\begin{aligned}
S^{(1)} &= (S^{(1)})^q_p\{a^p_q\}_n, && (15) \\
(S^{(1)})^q_p &= -i(-U)^q_p 2\pi\Delta_\gamma(\varepsilon_q - \varepsilon_p), && (16) \\
\langle\alpha|S^{(1)}|\alpha\rangle &= \frac{2iU^i_i}{\gamma}, && (17) \\
E^{(1)}_{3c} &= \frac{i\gamma}{2}\langle\alpha|S^{(1)}|\alpha\rangle = -U^i_i. && (18)
\end{aligned}
$$

The sum of $E^{(1)}_{3b}$ and $E^{(1)}_{3c}$ leads to the full first order energy

$$E^{(1)} = (\frac{1}{2}V_{HF} - U)^i_i, \qquad (19)$$

which agrees with Eq. (16) in Ref.[1].

Fig. (3d):

$$S^{(4)} = \frac{1}{2}(S^{(4)})^{rs}_{pq}\{a^{pq}_{rs}\}_n, \qquad (20)$$

$$
\begin{aligned}
(S^{(4)})_{pq}^{rs} = & \int\frac{dz_1}{2\pi}\int\frac{dz_2}{2\pi}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi} \\
\times & \langle pq|(-i)I(z_1;\vec{r}_2,\vec{r}_1)(-i)I(z_2;\vec{r}_3,\vec{r}_4) \\
\times & iS_F(\omega_1;\vec{r}_1,\vec{r}_4)iS_F(\omega_2;\vec{r}_2,\vec{r}_3)|rs\rangle \\
\times & 2\pi\Delta_\gamma(\varepsilon_r - z_2 - \omega_1)2\pi\Delta_\gamma(z_2+\varepsilon_s-\omega_2) \\
\times & 2\pi\Delta_\gamma(\omega_1-\varepsilon_p-z_1)2\pi\Delta_\gamma(z_1+\omega_2-\varepsilon_q) \quad (21)\\
\rightarrow & \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\langle pq|g(2,1)g(3,4) \\
\times & S_F(\omega_1;\vec{r}_1,\vec{r}_4)S_F(\omega_2;\vec{r}_2,\vec{r}_3)|rs\rangle \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_r+\varepsilon_s-\omega_1-\omega_2) \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_p+\varepsilon_q-\omega_1-\omega_2) \quad (22)\\
= & g_{pq}^{tu}g_{tu}^{rs}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\frac{1}{\omega_1-\varepsilon_t(1-i\eta)}\frac{1}{\omega_2-\varepsilon_u(1-i\eta)} \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_r+\varepsilon_s-\omega_1-\omega_2) \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_p+\varepsilon_q-\omega_1-\omega_2) \quad (23)\\
= & g_{pq}^{tu}g_{tu}^{rs}I_{22}^L(\varepsilon_t,\varepsilon_u;\varepsilon_r+\varepsilon_s,\varepsilon_p+\varepsilon_q,2\gamma), \quad (24)
\end{aligned}
$$

where the integral I_{22}^L is given in Eq. (117). From the expectation value

$$
\begin{aligned}
\langle\alpha|S^{(4)}|\alpha\rangle = & \tfrac{1}{2}g_{ij}^{tu}\bar{g}_{tu}^{ij}I_{22}^L(\varepsilon_t,\varepsilon_u;\varepsilon_i+\varepsilon_j,\varepsilon_i+\varepsilon_j,2\gamma) \quad (25)\\
= & \frac{g_{ij}^{tu}\bar{g}_{tu}^{ij}}{4i\gamma}\Big\{\frac{L_{tu}}{\varepsilon_i+\varepsilon_j-\varepsilon_t-\varepsilon_u+2i\gamma L_{tu}} \\
& +\frac{2i\gamma|L_{tu}|}{[\varepsilon_i+\varepsilon_j-\varepsilon_t-\varepsilon_u+2i\gamma L_{tu}]^2}\Big\} \quad (26)\\
= & \frac{g_{ij}^{tu}\bar{g}_{tu}^{ij}}{4i\gamma}\Big\{\frac{L_{tu}}{\varepsilon_i+\varepsilon_j-\varepsilon_t-\varepsilon_u}|_{\varepsilon_i+\varepsilon_j\neq\varepsilon_t+\varepsilon_u} \\
+ & \frac{1}{i\gamma}|_{\varepsilon_i+\varepsilon_j=\varepsilon_t+\varepsilon_u}\Big\}, \quad (27)
\end{aligned}
$$

we obtain (cf. Eq. (2))

$$
\begin{aligned}
E_{L,\gamma}^{(2)} = & \frac{i\gamma}{2}[4\langle\alpha|S^{(4)}|\alpha\rangle] \quad (28)\\
= & \frac{1}{4}\frac{\bar{g}_{ij}^{tu}\bar{g}_{tu}^{ij}L_{tu}}{\varepsilon_i+\varepsilon_j-\varepsilon_t-\varepsilon_u}|_{\varepsilon_i+\varepsilon_j\neq\varepsilon_t+\varepsilon_u}+\frac{\bar{g}_{ij}^{ij}\bar{g}_{ij}^{ij}}{2i\gamma}, \quad (29)
\end{aligned}
$$

where the first term can further be split into

$$
\begin{aligned}
E_{L++}^{(2)} = & \frac{1}{4}\frac{\bar{g}_{ij}^{ab}\bar{g}_{ab}^{ij}}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}, \quad (30)\\
E_{L--}^{(2)} = & -\frac{1}{4}\frac{\bar{g}_{ij}^{\bar{i}\bar{j}}\bar{g}_{\bar{i}\bar{j}}^{ij}}{\varepsilon_i+\varepsilon_j-\varepsilon_{\bar{j}}-\varepsilon_{\bar{i}}}, \quad (31)\\
E_{Lov}^{(2)} = & \frac{\bar{g}_{ij}^{aj}\bar{g}_{aj}^{ij}}{\varepsilon_i-\varepsilon_a}+\frac{1}{2}\frac{\bar{g}_{ij}^{ka}\bar{g}_{ka}^{ij}}{\varepsilon_i+\varepsilon_j-\varepsilon_k-\varepsilon_a}|_{i\neq j\neq k}, \quad (32)\\
E_{LOO}^{(2)} = & \frac{1}{8}\frac{\bar{g}_{ij}^{kl}\bar{g}_{kl}^{ij}}{\varepsilon_i+\varepsilon_j-\varepsilon_k-\varepsilon_l}+\frac{1}{8}\frac{\bar{g}_{kl}^{ij}\bar{g}_{ij}^{kl}}{\varepsilon_k+\varepsilon_l-\varepsilon_i-\varepsilon_j}=0. \quad (33)
\end{aligned}
$$

Fig. (3e):

$$
S^{(4)} = \frac{1}{2}(S^{(4)})_{pq}^{rs}\{a_{rs}^{pq}\}_n, \quad (34)
$$

$$
\begin{aligned}
(S^{(4)})_{pq}^{rs} = & \int\frac{dz_1}{2\pi}\int\frac{dz_2}{2\pi}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi} \\
\times & \langle pq|(-i)I(z_1;\vec{r}_2,\vec{r}_4)(-i)I(z_2;\vec{r}_3,\vec{r}_1) \\
\times & iS_F(\omega_1;\vec{r}_1,\vec{r}_4)iS_F(\omega_2;\vec{r}_2,\vec{r}_3)|rs\rangle \\
\times & 2\pi\Delta_\gamma(\varepsilon_r-z_1-\omega_1)2\pi\Delta_\gamma(\varepsilon_s+z_2-\omega_2) \\
\times & 2\pi\Delta_\gamma(\omega_1-z_2-\varepsilon_p)2\pi\Delta_\gamma(\omega_2+z_1-\varepsilon_q) \quad (35)\\
\rightarrow & \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\langle pq|g(2,4)g(3,1) \\
\times & S_F(\omega_1;\vec{r}_1,\vec{r}_4)S_F(\omega_2;\vec{r}_2,\vec{r}_3)|rs\rangle \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_r-\varepsilon_q-\omega_1+\omega_2) \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_s-\varepsilon_p+\omega_1-\omega_2) \quad (36)\\
= & g_{pu}^{ts}g_{tq}^{ru}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\frac{1}{\omega_1-\varepsilon_t(1-i\eta)}\frac{1}{\omega_2-\varepsilon_u(1-i\eta)} \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_r-\varepsilon_q-\omega_1+\omega_2) \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_s-\varepsilon_p+\omega_1-\omega_2) \quad (37)\\
= & g_{pu}^{ts}g_{tq}^{ru}I_{22}^X(\varepsilon_t,\varepsilon_u;\varepsilon_q-\varepsilon_r,\varepsilon_s-\varepsilon_p,2\gamma), \quad (38)
\end{aligned}
$$

where the integral I_{22}^X is given in Eq. (118). From the expectation value

$$
\begin{aligned}
\langle\alpha|S^{(4)}|\alpha\rangle = & \tfrac{1}{2}g_{iu}^{tj}g_{tj}^{iu}I_{22}^X(\varepsilon_t,\varepsilon_u;\varepsilon_j-\varepsilon_i,\varepsilon_j-\varepsilon_i,2\gamma) \\
& -\tfrac{1}{2}g_{iu}^{ti}g_{jt}^{uj}I_{22}^X(\varepsilon_t,\varepsilon_u;0,0,2\gamma) \quad (39)\\
= & \frac{1}{4i\gamma}\Big\{\frac{g_{iu}^{tj}g_{tj}^{iu}X_{tu}}{\varepsilon_j-\varepsilon_i+\varepsilon_t-\varepsilon_u}-\frac{g_{iu}^{ti}g_{jt}^{uj}X_{tu}}{\varepsilon_t-\varepsilon_u}\Big\}, \quad (40)
\end{aligned}
$$

we obtain (cf. Eq. (2))

$$
\begin{aligned}
E_X^{(2)} = & \frac{i\gamma}{2}[4\langle\alpha|S^{(4)}|\alpha\rangle] \quad (41)\\
= & -\frac{g_{i\bar{j}}^{pj}g_{pj}^{i\bar{j}}}{\varepsilon_i+\varepsilon_{\bar{j}}-\varepsilon_j-\varepsilon_p}+\frac{g_{i\bar{j}}^{pi}g_{jp}^{\bar{j}j}}{\varepsilon_{\bar{j}}-\varepsilon_p}, \quad (42)
\end{aligned}
$$

where the summation over p includes all the occupied and virtual PES. Note that $E_X^{(2)}$ vanishes for the same occupied orbitals (i.e., $i=j$).

Fig. (3f):

$$
S^{(3)} = (S^{(3)})_{pq}^{rs}\{a_{rs}^{pq}\}_n, \quad (43)
$$

$$
\begin{aligned}
(S^{(3)})_{pq}^{rs} = & \int\frac{dz}{2\pi}\int\frac{d\omega}{2\pi}\langle pq|(-i)I(z;\vec{r}_2,\vec{r}_3) \\
\times & (-i)[-U(\vec{r}_1)]iS_F(\omega;\vec{r}_1,\vec{r}_2)|rs\rangle \\
\times & 2\pi\Delta_\gamma(\varepsilon_r-\varepsilon_p-z)2\pi\Delta_\gamma(\varepsilon_s+z-\omega) \\
\times & 2\pi\Delta_\gamma(\omega-\varepsilon_q) \\
\rightarrow & i\int\frac{d\omega}{2\pi}\langle pq|g(2,3)U(1)S_F(\omega;\vec{r}_1,\vec{r}_2)|rs\rangle \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_r+\varepsilon_s-\varepsilon_p-\omega)2\pi\Delta_\gamma(\varepsilon_q-\omega) \quad (44)\\
= & ig_{pt}^{rs}U_q^t\int\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon_t(1-i\eta)} \\
\times & 2\pi\Delta_{2\gamma}(\varepsilon_r+\varepsilon_s-\varepsilon_p-\omega)2\pi\Delta_\gamma(\varepsilon_q-\omega) \quad (45)\\
= & ig_{pt}^{rs}U_q^tJ_{12}(\varepsilon_t;\varepsilon_q,\varepsilon_q,\gamma), \quad (46)
\end{aligned}
$$

where use of the energy-conserving relation $\varepsilon_r+\varepsilon_s-\varepsilon_p=\varepsilon_q$ and the integral J_{12} (111) has been made. From the expectation value

$$\langle\alpha|S^{(3)}|\alpha\rangle = i\bar{g}_{it}^{ij}U_j^t J_{12}(\varepsilon_t;\varepsilon_j,\varepsilon_j,\gamma) \quad (47)$$
$$= i\bar{g}_{it}^{ij}U_j^t\{\frac{2}{3\gamma}\frac{1}{\varepsilon_j-\varepsilon_t}|_{j\neq t}+\frac{1}{i\gamma^2}|_{j=t}\}, \quad (48)$$

we obtain (cf. Eq. (2))

$$E_{f,\gamma}^{(2)} = \frac{i\gamma}{2}[3\langle\alpha|S^{(3)}|\alpha\rangle] \quad (49)$$
$$= -\frac{(V_{HF})_t^j U_j^t}{\varepsilon_j-\varepsilon_t}|_{j\neq t}-\frac{3\bar{g}_{ij}^{ij}U_j^j}{2i\gamma}. \quad (50)$$

Fig. (3g):

The derivation is completely parallel to Fig. (3f), leading to

$$E_{g,\gamma}^{(2)} = -\frac{(V_{HF})_j^t U_t^j}{\varepsilon_j-\varepsilon_t}|_{j\neq t}-\frac{3\bar{g}_{ij}^{ij}U_j^j}{2i\gamma}. \quad (51)$$

The sum of $E_{f,\gamma}^{(2)}$ (50) and $E_{g,\gamma}^{(2)}$ (51) gives rise to

$$E_{fg,1+}^{(2)} = -\frac{(V_{HF})_j^a U_a^j+U_j^a(V_{HF})_a^j}{\varepsilon_j-\varepsilon_a}, \quad (52)$$
$$E_{fg,1-}^{(2)} = -\frac{(V_{HF})_j^{\bar{j}} U_{\bar{j}}^j+U_j^{\bar{j}}(V_{HF})_{\bar{j}}^j}{\varepsilon_j-\varepsilon_{\bar{j}}}, \quad (53)$$
$$E_{fg,\gamma}^{(2)} = -\frac{3\bar{g}_{ij}^{ij}U_j^j}{i\gamma}. \quad (54)$$

Fig. (3h):

$$S^{(2)}=(S^{(2)})_p^q\{a_q^p\}_n, \quad (55)$$

$$\begin{aligned}(S^{(2)})_p^q = & \int\frac{d\omega}{2\pi}\langle p|(-i)[-U(\vec{r}_1)](-i)[-U(\vec{r}_2)]\\ \times & iS_F(\omega;\vec{r}_1,\vec{r}_2)|q\rangle\\ \times & 2\pi\Delta_\gamma(\varepsilon_q-\omega)2\pi\Delta_\gamma(\omega-\varepsilon_p)\\ \rightarrow & -iU_p^tU_t^q\int\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon_t(1-i\eta)}\\ \times & 2\pi\Delta_\gamma(\varepsilon_p-\omega)2\pi\Delta_\gamma(\varepsilon_q-\omega) \quad (56)\\ = & -iU_p^tU_t^q I_{12}(\varepsilon_t;\varepsilon_p,\varepsilon_q,\gamma), \quad (57)\end{aligned}$$

where the integral I_{12} is given in Eq. (109). From the expectation value

$$\langle\alpha|S^{(2)}|\alpha\rangle = -iU_j^tU_t^jI_{12}(\varepsilon_t;\varepsilon_j,\varepsilon_j,\gamma) \quad (58)$$
$$= \frac{U_j^tU_t^j}{i\gamma(\varepsilon_j-\varepsilon_t)}|_{j\neq t}+\frac{2U_j^jU_j^j}{(i\gamma)^2}|_{j=t}, \quad (59)$$

we obtain (cf. Eq. (2))

$$E_{h,\gamma}^{(2)}=\frac{i\gamma}{2}[2\langle\alpha|S^{(2)}|\alpha\rangle]=\frac{U_j^tU_t^j}{\varepsilon_j-\varepsilon_t}|_{j\neq t}+\frac{2U_j^jU_j^j}{i\gamma}, \quad (60)$$

where the first term can further be split into two terms

$$E_{h,1+}^{(2)} = \frac{U_j^aU_a^j}{\varepsilon_j-\varepsilon_a}, \quad (61)$$
$$E_{h,1-}^{(2)} = \frac{U_j^{\bar{j}}U_{\bar{j}}^j}{\varepsilon_j-\varepsilon_{\bar{j}}}. \quad (62)$$

Fig. (3i):

$$S^{(4)}=(S^{(4)})_{pqr}^{ijk}\{a_{ijk}^{pqr}\}_n,\quad i\neq j\neq k, \quad (63)$$

where

$$\begin{aligned}(S^{(4)})_{pqr}^{ijk} = & \int\frac{dz1}{2\pi}\int\frac{dz2}{2\pi}\int\frac{d\omega}{2\pi}\langle pqr|(-i)I(z_1;\vec{r}_2,\vec{r}_1)\\ \times & (-i)I(z_2;\vec{r}_3,\vec{r}_4)iS_F(\omega;\vec{r}_2,\vec{r}_4)|ijk\rangle\\ \times & 2\pi\Delta_\gamma(\varepsilon_i-\varepsilon_p-z_1)2\pi\Delta_\gamma(\varepsilon_j-z_2-\omega)\\ \times & 2\pi\Delta_\gamma(\varepsilon_k+z_2-\varepsilon_r)2\pi\Delta_\gamma(z_1+\omega-\varepsilon_q)\\ \rightarrow & -i\int\frac{d\omega}{2\pi}\langle pqr|g(2,1)g(3,4)S_F(\omega;\vec{r}_2,\vec{r}_4)|ijk\rangle\\ \times & 2\pi\Delta_{2\gamma}(\varepsilon_i-\varepsilon_p-\varepsilon_q+\omega)\\ \times & 2\pi\Delta_{2\gamma}(\varepsilon_j+\varepsilon_k-\varepsilon_r-\omega) \quad (64)\\ = & -ig_{pq}^{it}g_{rt}^{kj}\int\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon_t(1-i\eta)}\\ \times & 2\pi\Delta_{2\gamma}(\varepsilon_p+\varepsilon_q-\varepsilon_i-\omega)\\ \times & 2\pi\Delta_{2\gamma}(\varepsilon_j+\varepsilon_k-\varepsilon_r-\omega) \quad (65)\\ = & -ig_{pq}^{it}g_{rt}^{kj}\\ \times & I_{12}(\varepsilon_t;\varepsilon_p+\varepsilon_q-\varepsilon_i,\varepsilon_j+\varepsilon_k-\varepsilon_r,2\gamma). \quad (66)\end{aligned}$$

From the expectation value (cf. Eq. (9))

$$\begin{aligned}\langle\alpha|S^{(4)}|\alpha\rangle = & -i\{\bar{g}_{ij}^{it}\bar{g}_{kt}^{kj}I_{12}(\varepsilon_t;\varepsilon_j,\varepsilon_j,2\gamma)-\frac{1}{2}\bar{g}_{kj}^{it}\bar{g}_{it}^{kj}\\ \times & I_{12}(\varepsilon_t;\varepsilon_j+\varepsilon_k-\varepsilon_i,\varepsilon_j+\varepsilon_k-\varepsilon_i,2\gamma)\} \quad (67)\\ = & \frac{\bar{g}_{ij}^{it}\bar{g}_{kt}^{kj}}{2i\gamma}[\frac{1}{\varepsilon_j-\varepsilon_t(1-2i\gamma)}+\frac{2i\gamma\,\mathrm{sgn}(\varepsilon_t)}{[\varepsilon_j-\varepsilon_t(1-2i\gamma)]^2}]\\ - & \frac{\bar{g}_{kj}^{it}\bar{g}_{it}^{kj}}{4i\gamma}[\frac{1}{\varepsilon_j+\varepsilon_k-\varepsilon_i-\varepsilon_t(1-2i\gamma)}\\ + & \frac{2i\gamma\,\mathrm{sgn}(\varepsilon_t)}{[\varepsilon_j+\varepsilon_k-\varepsilon_i-\varepsilon_t(1-2i\gamma)]^2}],\quad i\neq j\neq k \quad (68)\end{aligned}$$

and the relation

$$\sum_{i\neq k}\bar{g}_{ij}^{it}\bar{g}_{kt}^{kj}=(V_{HF})_j^t(V_{HF})_j^t-\sum_i\bar{g}_{ij}^{it}\bar{g}_{it}^{ij}, \quad (69)$$

we obtain (cf. Eq. (2))

$$\begin{aligned}E_{3i,\gamma}^{(2)} = & \frac{i\gamma}{2}[4\langle\alpha|S^{(4)}|\alpha\rangle] \quad (70)\\ = & \{\frac{(V_{HF})_i^t(V_{HF})_t^i}{\varepsilon_i-\varepsilon_t}|_{i\neq t}-\frac{\bar{g}_{ij}^{tj}\bar{g}_{tj}^{ij}}{\varepsilon_i-\varepsilon_t}|_{i\neq t}\\ - & \frac{1}{2}\frac{\bar{g}_{ij}^{kt}\bar{g}_{kt}^{ij}}{\varepsilon_i+\varepsilon_j-\varepsilon_k-\varepsilon_t}|_{i\neq j\neq k\neq t}\}+\frac{\bar{g}_{ij}^{ij}\bar{g}_{ik}^{ik}}{i\gamma}|_{i\neq j\neq k}, \quad (71)\end{aligned}$$

where the first term can further be split into

$$E^{(2)}_{3i,1+} = \frac{(V_{HF})^a_i (V_{HF})^i_a}{\varepsilon_i - \varepsilon_a}, \quad (72)$$

$$E^{(2)}_{3iov} = -\frac{\bar{g}^{aj}_{ij}\bar{g}^{ij}_{aj}}{\varepsilon_i - \varepsilon_a} - \frac{1}{2}\frac{\bar{g}^{ka}_{ij}\bar{g}^{ij}_{ka}}{\varepsilon_i + \varepsilon_j - \varepsilon_k - \varepsilon_a}|_{i\neq j\neq k} \quad (73)$$

$$= -E^{(2)}_{Lov}, \quad (74)$$

$$E^{(2)}_{3i,1-} = \frac{(V_{HF})^{\tilde{i}}_i (V_{HF})^i_{\tilde{i}}}{\varepsilon_i - \varepsilon_{\tilde{i}}} - \frac{\bar{g}^{\tilde{i}j}_{ij}\bar{g}^{ij}_{\tilde{i}j}}{\varepsilon_i - \varepsilon_{\tilde{i}}}, \quad (75)$$

$$E^{(2)}_{3i,2-} = -\frac{1}{2}\frac{\bar{g}^{k\tilde{i}}_{ij}\bar{g}^{ij}_{k\tilde{i}}}{\varepsilon_i + \varepsilon_j - \varepsilon_k - \varepsilon_{\tilde{i}}}|_{i\neq j\neq k}. \quad (76)$$

Note that the term $E^{(2)}_{3iov}$ (74) will cancel the term $E^{(2)}_{Lov}$ in Eq. (32).

Fig. (4a):

$$S^{(2)} = \frac{1}{2}(S^{(2)})^{rs}_{pq}\{a^{pq}_{rs}\}_n, \quad (77)$$

$$\begin{aligned}(S^{(4)})^{rs}_{pq} = & \langle pq|(-i)[-U(\vec{r}_1)](-i)[-U(\vec{r}_2)]|rs\rangle \\ \times & \ 2\pi\Delta_\gamma(\varepsilon_r - \varepsilon_p)2\pi\Delta_\gamma(\varepsilon_s - \varepsilon_q) \\ = & -U^r_p U^s_q 2\pi\Delta_\gamma(\varepsilon_r - \varepsilon_p)2\pi\Delta_\gamma(\varepsilon_s - \varepsilon_q), \quad (78)\end{aligned}$$

From the expectation value

$$\begin{aligned}\langle\alpha|S^{(2)}|\alpha\rangle = & \tfrac{1}{2}\{-U^i_i U^j_j[2\pi\Delta_\gamma(0)]^2 \\ & +U^j_i U^i_j[2\pi\Delta_\gamma(\varepsilon_i - \varepsilon_j)]^2\}|_{i\neq j}, \quad (79)\end{aligned}$$

we obtain (cf. Eq. (2))

$$E^{(2)}_{4a,\gamma} = \tfrac{i\gamma}{2}[2\langle\alpha|S^{(2)}|\alpha\rangle] \quad (80)$$

$$= \frac{2U^i_i U^j_j}{i\gamma}|_{i\neq j}, \quad (81)$$

because the second term of Eq. (79) vanishes in the limit $\gamma \to 0$.

Fig. (4b):

$$S^{(4)} = \frac{1}{8}(S^{(4)})^{rsvw}_{pqtu}\{a^{pqtu}_{rsvw}\}_n. \quad (82)$$

A direct evaluation of this diagram according to Eq. (82) is possible but is very lengthy. As observed in Fig. (4a), the transitions between the disconnected parts of a disconnected diagram all vanish in the limit $\gamma \to 0$. That is, the disconnected parts can be treated as infinitely separated in space and time. Therefore, the expectation of $S^{(4)}$ (82) can be factorized as

$$\begin{aligned}\langle\alpha|S^{(4)}|\alpha\rangle = & \tfrac{1}{8}(S^{(2)}_L)^{rs}_{pq}\langle\alpha|\{a^{rs}_{pq}\}_n|\alpha\rangle \\ \times & \ (S^{(2)}_R)^{vw}_{tu}\langle\alpha|\{a^{vw}_{tu}\}_n|\alpha\rangle, \quad (83) \\ = & \tfrac{1}{2}\langle\alpha|S^{(2)}_L|\alpha\rangle\langle\alpha|S^{(2)}_R|\alpha\rangle \quad (84) \\ = & \tfrac{1}{2}\tfrac{\bar{g}^{ij}_{ij}}{2i\gamma}\tfrac{\bar{g}^{kl}_{kl}}{2i\gamma}|_{i\neq j\neq k\neq l}, \quad (85)\end{aligned}$$

where use of the expression (13) has been made for both the left ($S^{(2)}_L$) and right ($S^{(2)}_R$) parts of the diagram. We then obtain (cf. Eq. (2))

$$E^{(2)}_{4b,\gamma} = \tfrac{i\gamma}{2}[4\langle\alpha|S^{(4)}|\alpha\rangle] \quad (86)$$

$$= \tfrac{\bar{g}^{ij}_{ij}\bar{g}^{kl}_{kl}}{4i\gamma}|_{i\neq j\neq k\neq l}. \quad (87)$$

Fig. (4c):

$$S^{(3)} = \frac{1}{2}(S^{(3)})^{rsu}_{pqt}\{a^{pqt}_{rsu}\}_n. \quad (88)$$

Like Fig. (4b), the expectation value of $S^{(3)}$ (88) can be factorized as

$$\langle\alpha|S^{(3)}|\alpha\rangle = \langle\alpha|S^{(2)}_L|\alpha\rangle\langle\alpha|S^{(1)}_R|\alpha\rangle \quad (89)$$

$$= \tfrac{\bar{g}^{ij}_{ij}}{2i\gamma}\tfrac{2iU^k_k}{\gamma}|_{i\neq j\neq k}, \quad (90)$$

where use of the expressions (13) and (17) has been made for the left ($S^{(2)}_L$) and right ($S^{(1)}_R$) parts of the diagram. We then obtain (cf. Eq. (2))

$$E^{(2)}_{4c,\gamma} = \tfrac{i\gamma}{2}[3\langle\alpha|S^{(3)}|\alpha\rangle] \quad (91)$$

$$= -\tfrac{3}{2i\gamma}\bar{g}^{ij}_{ij}U^k_k|_{i\neq j\neq k}. \quad (92)$$

Some remarks on the γ^{-1}-type of divergent terms should now be made. Note first that the second term in Eq. (60) can only be canceled out by the sum of Eq. (81) and the following term (cf. Eqs. (1) and (17))

$$\frac{i\gamma}{2}[-\langle\alpha|S^{(1)}|\alpha\rangle^2] = -\frac{2U^i_i U^j_j}{i\gamma} = -\frac{2U^j_j U^j_j}{i\gamma} - \frac{2U^i_i U^j_j}{i\gamma}|_{i\neq j}. \quad (93)$$

Likewise, the divergent term (54) can only be canceled out by the sum of Eq. (92) and the following term (cf. Eqs. (2), (13) and (17))

$$\frac{i\gamma}{2}[-3\langle\alpha|S^{(1)}|\alpha\rangle\langle\alpha|S^{(2)}|\alpha\rangle] = \frac{3\bar{g}^{ij}_{ij}U^j_j}{i\gamma}|_{i\neq j} + \frac{3\bar{g}^{ij}_{ij}U^k_k}{2i\gamma}|_{i\neq j\neq k}. \quad (94)$$

Similarly, the second terms of Eqs. (29) and (71) together can only be canceled out by the sum of Eq. (87) and the following term (cf. Eqs. (2) and (13))

$$\frac{i\gamma}{2}[-2\langle\alpha|S^{(2)}|\alpha\rangle^2] = -\frac{\bar{g}_{ij}^{ij}\bar{g}_{kl}^{kl}}{4i\gamma}|_{i\neq j,k\neq l} \quad (95)$$

$$= -\frac{\bar{g}_{ij}^{ij}\bar{g}_{ij}^{ij}}{2i\gamma}|_{i\neq j} - \frac{\bar{g}_{ij}^{ij}\bar{g}_{kl}^{kl}}{i\gamma}|_{i\neq j\neq k}$$

$$-\frac{\bar{g}_{ij}^{ij}\bar{g}_{kl}^{kl}}{4i\gamma}|_{i\neq j\neq k\neq l}. \quad (96)$$

It is therefore clear that the disconnected but linked diagrams in Fig. (4) are essential for removing the γ^{-1}-type of divergences from Fig. (3), although they do not contribute to the energy. Of course, Fig. (4b) appears only for systems of more than three electrons, whereas Fig. (4c) (and (3i)) only for systems of more than two electrons. The final two-body terms of $E^{(2)}$ include Eqs. (30), (31), (42), and (76), while the one-body terms in Eqs. (52), (53), (61), (62), (72), and (75) can be regrouped into

$$E^{(2)}_{QED,1+} = \frac{(V_{HF}-U)^a_i(V_{HF}-U)^i_a}{\varepsilon_i-\varepsilon_a} = E^{(2)}_{CS,1+}, \quad (97)$$

$$E^{(2)}_{QED,1-} = \frac{(V_{HF}-U)^{\tilde{i}}_i(V_{HF}-U)^i_{\tilde{i}}}{\varepsilon_i-\varepsilon_{\tilde{i}}} - \frac{\bar{g}^{\tilde{i}j}_{ij}\bar{g}^{ij}_{\tilde{i}j}}{\varepsilon_i-\varepsilon_{\tilde{i}}} \quad (98)$$

$$= E^{(2)}_{CS,1-} - \frac{\bar{g}^{\tilde{i}j}_{ij}\bar{g}^{ij}_{\tilde{i}j}}{\varepsilon_i-\varepsilon_{\tilde{i}}}. \quad (99)$$

Note in passing that, at variance with the above complete manipulations, the same results can alternatively be obtained by discarding the singular terms from the outset, including the terms with a negative sign in Eqs. (1) and (2), the last terms in the integrals (109), (110), (111), (117), and (118), as well as all the diagrams in Fig. (4). It is this 'shortcut' that is usually employed in the literature[3]. Retaining only the terms in Eqs. (30) and (97) goes back to the standard no-pair approximation that has an intrinsic error of order $(Z\alpha)^3$ and is dependent on the mean-field potential generating the orbitals. Fortunately, such an error as well as the potential dependence can largely be removed by further accounting for the simple counter terms (53) and (62), leading to a 'potential-independent (hybrid) no-pair approximation'.

The algebraic equations for the diagrams in Fig. (5) can in principle be derived in the same way. However, they require delicate regularization and renormalization that go beyond the scope of the present work. The results are therefore not to be documented here. Yet, we can discuss briefly the vacuum density ρ_{vp}

$$\rho_{vp}(\vec{r}) = i|e|Tr[S_F(x_1,x_2)] \quad (100)$$

$$= \frac{|e|}{2}(\rho_+(\vec{r})-\rho_-(\vec{r})), \quad (101)$$

$$\rho_+(\vec{r}) = \sum_i \varphi_i^\dagger(\vec{r})\varphi_i(\vec{r}), \quad (102)$$

$$\rho_-(\vec{r}) = \sum_{\tilde{i}} \varphi_{\tilde{i}}^\dagger(\vec{r})\varphi_{\tilde{i}}(\vec{r}), \quad (103)$$

where Eq. (101) arises from the equal-time electron propagator (see Eq. (112)) and the summations in Eqs. (102) and (103) involve the whole PES and NES, respectively. Obviously, $\rho_{vp}(\vec{r})$ vanishes pointwise for free particles. However, in the presence of a pointlike nucleus, the induced charge density ρ_{vp} has a profound feature[4]: The PES are occupied by positrons e^+, while the NES are occupied by electrons e^-; Since the positive energy functions φ_i are pulled closer to the nucleus by the Coulomb field, whereas the negative energy functions $\varphi_{\tilde{i}}$ are pushed away from the nucleus, the induced charge density ρ_{vp} has a positively charged part localized at the position of the nucleus and a negatively charged polarization cloud marginally spread out from the nucleus, in accordance with the condition $Q_{vp} = \int \rho_{vp}(\vec{r})d\vec{r} = 0$. That is, the dipole moments of e^+e^- pairs are oriented with e^+ closer to the nucleus. This is completely opposite to an ordinary polarizable medium, where positive and negative charges are usually alternating. Since the radial extension of ρ_{vp} is extremely short ranged (in the order of $\hbar/mc \approx 386$ fm), the vacuum polarization can effectively be visualized as an enlargement of the nucleus charge and thereby behaves as an attractive force. Note that this pictorial interpretation is independent of the charge renormalization.

B Useful integrals

We first define[3]

$$\int_{-\infty}^{+\infty} dt e^{i\omega t}e^{-\gamma|t|} = \frac{2\gamma}{\omega^2+\gamma^2} = 2\pi\Delta_\gamma(\omega), \quad (104)$$

where $\Delta_\gamma(\omega)$ is an even function of ω and has the following properties

$$\lim_{\gamma\to 0}\Delta_\gamma(\omega) = \delta(\omega), \quad (105)$$

$$\lim_{\gamma\to 0}\pi\gamma\Delta_\gamma(\omega) = \delta_0^\omega, \quad (106)$$

$$\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}2\pi\Delta_\alpha(a-\omega)2\pi\Delta_\beta(b+\omega) = 2\pi\Delta_{\alpha+\beta}(a+b). \quad (107)$$

The integral I_{11} with one electron propagator and one Δ function reads

$$I_{11}(\varepsilon_t;a,\gamma) = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon_t(1-i\eta)}2\pi\Delta_\gamma(a-\omega) = \frac{1}{a-\varepsilon_t(1-i\gamma)}, \quad (108)$$

where η is an infinitesimally positive number, whereas γ is a small but finite positive number (i.e., $\eta+\gamma\approx\gamma$). The integral I_{12} with one electron propagator and two Δ functions reads

$$\begin{aligned} I_{12}(\varepsilon_t;a,b,\gamma) &= \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon_t(1-i\eta)}2\pi\Delta_\gamma(a-\omega)2\pi\Delta_\gamma(b-\omega)\\ &= 2\pi\Delta_{2\gamma}(a-b)\{\frac{1}{2[a-\varepsilon_t(1-i\gamma)]}+\frac{1}{2[b-\varepsilon_t(1-i\gamma)]}\\ &\quad+\frac{i\gamma\mathrm{sgn}(\varepsilon_t)}{[a-\varepsilon_t(1-i\gamma)][b-\varepsilon_t(1-i\gamma)]}\}, \end{aligned} \quad (109)$$

which reduces to

$$I_{12}(\varepsilon_t;a,a,\gamma) = \frac{\gamma^{-1}}{a-\varepsilon_t(1-i\gamma)}+\frac{i\,\mathrm{sgn}(\varepsilon_t)}{[a-\varepsilon_t(1-i\gamma)]^2} \quad (110)$$

in the case of $a=b$. Likewise,

$$\begin{aligned} J_{12}(\varepsilon_t;a,a,\gamma) &= \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon_t(1-i\eta)}2\pi\Delta_\gamma(a-\omega)2\pi\Delta_{2\gamma}(a-\omega)\\ &= \frac{2}{3\gamma}\{\frac{2}{a-\varepsilon_t(1-i\gamma)}-\frac{1}{a-\varepsilon_t(1-2i\gamma)}\}\\ &= \begin{cases} \frac{2}{3\gamma}\frac{1}{a-\varepsilon_t}, & \text{if } a\neq\varepsilon_t,\\ \frac{1}{i\gamma^2\,\mathrm{sgn}(\varepsilon_t)}, & \text{if } a=\varepsilon_t. \end{cases} \end{aligned} \quad (111)$$

Further in view of the identities

$$I_{10}(a,\varepsilon_t) = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{a\pm\omega-\varepsilon_t(1-i\eta)} = \frac{1}{2i}\mathrm{sgn}(\varepsilon_t), \quad (112)$$

$$\begin{aligned} I_{20}^L(a,\varepsilon_t,b,\varepsilon_u) &= \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{a\mp\omega-\varepsilon_t(1-i\eta)}\frac{1}{b\pm\omega-\varepsilon_u(1-i\delta)}\\ &= \frac{-iL_{tu}}{[a-\varepsilon_t(1-i\eta)]+[b-\varepsilon_u(1-i\delta)]} \end{aligned} \quad (113)$$

with

$$L_{tu} = L_{++} = -L_{--} = 1, \quad L_{tu} = L_{+-} = L_{-+} = 0, \quad (114)$$

and

$$\begin{aligned} I_{20}^X(a,\varepsilon_t,b,\varepsilon_u) &= \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{a\pm\omega-\varepsilon_t(1-i\eta)}\frac{1}{b\pm\omega-\varepsilon_u(1-i\delta)}\\ &= \frac{iX_{tu}}{[a-\varepsilon_t(1-i\eta)]-[b-\varepsilon_u(1-i\delta)]} \end{aligned} \quad (115)$$

with

$$X_{tu} = X_{++} = X_{--} = 0, \quad X_{tu} = X_{+-} = -X_{-+} = 1, \quad (116)$$

the integrals with two Δ functions and two electron propagators can readily be evaluated as

$$\begin{aligned} I_{22}^L(\varepsilon_t,\varepsilon_u;a,b,\gamma) &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{1}{\omega_1-\varepsilon_t(1-i\eta)}\frac{1}{\omega_2-\varepsilon_u(1-i\eta)}\\ &\quad\times2\pi\Delta_\gamma(a-\omega_1-\omega_2)2\pi\Delta_\gamma(b-\omega_1-\omega_2)\\ &= 2\pi\Delta_{2\gamma}(a-b)\{\frac{L_{tu}}{2i[a-\varepsilon_t-\varepsilon_u+i\gamma L_{tu}]}\\ &\quad+\frac{L_{tu}}{2i[b-\varepsilon_t-\varepsilon_u+i\gamma L_{tu}]}\\ &\quad+\frac{\gamma|L_{tu}|}{[a-\varepsilon_t-\varepsilon_u+i\gamma L_{tu}][b-\varepsilon_t-\varepsilon_u+i\gamma L_{tu}]}\}, \end{aligned} \quad (117)$$

$$\begin{aligned} I_{22}^X(\varepsilon_t,\varepsilon_u;a,b,\gamma) &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{1}{\omega_1-\varepsilon_t(1-i\eta)}\frac{1}{\omega_2-\varepsilon_u(1-i\eta)}\\ &\quad\times2\pi\Delta_\gamma(a+\omega_1-\omega_2)2\pi\Delta_\gamma(b+\omega_1-\omega_2)\\ &= 2\pi\Delta_{2\gamma}(a-b)\{\frac{X_{tu}}{2i[a+\varepsilon_t-\varepsilon_u-i\gamma X_{tu}]}\\ &\quad+\frac{X_{tu}}{2i[b+\varepsilon_t-\varepsilon_u-i\gamma X_{tu}]}\\ &\quad-\frac{\gamma|X_{tu}|}{[a+\varepsilon_t-\varepsilon_u-i\gamma X_{tu}][b+\varepsilon_t-\varepsilon_u-i\gamma X_{tu}]}\}, \end{aligned} \quad (118)$$

$$\begin{aligned} I_{22}^Y(\varepsilon_t,\varepsilon_u;a,b,\gamma) &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{1}{\omega_1-\varepsilon_t(1-i\eta)}\frac{1}{\omega_2-\varepsilon_u(1-i\eta)}\\ &\quad\times2\pi\Delta_\gamma(a-\omega_1+\omega_2)2\pi\Delta_\gamma(b+\omega_1-\omega_2)\\ &= I_{22}^X(\varepsilon_t,\varepsilon_u;-a,b,\gamma). \end{aligned} \quad (119)$$

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