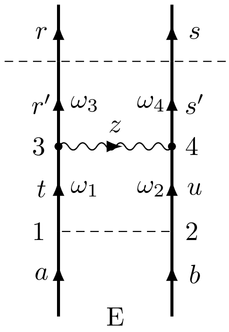
Two-photon interaction with one Coulomb Ladder diagram

Ingvar Lindgren 2004.09.02



The matrix element of the evolution operator for two-photon ladder with one Coulomb is given by (leaving out the time integrals)

$$\langle rs|U_{\rm Cov}^{(y)}|ab\rangle = -\Big\langle rs\Big|\int\frac{{\rm d}z}{2\pi}\iiiint\frac{{\rm d}\omega_4}{2\pi}\,\frac{{\rm d}\omega_3}{2\pi}\,\frac{{\rm d}\omega_2}{2\pi}\,\frac{{\rm d}\omega_1}{2\pi}\,\frac{|s'\rangle\langle s'|}{(\omega_4-\varepsilon_{s'}+{\rm i}\eta_{s'})}\,\frac{|r'\rangle\langle r'|}{(\omega_3-\varepsilon_{r'}+{\rm i}\eta_{r'})}$$
$$\times\ \frac{|u\rangle\langle u|}{(\omega_2-\varepsilon_u+{\rm i}\eta_u)}\,\frac{|t\rangle\langle t|}{(\omega_1-\varepsilon_t+{\rm i}\eta_t)}\,I_{34}(z\,)\,\frac{e^2}{4\pi r_{12}}\Big|ab\Big\rangle \tag{1}$$

where

$$I_{34}(z)=\int_0^\infty\frac{2k\,f_{34}(k)}{z^2-k^2+{\rm i}\eta}\qquad f_{34}(k)=-\frac{e^2}{4\pi^2 r_{34}}(1-\boldsymbol{\alpha_3}\cdot\boldsymbol{\alpha_4})\sin(kr_{34})$$

With

$$\frac{\sin(kr_{12})}{kr_{12}}=\sum_{l=0}^{\infty}(2l+1)j_l(kr_1)j_l(kr_2)\boldsymbol{C}^k(1)\cdot\boldsymbol{C}^k(1)$$

$f_{34}(k)$ can be expressed

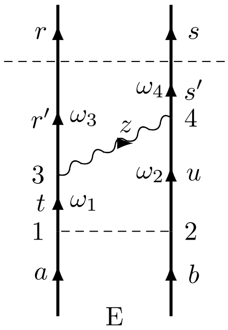
$$f_{34}(k)=\mathcal{H}_l(4,k)\mathcal{H}_l(3,k)$$

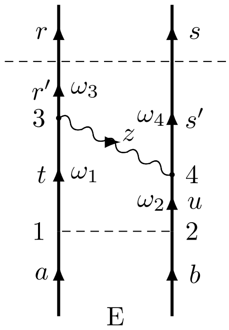
summed over l.

The Coulomb interaction is instantaneous with $t_1=t_2$. Time integration then leads to $2\pi\delta(\varepsilon_a+\varepsilon_b-\omega_1-\omega_2$; $2\pi\delta(\omega_1-z-\omega_3)$ and $2\pi\delta(\omega_2+z-\omega_4)$. With $E=\varepsilon_a+\varepsilon_b$ this gives the matrix element (1), leaving out the z,ω integrals and the factor $e^2/4\pi$

$$-\frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l|u\rangle\ \ \langle s'|\mathcal{H}_l|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle\ \ 2k}{(\omega_1-z-\varepsilon_r+{\rm i}\eta_r)(E-\omega_1+z-\varepsilon_s+{\rm i}\eta_s)(\omega_1-\varepsilon_t+{\rm i}\eta_t)(E-\omega_1-\varepsilon_u+{\rm i}\eta_u)(z^2-k^2+{\rm i}\eta)} \tag{2}$$

No virtual pair





Integrations yield

$$\langle rs|U_{\rm Cov}^{(y)}|ab\rangle = \frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l(k)|u\rangle\ \ \langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(E-r-s)\ \ (E-t-u)} \times \Big[\frac{1}{E-r-u-k}+\frac{1}{E-s-t-k}\Big] \tag{3}$$

We can define pair functions by

$$\langle rs|U_{\rm Cov}^{(y)}|ab\rangle = \big\langle rs\big|r's'\big\rangle\big[\rho_{ab1}^{++}(r's')+\rho_{ab2}^{++}(r's')\big\rangle\big] \tag{4}$$

where the first function can be expressed

$$\rho_{ab1}^{++}(r's') = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle\ \ \langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(E-r-s)\ (E-r-u-k)\ (E-t-u)} = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle\ \ \rho_{ab}^{+}(r',u,k)}{E-r-s} \tag{5}$$

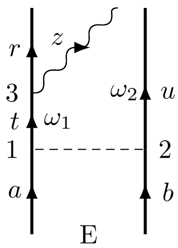
summed over u

$$\rho_{ab}^{+}(r',u,k) = \frac{\langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(E-r-u-k)\ \ (E-t-u)} = \frac{\langle r'|\mathcal{H}_l(k)|t\rangle\ \ \rho_{ab}(t,u)}{E-r-u-k} \tag{6}$$

summed over t and

$$\rho_{ab}(t,u) = \frac{\langle tu|1/r_{12}|ab\rangle}{E-t-u} \tag{7}$$

(6) represents a pair function with an uncontracted photon (see Fig.)



The coordinate representation of (7)

$$\rho_{ab}(x,y) = \frac{\langle xy|tu\rangle\langle tu|1/r_{12}|ab\rangle}{E-t-u} \tag{8}$$

satisfies the ordinary pair equation

$$\big[E-h_0(x)-h_0(y)\big]\ \rho_{ab}(x,y) = Q\langle xy|tu\rangle\langle tu|1/r_{12}|ab\rangle \qquad \textbf{DF=2} \tag{9}$$

Q is the appropriate projection operator, in this case projecting out the positive-energy states. This equation has **two degrees of freedom (DF=2)**.

The coordinate representation of (6)

$$\rho^+_{ab}(x,y,k) = \langle xy|r'u'\rangle\ \rho^+_{ab}(r',u,k) \tag{10}$$

satisfies the pair equation

$$\big[E - h_0(x) - h_0(y) - k\big]\rho^+_{ab}(x,y,k) = Q\langle xy|r'u\rangle\langle r'|\mathcal{H}_l(k)|t\rangle\ \ \rho_{ab}(t,u) \qquad \textbf{DF=3} \tag{11}$$

This is a pair equation to be solved for each value of k, i.e., **three degrees of freedom (DF=3)**.

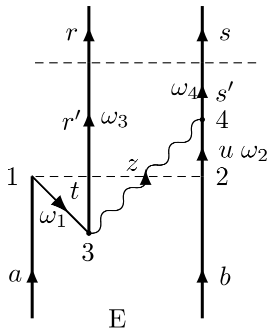
The coordinate representation of (5)

$$\rho^{++}_{ab1}(x,y) = \langle xy|r's'\rangle\ \rho^{++}_{ab1}(r's') \tag{12}$$

is a solution to

$$\big[E - h_0(x) - h_0(y)\big]\rho^{++}_{ab}(x,y) = Q\langle xy|r's'\rangle\langle s'|\mathcal{H}_l(k)|u\rangle\ \ \rho^+_{ab}(r',u,k) \qquad \textbf{DF=3} \tag{13}$$

Single virtual pair

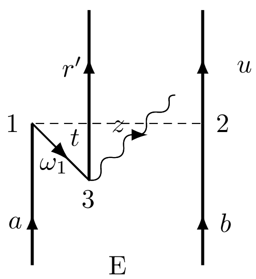


Integrations yield

$$\langle rs|U^{(y)}_{\rm Cov}|ab\rangle = -\frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l(k)|u\rangle\ \ \langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(E-r-s)\ (t-r-k)\ (E-u-r-k)} = -\langle rs|r's'\rangle\ \rho^{+-}_{ab}(r',s') \tag{14}$$

where the pair function is quite analogous to (5)

$$\rho^{+-}_{ab}(r',s') = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle\ \ \rho^-_{ab}(r',u,k)}{E-r-s} \tag{15}$$



The pair function with an uncontracted photon (see Fig.) becomes

$$\rho^-_{ab}(r',u,k) = \frac{\langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(t-r-k)\ \ (E-r-u-k)} = \frac{\rho(r',t,k)\ \ \langle tu|1/r_{12}|ab\rangle}{E-r-u-k} \tag{16}$$

where

$$\rho(r',t,k)=\frac{\langle r'|\mathcal{H}_l(k)|t\rangle}{t-r-k}$$

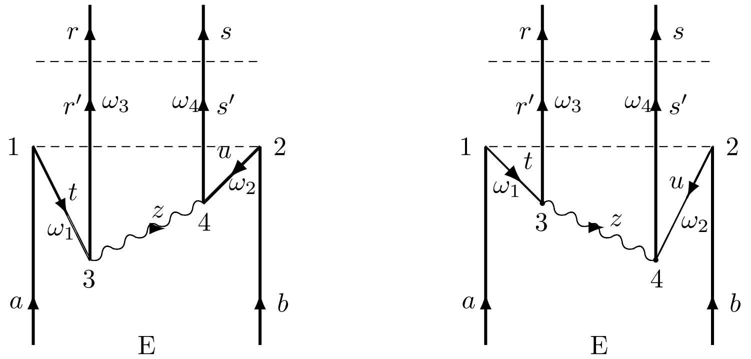
is in the coordinate representation solution to

$$\big[t-h_0(x)-k\big]\rho(3',t,k)=Q\langle x|r'\rangle\langle r'|\mathcal{H}_l(k)|t\rangle \qquad \textbf{DF=3}$$

The coordinate representation of $\rho^{-}_{ab}(r',u,k)$ is a solution to

$$\big[E-h_0(x)-h_0(y)-k\big]\ \rho^{-}_{ab}(x,y,k)=Q\langle x'y|r'u\rangle\ \rho(r',t,k)\ \ \langle tu|1/r_{12}|ab\rangle \qquad \textbf{DF=3}$$

Double virtual pairs



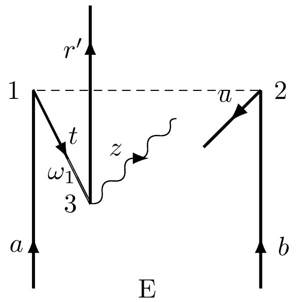
Integrations yield

$$\begin{aligned}\langle rs|U^{(y)}_{\rm Cov}|ab\rangle &= \frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l(k)|u\rangle\ \ \langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(E-r-s)\ \ (t+u-E)}\Big[\frac{1}{t-r-k}+\frac{1}{u-s-k}\Big]\\ &= \langle rs|r's'\rangle\big[\rho^{--}_{ab1}(r',s')+\rho^{--}_{ab2}(r',s')\big] \end{aligned} \qquad (17)$$

where the first pair function is

$$\rho^{--}_{ab1}(r',s')=\frac{\langle s'|\mathcal{H}_l(k)|u\rangle\ \ \rho^{-}_{ab1}(r',u,k)}{(E-r-s)} \qquad (18)$$

analogous to (5).



The pair function with an uncontracted photon (see Fig.) becomes

$$\rho^{-}_{ab1}(r',u,k)=\frac{\langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(t-r-k)\ \ (t+u-E)}=\rho(r',t,k)\ \ \rho^{--}_{ab}(t,u) \qquad (19)$$

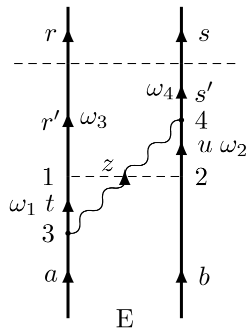
where $\rho(r', t, k)$ is the sing. part. function in (16) and $\rho_{ab}^{--}(t,u)$ is a standard pair function with negative energy states

$$\rho_{ab}^{--}(t,u) = \frac{\langle tu|1/r_{12}|ab\rangle}{(t+u-E)}$$

in coordinate representation solution to equation

$$\left[h_0(x) + h_0(y) - E\right]\rho_{ab}^{--}(x,y) = Q\langle xy|tu\rangle\langle tu|1/r_{12}|ab\rangle \qquad \textbf{DF=2}$$

Crossed diagram



The matrix element of the evolution operator for two-photon cross with one Coulomb is the same as for ladder (1)

$$\begin{aligned}\langle rs|U_{\rm Cov}^{(y)}|ab\rangle &= -\Big\langle rs\Big|\int\frac{{\rm d}z}{2\pi}\iiiint\frac{{\rm d}\omega_4}{2\pi}\,\frac{{\rm d}\omega_3}{2\pi}\,\frac{{\rm d}\omega_2}{2\pi}\,\frac{{\rm d}\omega_1}{2\pi}\,\frac{|s'\rangle\langle s'|}{(\omega_4-\varepsilon_{s'}+{\rm i}\eta_{s'})}\,\frac{|r'\rangle\langle r'|}{(\omega_3-\varepsilon_{r'}+{\rm i}\eta_{r'})}\\ &\times\ \frac{|u\rangle\langle u|}{(\omega_2-\varepsilon_u+{\rm i}\eta_u)}\,\frac{|t\rangle\langle t|}{(\omega_1-\varepsilon_t+{\rm i}\eta_t)}\,I_{34}(z)\frac{e^2}{4\pi r_{12}}\Big|ab\Big\rangle \qquad (20)\end{aligned}$$

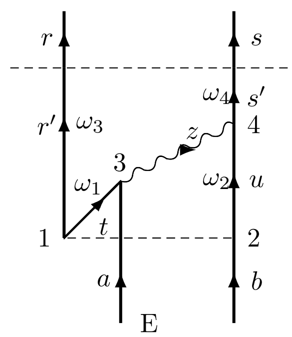
Time integrations yield $2\pi\delta(\omega_1+\varepsilon_b-\omega_3-\omega_2$; $2\pi\delta(\varepsilon_a-z-\omega_1)$ and $2\pi\delta(\omega_2+z-\omega_4)$. With $E=\varepsilon_a+\varepsilon_b$ this gives the matrix element (1), leaving out the z,ω integrals and the factor $e^2/4\pi$

$$-\frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l|u\rangle\ \ \langle t|\mathcal{H}_l|a\rangle\ \ \langle tb|1/r_{12}|r'u\rangle\ \ 2k}{(\omega_2+z-s+{\rm i}s)(E-z-\omega_2-r+{\rm i}r)(\omega_2-u-{\rm i}u)(a-z-t+{\rm i}t)(z^2-k^2+{\rm i}\eta)} \qquad (21)$$

No virtual pair

This can be handled in he one-photon approach

Single virtual pair



Integrations yield

$$\begin{aligned}\langle rs|U_{\rm Cov}^{(y)}|ab\rangle &= -\frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l(k)|u\rangle\ \ \langle t|\mathcal{H}_l(k)|a\rangle\ \ \langle r'u|1/r_{12}|tb\rangle}{(E-r-s)\ (b+t-r-u)}\Big[\frac{1}{a-t-k}+\frac{1}{E-r-u-k}\Big]\\ &= -\big\langle rs\big|r's'\big\rangle\big[\rho^{-+}_{ab1}(r's')+\rho^{-+}_{ab2}(r's')\big\rangle\big] \qquad (22)\end{aligned}$$

where the pair functions are analogous to the ladder case (5)

$$\rho_{ab1}^{-+}(r's') = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle \ \langle r'u|1/r_{12}|tb\rangle \ \langle t|\mathcal{H}_l(k)|a\rangle}{(E-r-s)\,(b+t-r-u)\,(a-t-k)} = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle \ \rho_{ab1}^{-+}(r',u,k)}{E-r-s} \tag{23}$$

$$\rho_{ab2}^{-+}(r's') = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle \ \langle r'u|1/r_{12}|tb\rangle \ \langle t|\mathcal{H}_l(k)|a\rangle}{(E-r-s)\,(b+t-r-u)\,(E-r-u-k)} = \frac{\langle s'|\mathcal{H}_l(k)|u\rangle \ \rho_{ab2}^{-+}(r',u,k)}{E-r-s} \tag{24}$$

The first pair function with an uncontracted photon becomes

$$\rho_{ab1}^{-+}(r',u,k) = \frac{\langle r'u|1/r_{12}|tb\rangle \ \langle t|\mathcal{H}_l(k)|a\rangle}{(b+t-r-u) \ \ (a-t-k)} = \frac{\langle r'u|1/r_{12}|tb\rangle \ \rho(r',t,k)}{b+t-r-u} \tag{25}$$

where

$$\rho_a(t,k) = \frac{\langle t|\mathcal{H}_l(k)|a\rangle}{a-t-k}$$

is a sing.part. function with negative output, in the coordinate representation solution to

$$\big[a-h_0(x)-k\big]\rho_a(x,k) = Q\langle x|t\rangle\langle t|\mathcal{H}_l(k)|a\rangle \qquad \textbf{DF=2}$$

The coordinate representation of $\rho_{ab1}^{-}(r',u,k)$ is a solution to

$$\big[E-h_0(x)-h_0(y)-k\big] \ \rho_{ab1}^{-}(x,y,k) = Q\langle x'y|r'u\rangle \ \langle r'u|1/r_{12}|tb\rangle \ \rho_a(t,k) \qquad \textbf{DF=3}$$

The second pair function with an uncontracted photon (24) becomes

$$\rho_{ab1}^{-+}(r',u,k) = \frac{\langle r'u|1/r_{12}|tb\rangle \ \langle t|\mathcal{H}_l(k)|a\rangle}{(b+t-r-u) \ \ (E-r-u-k)} = \frac{\langle t|\mathcal{H}_l(k)|a\rangle \ \ \rho_t(r',u)}{E-r-u-k} \tag{26}$$

where

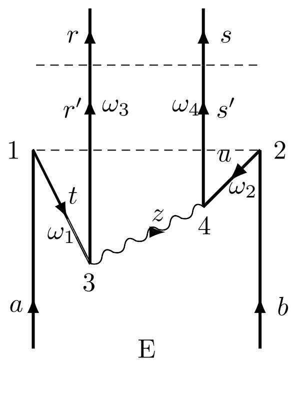
$$\rho_t(r',u) = \frac{\langle r'u|1/r_{12}|tb\rangle}{b+t-r-u}$$

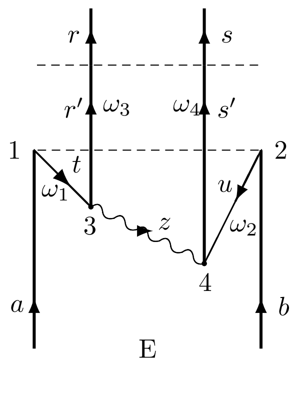
is in the coordinate reprsentation a solution to the pair equation

$$\big[b+t-h_0(x)-h_0(y)\big] \ \rho_t(r',u) = Q\langle x'y|r'u\rangle \ \langle r'u|1/r_{12}|tb\rangle \ \rho_a(t,k) \qquad \textbf{DF=3}$$

This represents a standard pair function for each negative orbital t.

Double virtual pairs





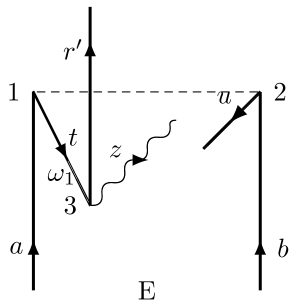
Integrations yield

$$\begin{aligned}\langle rs|U_{\rm Cov}^{(y)}|ab\rangle &= \frac{\langle rs|r's'\rangle\ \ \langle s'|\mathcal{H}_l(k)|u\rangle\ \ \langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(E-r-s)\ \ (t+u-E)}\Big[\frac{1}{t-r-k}+\frac{1}{u-s-k}\Big] \\ &= \langle rs|r's'\rangle\big[\rho_{ab1}^{--}(r',s')+\rho_{ab2}^{--}(r',s')\big] \qquad (27)\end{aligned}$$

where the first pair function is

$$\rho_{ab1}^{--}(r',s')=\frac{\langle s'|\mathcal{H}_l(k)|u\rangle\ \ \rho_{ab1}^{-}(r',u,k)}{(E-r-s)} \qquad (28)$$

analogous to (5).



The pair function with an uncontracted photon (see Fig.) becomes

$$\rho_{ab1}^{-}(r',u,k)=\frac{\langle r'|\mathcal{H}_l(k)|t\rangle\ \ \langle tu|1/r_{12}|ab\rangle}{(t-r-k)\ \ (t+u-E)}=\rho(r',t,k)\ \ \rho_{ab}^{--}(t,u) \qquad (29)$$

where $\rho(r',t,k)$ is the sing. part. function in (16) and $\rho_{ab}^{--}(t,u)$ is a standard pair function with negative energy states

$$\rho_{ab}^{--}(t,u)=\frac{\langle tu|1/r_{12}|ab\rangle}{(t+u-E)}$$

in coordinate representation solution to equation

$$\big[h_0(x)+h_0(y)-E\big]\rho_{ab}^{--}(x,y)=Q\langle xy|tu\rangle\langle tu|1/r_{12}|ab\rangle \qquad \textbf{DF=2}$$