Valence-hole excitation in a closed shell system: QED approach

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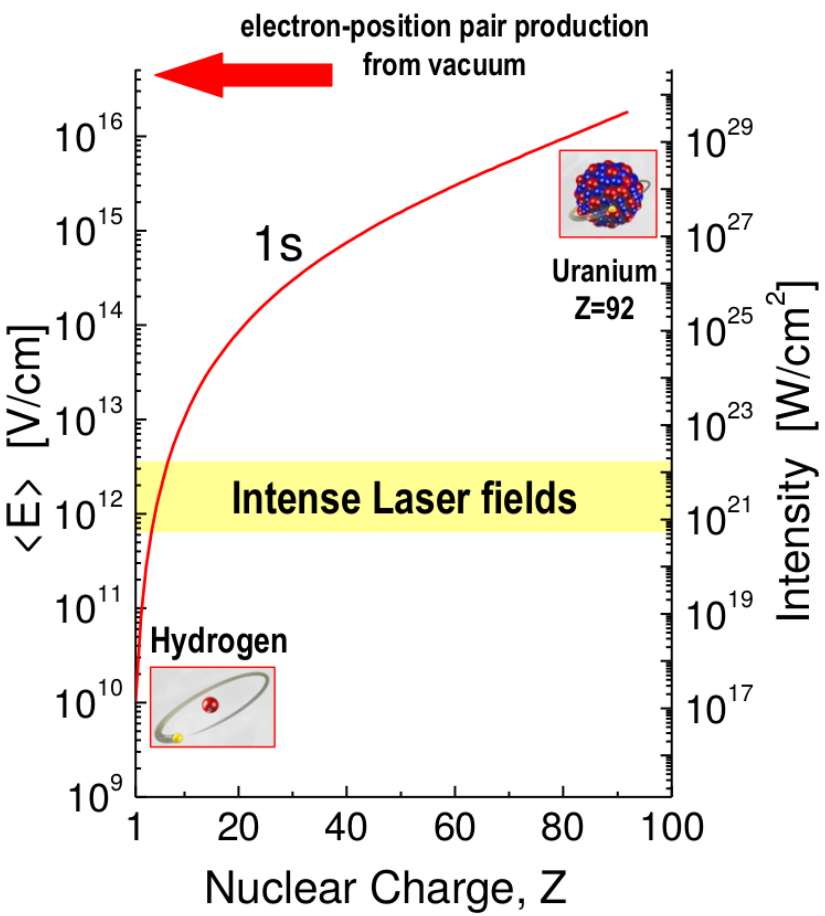
Outline

Motivation

Why interest in highly charged ions?

- Provide stringent test on bound state QED
- Precise determination of physical constants (α, m_e, g_μ,...)
- Test of Standard Model and constraint new physics



Motivations

- Application in atomic clocks for valence-hole transitions in B^+, Al^+, In^+, and Tl^+ ions
- Possible explanation of the disagreement in oscillator-strength ratio in Ne-like Fe

A. D. Ludlow *et al.*, Rev. Mod. Phys. **87**, 637 (2015)
S. Kühn *et al.*, https://arxiv.org/abs/2201.09070

Motivations

- Application in atomic clocks for valence-hole transitions in B^+, Al^+, In^+, and Tl^+ ions
- Possible explanation of the disagreement in oscillator-strength ratio in Ne-like Fe

- Natural next step after previous works (single valence and single hole cases)
- Devise an *ab initio* derivation of BSQED perturbation theory for a valence-hole excitation in a closed shell.

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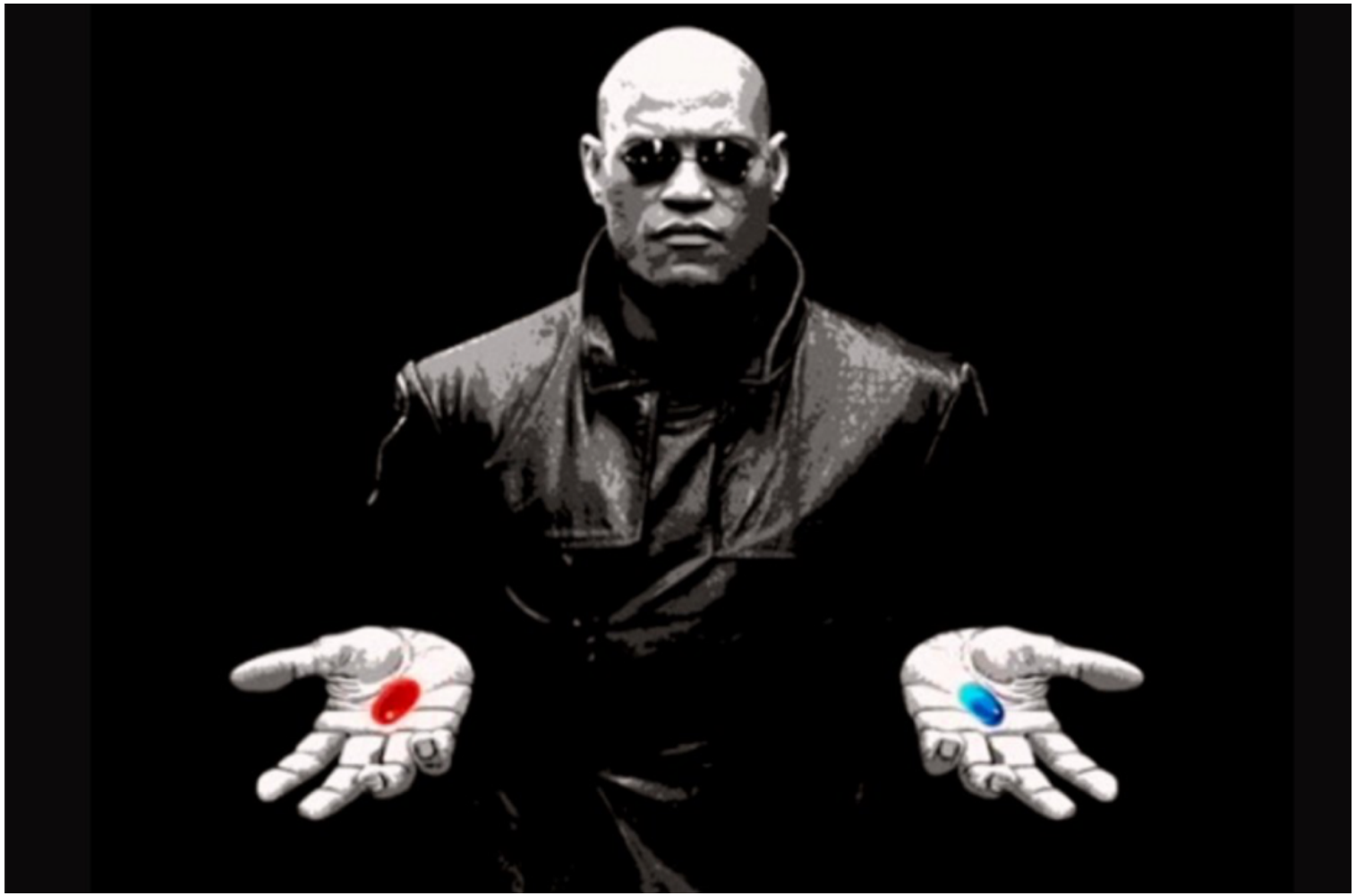
Emergency exit?!



https://www.linkedin.com/pulse/de-reis-van-held-red-pill-blue-edward-stronach-hardy

4-point Green's function

2-body system $\rightarrow$ generic 4-point Green's function:

$$G(t_1', \mathbf{x}_1, t_2', \mathbf{x}_2, t_1, \mathbf{y}_1, t_2, \mathbf{y}_2) = \langle 0| \, T \left[\psi(t_1', \mathbf{x}_1)\psi(t_2', \mathbf{x}_2)\bar{\psi}(t_2, \mathbf{y}_2)\bar{\psi}(t_1, \mathbf{y}_1)\right] |0\rangle$$

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- It contains all the information about the two-particle dynamics in presence of the nuclear Coulomb field.
- It is enough to consider a two-time Green's function.

Usual two-time Green's function

Shabaev's equal-time choice: $t_1' = t_2' = t'$ and $t_1 = t_2 = t$

$$G(t', \mathbf{x}_1, t', \mathbf{x}_2, t, \mathbf{y}_1, t, \mathbf{y}_2) = \langle 0| \, T \left[\psi(t', \mathbf{x}_1)\psi(t', \mathbf{x}_2)\bar{\psi}(t, \mathbf{y}_2)\bar{\psi}(t, \mathbf{y}_1)\right] |0\rangle$$

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Its spectral representation reveals poles only for pure electron (charge $2e$) or positron (charge $-2e$) states contributing to A and B respectively in the $\mathcal{N}$ summation.

$$\hookrightarrow g_{\alpha, i_1 i_2 j_1 j_2}(E) = \sum_{\mathcal{N}} \frac{A_{i_1 i_2 j_1 j_2}}{E - E_{\mathcal{N}} + i\varepsilon} - \sum_{\mathcal{N}} \frac{B_{i_1 i_2 j_1 j_2}}{E + E_{\mathcal{N}} - i\varepsilon}$$

Another equal-time choice

Let's select $t_1' = t_1 = t$ and $t_2' = t_2 = t'$

$$G(t, \mathbf{x}_1, t', \mathbf{x}_2, t, \mathbf{y}_1, t', \mathbf{y}_2) = \langle 0| \, T \left[\psi(t, \mathbf{x}_1)\psi(t', \mathbf{x}_2)\bar{\psi}(t', \mathbf{y}_2)\bar{\psi}(t, \mathbf{y}_1)\right] |0\rangle$$

Similar Green's function investigated in the literature:

- Logunov and Tavkhelidze, Quasi-optical approach in quantum field theory (1963)
- Fetter and Walecka, Quantum Theory of Many-Particle Systems (1971)
- J. Oddershede and P. Jørgensen, An order analysis of the particle–hole propagator (1976)
- C-M. Liegner, On the poles of the particle-hole Green's function (1981)

Towards spectral representation I

2-body TTGF in redefined vacuum framework:

$$G_\alpha(t_1, t_2; \mathbf{x}_1, \mathbf{x}_2, \mathbf{y}_1, \mathbf{y}_2) = \langle\alpha| \, T \left[\psi_\alpha(t_1, \mathbf{x}_1)\psi_\alpha(t_2, \mathbf{x}_2)\bar{\psi}_\alpha(t_2, \mathbf{y}_2)\bar{\psi}_\alpha(t_1, \mathbf{y}_1)\right.$$
$$\left. - (\mathbf{x}_1 \leftrightarrow \mathbf{x}_2) - (\mathbf{y}_1 \leftrightarrow \mathbf{y}_2) + (\mathbf{x}_1 \leftrightarrow \mathbf{x}_2, \mathbf{y}_1 \leftrightarrow \mathbf{y}_2)\right] |\alpha\rangle$$

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Steps to carry out:

- Recall for equal time: $\{\psi_a(t, \mathbf{x}), \psi_b^\dagger(t, \mathbf{y})\} = \delta^{(3)}(\mathbf{x} - \mathbf{y})\delta_{ab}$,
- Time ordering: $T\{\psi(t, \mathbf{x})\psi^\dagger(t', \mathbf{y})\} =$ $\theta(t - t')\psi(t, \mathbf{x})\psi^\dagger(t', \mathbf{y}) - \theta(t' - t)\psi^\dagger(t', \mathbf{y})\psi(t, \mathbf{x})$
- Completeness relation : $1 = \sum_\beta |\beta\rangle \langle\beta|$
- Heisenberg picture: $\psi_\alpha(t, \mathbf{x}) = e^{iHt}\psi_\alpha(0, \mathbf{x})e^{-iHt}$ with $H = H_0 + H_{\text{int}}$
- Integral representation $\theta(x) = \lim_{\varepsilon\to 0^+} \mp\frac{1}{2\pi i}\int d\omega \frac{e^{\mp ix\omega}}{\omega \pm i\varepsilon}$

Towards spectral representation II

Introduce the Fourier transform of G_α

$$\mathcal{G}_\alpha(E;\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2)\delta(E-E') = \frac{1}{2\pi i}\frac{1}{2!}\int dt_1 dt_2 e^{iEt_1 - iE't_2} G_\alpha(t_1,t_2;\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2)$$

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where

$$\begin{aligned}\mathcal{A}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2) &= \langle\alpha|\left[\psi_\alpha(0,\mathbf{x}_1)\bar{\psi}_\alpha(0,\mathbf{y}_1)|\beta\rangle\langle\beta|\psi_\alpha(0,\mathbf{x}_2)\bar{\psi}_\alpha(0,\mathbf{y}_2)\right.\\ &- \left.(\mathbf{x}_1\leftrightarrow\mathbf{x}_2)-(\mathbf{y}_1\leftrightarrow\mathbf{y}_2)+(\mathbf{x}_1\leftrightarrow\mathbf{x}_2,\mathbf{y}_1\leftrightarrow\mathbf{y}_2)\right]|\alpha\rangle\end{aligned}$$

Spectral representation

$$\mathcal{G}_\alpha(E;\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2) = \frac{1}{2!}\left\{\sum_\beta \frac{\mathcal{A}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2)}{E-E_\beta+i\varepsilon} - \sum_\beta \frac{\mathcal{B}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2)}{E+E_\beta-i\varepsilon}\right\}$$

Only consistent zeroth-order $|\beta\rangle$ states:

$$|\beta\rangle = \left\{|vh\rangle = a_v^\dagger b_h^\dagger |\alpha\rangle\,,\ |\alpha\rangle\right\}$$

Presence of poles at the valence-hole excitation energies E_{vh} and $-E_{vh}$ as well as at the zero (vacuum energy). Neutral states!

Towards contour integral formula I

Introduce

$$g_\alpha(E) = \frac{1}{2!}\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 d^3\mathbf{y}_1 d^3\mathbf{y}_2 \; : \psi_\alpha^{(0)\dagger}(\mathbf{x}_1)\psi_\alpha^{(0)\dagger}(\mathbf{x}_2)\mathcal{G}_\alpha(E;\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2)$$
$$\times \; \gamma_1^0\gamma_2^0\psi_\alpha^{(0)}(\mathbf{y}_2)\psi_\alpha^{(0)}(\mathbf{y}_1) :$$

and the valence-hole state

$$|(vh)_{JM}\rangle = \sum_{m_v,m_h} \langle j_v m_v j_h - m_h | JM\rangle \, (-1)^{j_h - m_h} a_v^\dagger b_h^\dagger \, |\alpha\rangle \equiv F_{vh} a_v^\dagger b_h^\dagger \, |\alpha\rangle$$

Towards contour integral formula II

In second quantization language:

$$g_\alpha(E) \cong \frac{1}{2!}\left\{ \sum_{i,l>E_\alpha^F, j,k<E_\alpha^F} a_i^\dagger a_l b_k^\dagger b_j + \sum_{j,k>E_\alpha^F, i,l<E_\alpha^F} a_j^\dagger a_k b_l^\dagger b_i - \sum_{i,k>E_\alpha^F, j,l<E_\alpha^F} a_i^\dagger a_k b_l^\dagger b_j - \sum_{j,l>E_\alpha^F, i,k<E_\alpha^F} a_j^\dagger a_l b_k^\dagger b_i \right\} g_{\alpha,ijkl}(E)$$

Towards contour integral formula II

In second quantization language:

$$g_\alpha(E) \cong \frac{1}{2!}\left\{\sum_{i,l>E_\alpha^F,j,k<E_\alpha^F} a_i^\dagger a_l b_k^\dagger b_j + \sum_{j,k>E_\alpha^F,i,l<E_\alpha^F} a_j^\dagger a_k b_l^\dagger b_i - \sum_{i,k>E_\alpha^F,j,l<E_\alpha^F} a_i^\dagger a_k b_l^\dagger b_j - \sum_{j,l>E_\alpha^F,i,k<E_\alpha^F} a_j^\dagger a_l b_k^\dagger b_i\right\} g_{\alpha,ijkl}(E)$$

Matrix element of interest:

$$\langle (vh)_{JM}|\, g_\alpha(E)\, |(vh)_{JM}\rangle = F_{v_1h_1}F_{v_2h_2}\left[g_{\alpha,v_1h_2h_1v_2}(E) - g_{\alpha,v_1h_2v_2h_1}(E)\right]$$

with

$$g_{\alpha,ijkl}(E) = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 d^3\mathbf{y}_1 d^3\mathbf{y}_2 \phi_i^\dagger(\mathbf{x}_1)\phi_j^\dagger(\mathbf{x}_2)\mathcal{G}_\alpha(E;\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2) \times \gamma_1^0\gamma_2^0\phi_k(\mathbf{y}_1)\phi_l(\mathbf{y}_2)$$

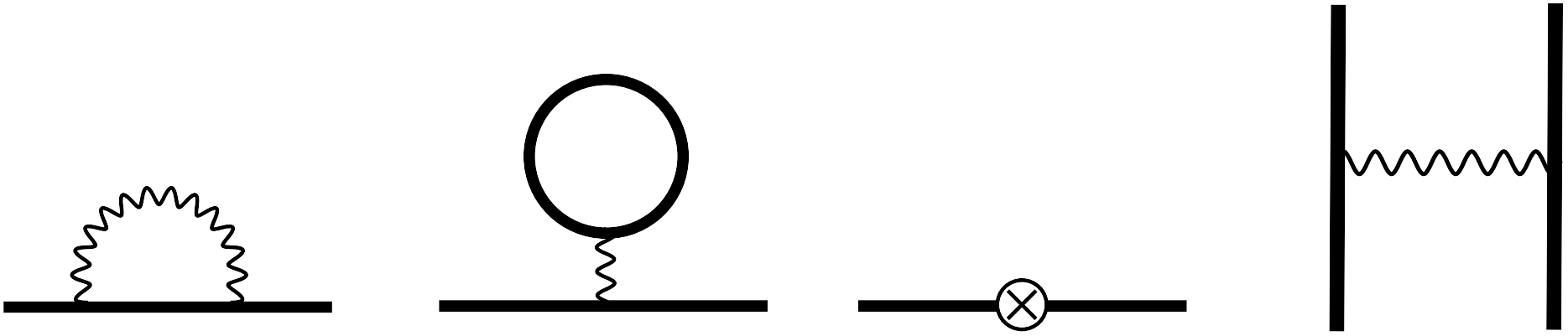
Contour integral formula

Focusing on $\mathcal{A}$ term along with the contour Γ_{vh} surrounding only the pole $E \sim E_{vh}^{(0)}$:

$$\Delta E_{vh} = \frac{\frac{1}{2\pi i}\oint_{\Gamma_{vh}} dE(E - E_{vh}^{(0)}) \langle (vh)_{JM} | \Delta g_{\alpha}(E) | (vh)_{JM} \rangle}{1 + \frac{1}{2\pi i}\oint_{\Gamma_{vh}} dE \langle (vh)_{JM} | \Delta g_{\alpha}(E) | (vh)_{JM} \rangle}$$

Diagrams: 1-particle and 2-particle terms

$$\Delta E_{vh}^{(1)} = \frac{1}{2\pi i} F_{v_1 h_1} F_{v_2 h_2} \oint_{\Gamma_{vh}} dE (E - E_{vh}^{(0)}) \left[\Delta g^{(1)}_{\alpha, v_1 h_2 h_1 v_2}(E) - \Delta g^{(1)}_{\alpha, v_1 h_2 v_2 h_1}(E) \right]$$



(a) (b)

$$\Delta E_{vh}^{(1)} = \Delta E_{vh}^{(1)1} + \Delta E_{vh}^{(1)2}$$

1-particle contributions: SE valence graph

CAUTION: p_0^2 is the hole energy, flowing backward in time!

$$\Delta g^{(1)\mathrm{SE}v}_{\alpha,v_1h_2v_2h_1}(E)\delta(E-E') \propto \delta(E-p_1^0+p_2^0)\delta(E'-p_1^0+p_2^0)$$
$$\times \frac{I_{v_1jjv_2}(\omega)}{k^0-\epsilon_j+i\varepsilon(\epsilon_j-E_\alpha^F)}\frac{\delta(p_1^0-\omega-k^0)}{\left[p_1^0-\epsilon_v+i\varepsilon\right]^2}\frac{\delta_{h_1h_2}}{p_2^0-\epsilon_h-i\varepsilon}$$

Extract most singular part:

$$\frac{1}{\left[p_1^0-\epsilon_v+i\varepsilon\right]^2}\frac{1}{p_1^0-E-\epsilon_h-i\varepsilon}=$$
$$\frac{1}{(E-E_{vh}^{(0)})^2}\left[\frac{1}{p_1^0-E-\epsilon_h-i\varepsilon}-\frac{1}{p_1^0-\epsilon_v+\varepsilon}\right]+\text{less singular}$$

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$$\times \frac{I_{v_1jjv_2}(\omega)}{k^0-\epsilon_j+i\varepsilon(\epsilon_j-E^F_\alpha)}\frac{\delta(p_1^0-\omega-k^0)}{\left[p_1^0-\epsilon_v+i\varepsilon\right]^2}\frac{\delta_{h_1h_2}}{p_2^0-\epsilon_h-i\varepsilon}$$

Separating singularities in $E-E^{(0)}_{vh}$ and keeping the most singular one:

$$\begin{aligned}\Delta E^{(1)\mathrm{SE}v}_{vh} &= \frac{i}{2\pi}F_{v_1h_1}F_{v_2h_2}\int d\omega\sum_j\frac{I_{v_1jjv_2}(\omega)\delta_{h_1h_2}}{\epsilon_v-\omega-\epsilon_j+i\varepsilon(\epsilon_j-E^F_\alpha)}\\ &\equiv F_{v_1h_1}F_{v_2h_2}\delta_{h_1h_2}\left\langle v_1\right|\Sigma_\alpha(\epsilon_v)\left|v_2\right\rangle\end{aligned}$$

1-particle contributions: SE hole graph

$$\Delta g^{(1)\mathrm{SE}h}_{\alpha,v_1h_2v_2h_1}(E)\delta(E-E') = \left(\frac{i}{2\pi}\right)^2 \int dp_2^0 d\omega \sum_j$$

$$\times \frac{I_{h_2jjh_1}(\omega)}{p_2^0-\omega-\epsilon_j+i\varepsilon(\epsilon_j-E_\alpha^F)} \frac{1}{\left[p_2^0-\epsilon_h-i\varepsilon\right]^2} \frac{\delta_{v_1v_2}}{E+p_2^0-\epsilon_v+i\varepsilon}$$

Keeping the most singular part in $E-E_{vh}^{(0)}$:

$$\begin{aligned}\Delta E_{vh}^{(1)\mathrm{SE}h} &= -\frac{i}{2\pi}F_{v_1h_1}F_{v_2h_2}\int d\omega \sum_j \frac{I_{h_2jjh_1}(\omega)\delta_{v_1v_2}}{\epsilon_{h_1}-\omega-\epsilon_j+i\varepsilon(\epsilon_j-E_\alpha^F)} \\ &\equiv -F_{v_1h_1}F_{v_2h_2}\delta_{v_1v_2}\left\langle h_2\right|\Sigma_\alpha(\epsilon_h)\left|h_1\right\rangle\end{aligned}$$

Total 1-particle contributions

Extended to VP graph under the modification:

$$\langle v_1 | \Sigma_\alpha(\epsilon_v) | v_2 \rangle \to \langle v_1 | \Upsilon_\alpha | v_2 \rangle = -\frac{i}{2\pi} \int d\omega \sum_j \frac{I_{v_1 j v_2 j}(0)}{\omega - \epsilon_j + i\varepsilon(\epsilon_j - E_\alpha^F)}$$

Total 1-particle contributions

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Total one-particle contribution:

$$\Delta E_{vh}^{(1)1} = \langle v | \Sigma_\alpha(\epsilon_v) | v \rangle + \langle v | \Upsilon_\alpha | v \rangle - U_{vv} - \langle h | \Sigma_\alpha(\epsilon_h) | h \rangle - \langle h | \Upsilon_\alpha | h \rangle + U_{hh}$$

One-photon exchange: direct part

$$\Delta E_{vh}^{(1)2\mathrm{dir}} = -\frac{1}{2\pi i} F_{v_1 h_1} F_{v_2 h_2} \oint_{\Gamma_{vh}} dE (E - E_{vh}^{(0)}) \Delta g_{\alpha, v_1 h_2 v_2 h_1}^{(1)2\mathrm{dir}}(E)$$

One has

$$\Delta g_{\alpha, v_1 h_2 v_2 h_1}^{(1)\mathrm{dir}}(E)\delta(E - E') \propto \delta(E - p_1^0 + p_2^0)\delta(E' - p_1'^0 + p_2'^0)$$
$$\times \frac{\delta(p_1^0 - \omega - p_1'^0)}{p_1'^0 - \epsilon_v + i\varepsilon} \frac{\delta(p_2'^0 + \omega - p_2^0)}{p_2'^0 - \epsilon_h - i\varepsilon} \frac{I_{v_1 h_2 v_2 h_1}(\omega)}{p_1^0 - \epsilon_v + i\varepsilon} \frac{1}{p_2^0 - \epsilon_h - i\varepsilon}$$

One-photon exchange: direct part

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Need to extract singular parts, to get in the end:

$$\Delta E_{vh}^{(1)2\mathrm{dir}} = -F_{v_1 h_1} F_{v_2 h_2} I_{v_1 h_2 v_2 h_1}(0)$$

One-photon exchange: exchange part

$$\Delta E_{vh}^{(1)2\mathrm{exc}} = \frac{1}{2\pi i} F_{v_1 h_1} F_{v_2 h_2} \oint_{\Gamma_{vh}} dE (E - E_{vh}^{(0)}) \Delta g_{\alpha, v_1 h_2 h_1 v_2}^{(1)2\mathrm{exc}}(E)$$

with

$$\Delta g_{\alpha, v_1 h_2 h_1 v_2}^{(1)2\mathrm{exc}}(E)\delta(E - E') = \delta(E - p_1^0 + p_2^0)\delta(E' - p_1'^0 + p_2'^0)$$
$$\times \frac{\delta(p_2^0 - \omega - p_1'^0)}{p_1'^0 - \epsilon_v + i\varepsilon} \frac{\delta(p_2'^0 + \omega - p_1^0)}{p_2'^0 - \epsilon_h - i\varepsilon} \frac{I_{v_1 h_2 h_1 v_2}(\omega)}{p_2^0 - \epsilon_h - i\varepsilon} \frac{1}{p_1^0 - \epsilon_v + i\varepsilon}$$

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$$\Delta g_{\alpha, v_1 h_2 h_1 v_2}^{(1)2\mathrm{exc}}(E)\delta(E - E') = \delta(E - p_1^0 + p_2^0)\delta(E' - p_1'^0 + p_2'^0)$$
$$\times \frac{\delta(p_2^0 - \omega - p_1'^0)}{p_1'^0 - \epsilon_v + i\varepsilon} \frac{\delta(p_2'^0 + \omega - p_1^0)}{p_2'^0 - \epsilon_h - i\varepsilon} \frac{I_{v_1 h_2 h_1 v_2}(\omega)}{p_2^0 - \epsilon_h - i\varepsilon} \frac{1}{p_1^0 - \epsilon_v + i\varepsilon}$$

After extraction of the most singular part:

$$\Delta E_{vh}^{(1)2\mathrm{exc}} = F_{v_1 h_1} F_{v_2 h_2} I_{v_1 h_2 h_1 v_2}(\Delta_{hv})$$

Total 2-particle contributions:

$$\Delta E_{vh}^{(1)2} = F_{v_1 h_1} F_{v_2 h_2} \left[I_{v_1 h_2 h_1 v_2}(\Delta_{hv}) - I_{v_1 h_2 v_2 h_1}(0) \right] .$$

First order corrections in redefined vacuum state

$$
\begin{aligned}
\Delta E_{vh}^{(1)} &= F_{v_1 h_1} F_{v_2 h_2} \left[I_{v_1 h_2 h_1 v_2}(\Delta_{hv}) - I_{v_1 h_2 v_2 h_1}(0) \right] \\
&+ \langle v | \Sigma_{\alpha}(\epsilon_v) | v \rangle + \langle v | \Upsilon_{\alpha} | v \rangle - U_{vv} \\
&- \langle h | \Sigma_{\alpha}(\epsilon_h) | h \rangle - \langle h | \Upsilon_{\alpha} | h \rangle + U_{hh} \,,
\end{aligned}
$$

So far no interactions with core electrons, must be extracted!

Vacuum states

- Original (Fock) vacuum state:

$$a_j \left|0\right\rangle = 0 \quad \forall j : \epsilon_j > E^F = 0$$

- Redefined (Fock) vacuum state $\left|\alpha\right\rangle$:

$$\left|\alpha\right\rangle = a_a^\dagger a_b^\dagger ... \left|0\right\rangle \text{ such that } b_a \left|\alpha\right\rangle = 0$$

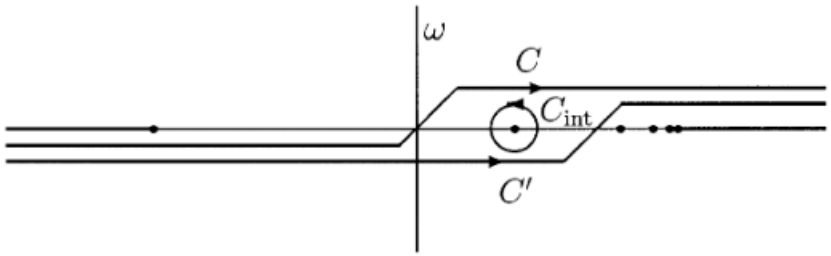
with associated Fermi level: $E_\alpha^F \in (\epsilon_a, \epsilon_v)$

- Effect on the electron propagator:

$$\left\langle\alpha\right| T\ [\psi_\alpha^{(0)}(x)\psi_\alpha^{(0)\dagger}(y)\ ] \left|\alpha\right\rangle =$$
$$\frac{i}{2\pi}\int d\omega \sum_j \frac{\phi_j(\boldsymbol{x})\phi_j^\dagger(\boldsymbol{y})\exp\left[-i(x^0-y^0)\omega\right]}{\omega - \epsilon_j + i\varepsilon(\epsilon_j - E_\alpha^F)}$$

Effect of vacuum state redefinition (E_α^F)

- Core electrons promoted into Dirac sea



C path: $1 - i\varepsilon$ prescription
$C^{'}$ path: $1 + i\varepsilon$ prescription
$C_{int} = C^{'} - C$

- Benefits:
  1. C_{int} describes interactions of the particle of interest with core electrons, accounted via loop and raditive corrections.
  2. Vacuum redefintion allows to selectively encircles the interaction partner of the corresponding state of interest.

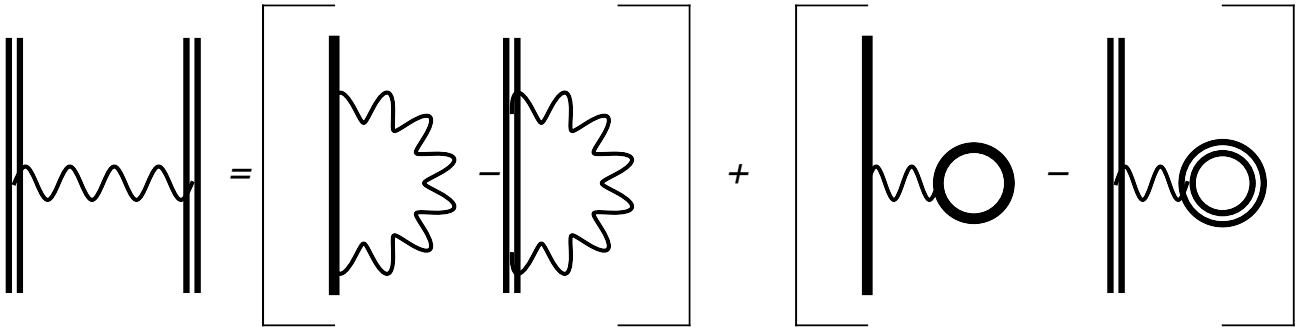
V. M. Shabaev, Phys. Rep. **365**, 119 (2002)

How to extract many-electron corrections

At one-loop level:

$$\Delta E_v^{(1)} = \Delta E_v^{(1L)} + \Delta E_v^{(1I)}$$

Graphically:



Sokhotski theorem:

$$\sum_j \frac{\phi_j(\boldsymbol{x})\bar{\phi}_j(\boldsymbol{y})}{[\omega - \epsilon_j + i\varepsilon(\epsilon_j - E_\alpha^F)]^p} - \sum_j \frac{\phi_j(\boldsymbol{x})\bar{\phi}_j(\boldsymbol{y})}{[\omega - \epsilon_j + i\varepsilon(\epsilon_j - E^F)]^p}$$

$$= \frac{2\pi i(-1)^p}{(p-1)!} \frac{d^{(p-1)}}{d\omega^{(p-1)}} \sum_a \delta(\omega - \epsilon_a)\phi_a(\boldsymbol{x})\bar{\phi}_a(\boldsymbol{y})$$

From a redefined vacuum state to the standard one

Linkage:

$$\begin{aligned} \langle v| \Sigma_{\alpha}(\epsilon_v) |v\rangle &= \langle v| \Sigma(\epsilon_v) |v\rangle - \sum_a I_{vaav}(\Delta_{va}) \\ \langle v| \Upsilon_{\alpha} |v\rangle &= \langle v| \Upsilon |v\rangle + \sum_a I_{vava}(0) \end{aligned}$$

From a redefined vacuum state to the standard one

Linkage:

$$\begin{aligned}\langle v|\,\Sigma_{\alpha}(\epsilon_v)\,|v\rangle &= \langle v|\,\Sigma(\epsilon_v)\,|v\rangle - \sum_a I_{vaav}(\Delta_{va})\\ \langle v|\,\Upsilon_{\alpha}\,|v\rangle &= \langle v|\,\Upsilon\,|v\rangle + \sum_a I_{vava}(0)\end{aligned}$$

Total first order corrections

$$\begin{aligned}\Delta E^{(1)}_{vh} &= \sum_a [I_{vava}(0) - I_{vaav}(\Delta_{va})] - \sum_a [I_{haha}(0) - I_{haah}(\Delta_{ha})]\\ &+ F_{v_1h_1}F_{v_2h_2}\,[I_{v_1h_2h_1v_2}(\Delta_{hv}) - I_{v_1h_2v_2h_1}(0)]\\ &+ \langle v|\,\Sigma(\epsilon_v)\,|v\rangle + \langle v|\,\Upsilon\,|v\rangle - U_{vv}\\ &- \langle h|\,\Sigma(\epsilon_h)\,|h\rangle - \langle h|\,\Upsilon\,|h\rangle + U_{hh}\,.\end{aligned}$$

R. N. Soguel, *et al.*,Phys. Rev. A **106**, 012802 (2022)

Conclusion and outlooks

- Two-time Green's function for valence-hole excitation derived
- Possible to account for full first order QED corrections in α
- Identification of gauge invariant subsets

Conclusion and outlooks

- Two-time Green's function for valence-hole excitation derived
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- Ne-like Ge: agreement up to 10^{-4} relative uncertainty between MBPT calculations and measured values!
  $\hookrightarrow$ First order radiative QED effects via Model Lamb-shift-operator
  $\hookrightarrow$ Interelectronic interaction via frequency independent Breit interaction
- Ne-like Eu: agreement of the order of 1 eV, in absolute value, between MBPT predictions and experimental values.

P. Beiersdorfer *et al.*, Phys. Rev. A **100**, 032516 (2019)
P. Beiersdorfer, *et al.*, Can. J. Phys. **98**, 239 (2020)