Vacuum polarization in the finite basis Dirac problem

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EMMI Workshop "Accurate relativistic treatment of multi-electron atoms and applications to Super-Heavy elements"

Plan and motivations

Presentation plan

1. The Dirac equation
   1. Charge conjugation symmetry
   2. Finite basis approximation: Kinetic Balances

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      1. Qualitative journey: the full α VP density
      2. Quantitative goal: the $\alpha\,(Z\alpha)^{n\geq 3}$ VP density

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Motivations to construct QED corrections from numerical Dirac solutions

- Effective VP potentials are not suited for practical calculations.[a]

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Motivations to construct QED corrections from numerical Dirac solutions

- Effective VP potentials are not suited for practical calculations.[a]
- Effective SE potentials are parameterized to fit exact 1e SE energy-shift.[bcd]

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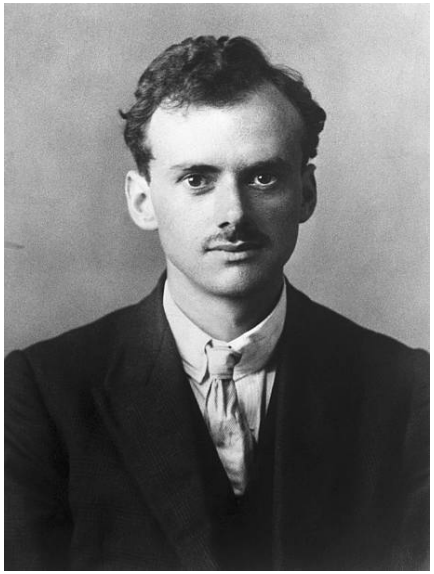
[a] Blomqvist, J. Nuc. Phys. B 48.1 (1972): 95-103.
[b] Pyykkö and Zhao. Journal of Physics B:36.8 (2003): 1469.
[c] Flambaum and Ginges. Phys. Rev. A 72.5 (2005): 052115.
[d] Shabaev et al. Phys. Rev. A 88.1 (2013): 012513.

Relativistic electron/positron theory

The electron behavior is, up to a large extent, predicted by the Dirac equation

$$\left[i\hbar\gamma^{\mu}\partial_{\mu} - mc\right]\psi^{e}(x) = 0. \tag{1}$$



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In the presence of a general external four-potential $A^{\mu} = (\phi, \boldsymbol{A})^{\mu}$, this equation becomes ($q_{\text{electron}} = -e$)

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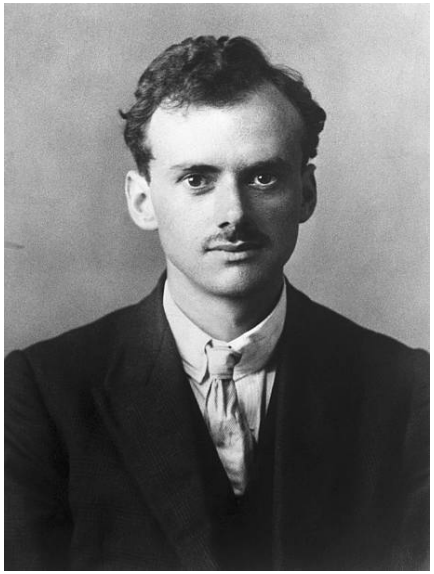

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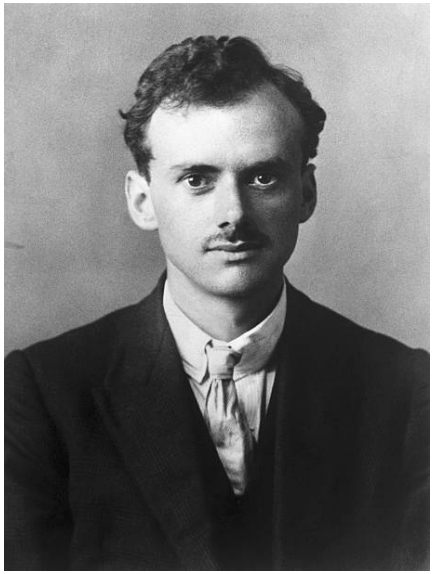
The positron's (electron's antiparticle partner) wavefunction obeys

$$\left[\gamma^{\mu}\left(i\hbar\partial_{\mu}\boxed{-e}A_{\mu}(x)\right) - mc\right]\psi^{p}(x) = 0. \tag{3}$$



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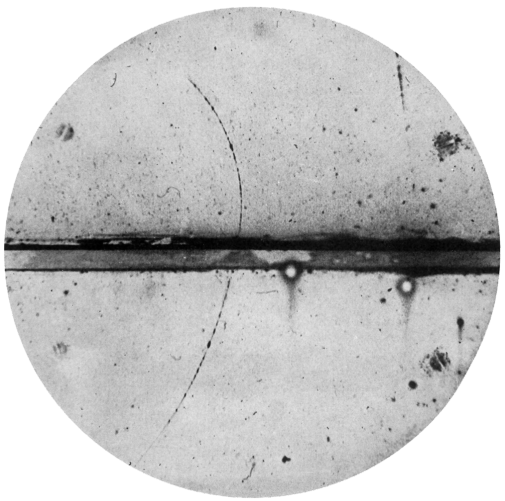

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The two wavefunctions are related by the charge conjugation operation

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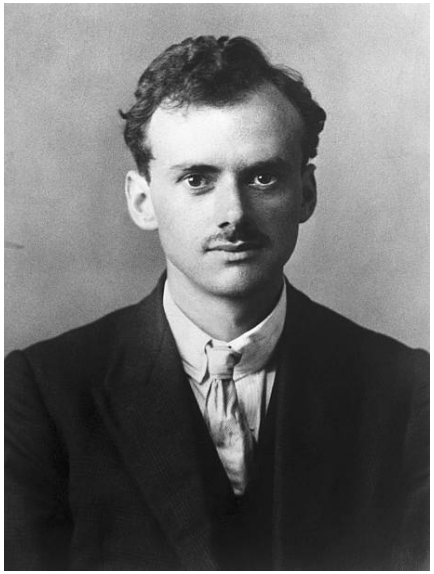

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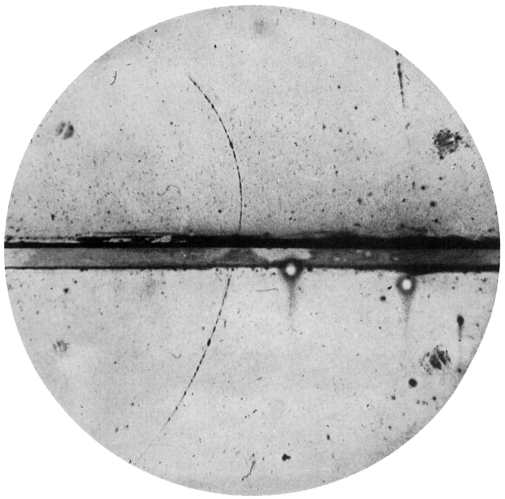

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$\mathcal{C}$-symmetry in the time-independent problem

In the time-independent potential case: $A(x) = A(\boldsymbol{x})$, one can write

$$\psi_n(x) = e^{-\frac{i}{\hbar}E_n t}\psi_n(\boldsymbol{x}) \tag{5}$$

where $\{E_n, \psi_n(\boldsymbol{x})\}$ forms a solution of the time-independent Dirac equation:

$$\left[-c\boldsymbol{\alpha}\cdot\left[+i\hbar\boldsymbol{\nabla}-e\boldsymbol{A}(\boldsymbol{x})\right]+\beta mc^2-e\phi(\boldsymbol{x})\right]\ \psi(\boldsymbol{x}) = \boxed{+E}\ \psi(\boldsymbol{x}). \tag{6}$$

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The charge-conjugated solution $\mathcal{C}\psi(\boldsymbol{x})$ (positron), obeys:

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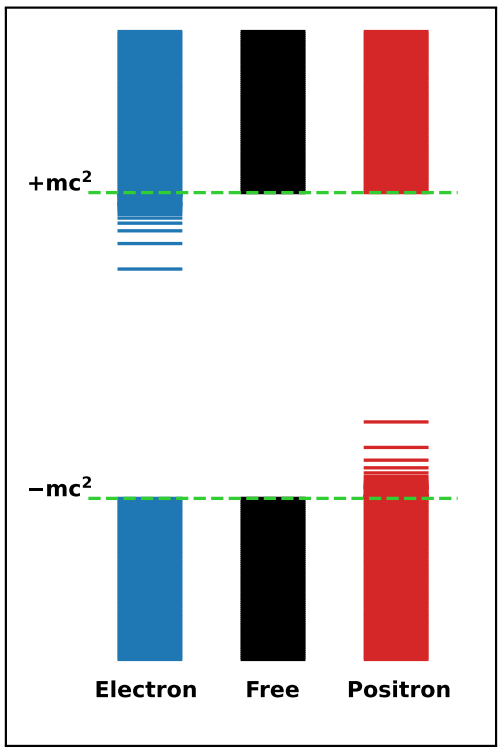

	Electron	Positron
Charge	$-e$	$+e$
Wavefunction	$\psi(\boldsymbol{x}) = \begin{bmatrix}\psi^L(\boldsymbol{x})\\ \psi^S(\boldsymbol{x})\end{bmatrix}$	$\mathcal{C}\psi(\boldsymbol{x}) = \begin{bmatrix}\sigma_2\psi^{S*}(\boldsymbol{x})\\ -\sigma_2\psi^{L*}(\boldsymbol{x})\end{bmatrix}$
Energy	$+E$	$-E$

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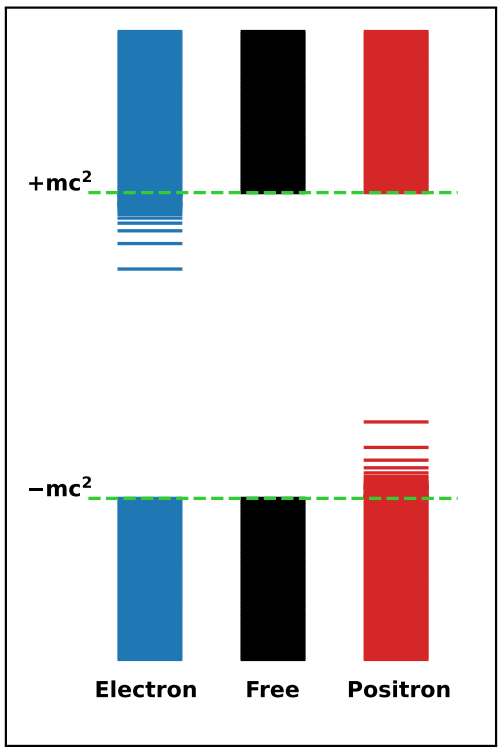

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Energy	$+E$	$-E$

In the free-particle case (black spectrum), we have:

$$\left[-c\boldsymbol{\alpha}\cdot i\hbar\boldsymbol{\nabla}+\beta mc^2\right]\ \psi(\boldsymbol{x}) = \boxed{+E}\ \psi(\boldsymbol{x}). \tag{8}$$

$$\left[-c\boldsymbol{\alpha}\cdot i\hbar\boldsymbol{\nabla}+\beta mc^2\right]\mathcal{C}\psi(\boldsymbol{x}) = \boxed{-E}\,\mathcal{C}\psi(\boldsymbol{x}). \tag{9}$$

Relativistic electron theory in the finite basis problem

The radial Dirac equation reads

$$\begin{bmatrix} mc^2 - e\phi(r) - E_{n,\kappa} & -c\hbar\left[\frac{d}{dr} - \frac{\kappa}{r}\right] \\ c\hbar\left[\frac{d}{dr} + \frac{\kappa}{r}\right] & -mc^2 - e\phi(r) - E_{n,\kappa} \end{bmatrix} \begin{bmatrix} P_{n,\kappa} \\ Q_{n,\kappa} \end{bmatrix} = 0 \tag{10}$$

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L and S component functions ($P_{n,\kappa}$ and $Q_{n,\kappa}$) are expanded in L and S basis sets:

$$\begin{bmatrix} P_{n,\kappa} \\ Q_{n,\kappa} \end{bmatrix} \approx \begin{bmatrix} \mathcal{P}_{\alpha,\kappa} \\ \mathcal{Q}_{\alpha,\kappa} \end{bmatrix} = \sum_{i=1}^{n_\kappa^L} c_{\alpha,\kappa,i}^L \begin{bmatrix} \pi_{\kappa,i}^L(r) \\ 0 \end{bmatrix} + \sum_{i=1}^{n_\kappa^S} c_{\alpha,\kappa,i}^S \begin{bmatrix} 0 \\ \pi_{\kappa,i}^S(r) \end{bmatrix} \tag{11}$$

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The problem

Arbitrary choices of radial functions $\pi_{\kappa,i}^L$ and $\pi_{\kappa,i}^S$ lead to:

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The solution

Respect the right (or at least the approximated) coupling between large and small component functions: Kinetic balance!

Kinetic balances

The radial Dirac equation can be written as:

$$Q_{n,\kappa} = \frac{\hbar}{mc} \frac{1}{1 + (e\phi + E_{n,\kappa})/mc^2} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{n,\kappa} \tag{12}$$

$$P_{n,\kappa} = \frac{\hbar}{mc} \frac{1}{1 - (e\phi + E_{n,\kappa})/mc^2} \left[\frac{d}{dr} - \frac{\kappa}{r} \right] Q_{n,\kappa}. \tag{13}$$

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$\mathcal{C}$-DKB with Gaussian functions

The spherical Gaussian basis functions are:

$$\pi^L_{\kappa,i} = r^{\left|\kappa+\frac{1}{2}\right|+\frac{1}{2}} e^{-\zeta^L_{\kappa,i} r^2} \tag{16}$$
$$\pi^S_{\kappa,i} = r^{\left|\kappa-\frac{1}{2}\right|+\frac{1}{2}} e^{-\zeta^S_{\kappa,i} r^2} \tag{17}$$

Gaussian DKB becomes $\mathcal{C}$-symmetric with

κ	-1	$+1$	-2	$+2$	$\ldots$
ζ^L_κ	●	●	●	●	$\ldots$
ζ^S_κ	●	●	●	●	$\ldots$

Table: Same color dots = same set of exponents.

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Bound-state QED

A fundamental quantity in the QED problem is the scattering matrix ($\hat{\mathcal{S}}$-matrix)

$$\hat{\mathcal{S}}(\epsilon,\lambda) = \mathsf{T}\left[\exp\left(\frac{\lambda}{i\hbar c}\int d^4x e^{-\frac{\epsilon}{\hbar}|t|}\hat{\mathcal{H}}_I^{\mathsf{QED}}(x)\right)\right], \qquad \text{with} \quad x=(ct,\boldsymbol{x}) \tag{18}$$

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This equation couples the electron field operator $\hat{\Psi}(x)$ that solves

$$\left[\gamma^\mu\left(i\hbar\partial_\mu + eA_\mu^e(x)\right) - mc\right]\hat{\Psi}(x) = 0, \quad \text{with} \quad A_\mu^e(x)\text{: external potential,} \tag{20}$$

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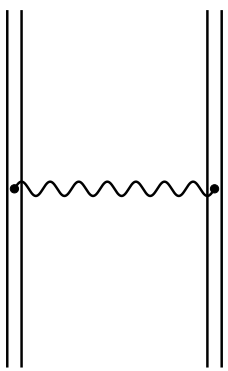

(a) Single-photon exchange

Figure: The no-real-photon e^2-order BSQED corrections ($\hat{\mathcal{S}}^{(2)}$)

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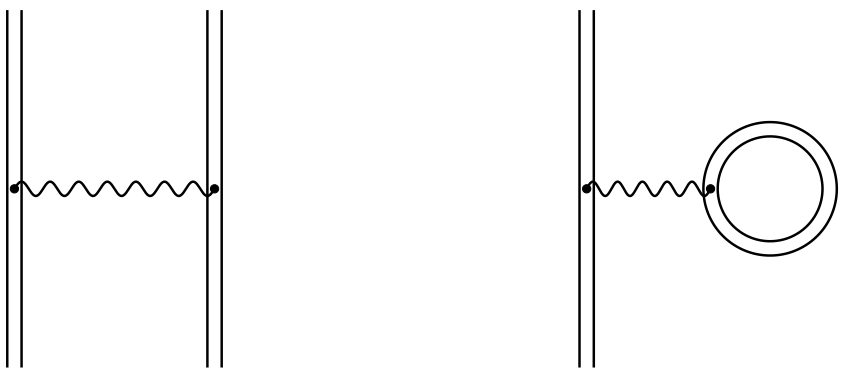

(a) Single-photon exchange (b) Vacuum polarization

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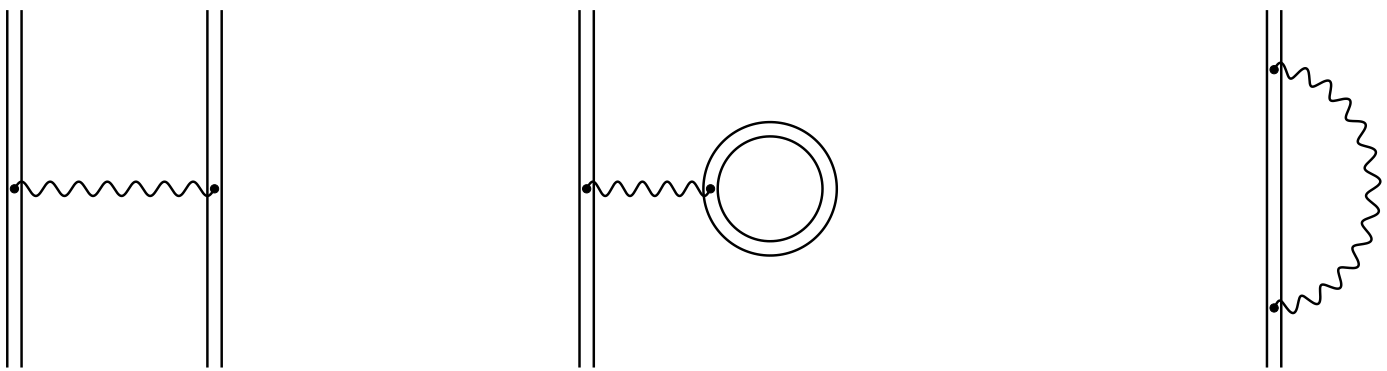
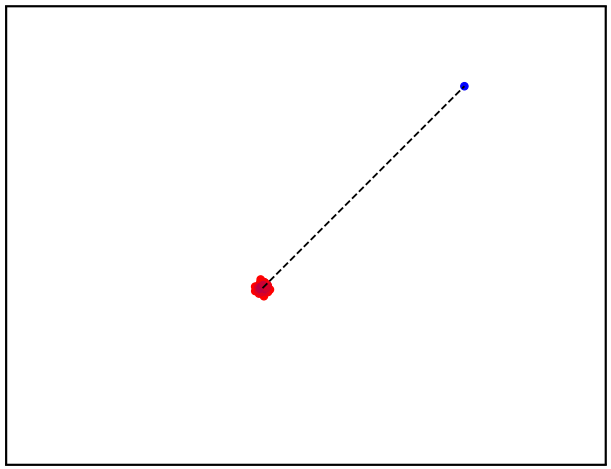


(a) Single-photon exchange (b) Vacuum polarization (c) Self-energy

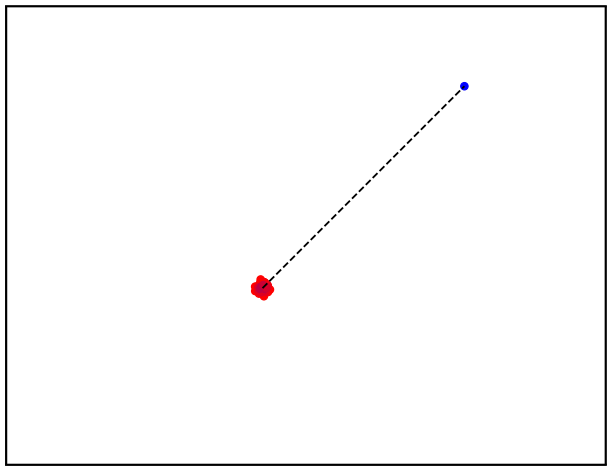
Figure: The no-real-photon e^2-order BSQED corrections ($\hat{\mathcal{S}}^{(2)}$)

Vacuum polarization



(a) The hydrogen problem

Vacuum polarization



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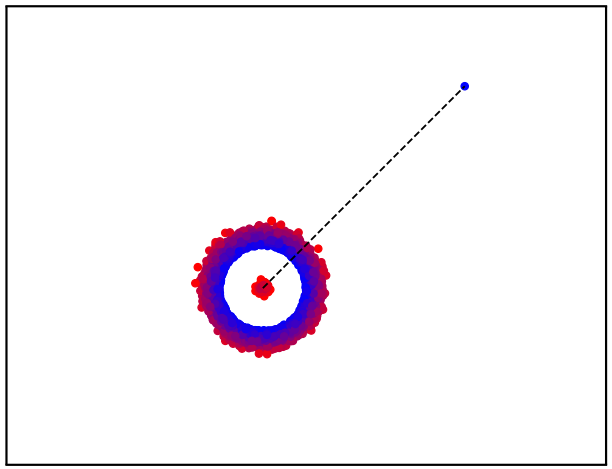

(b) The real hydrogen problem

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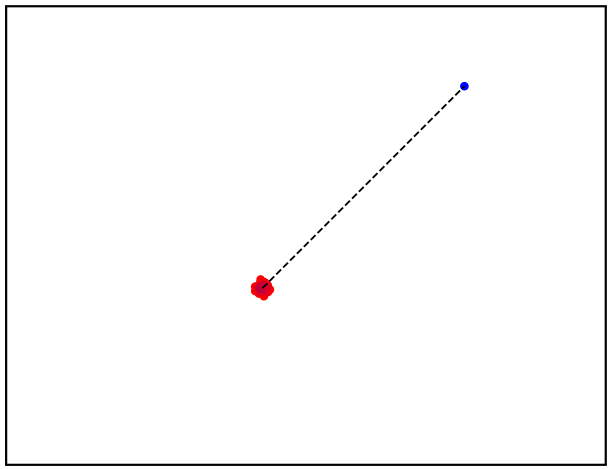

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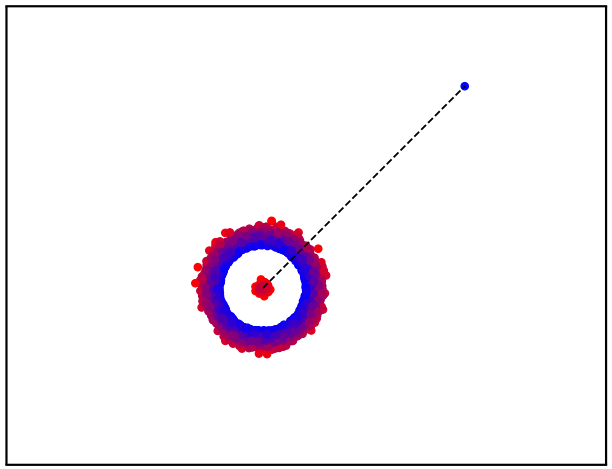

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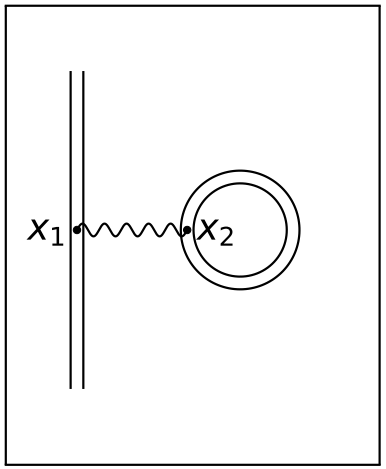

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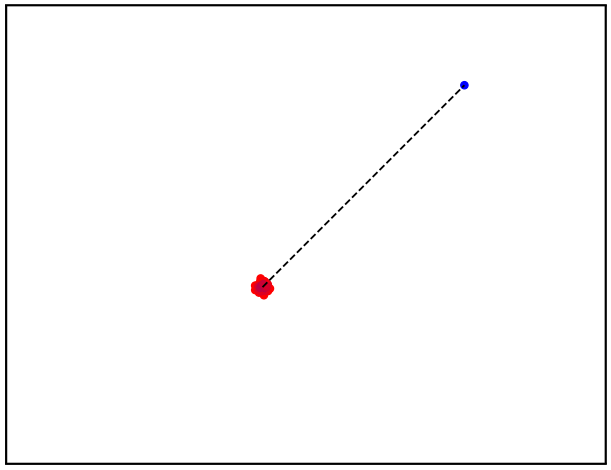

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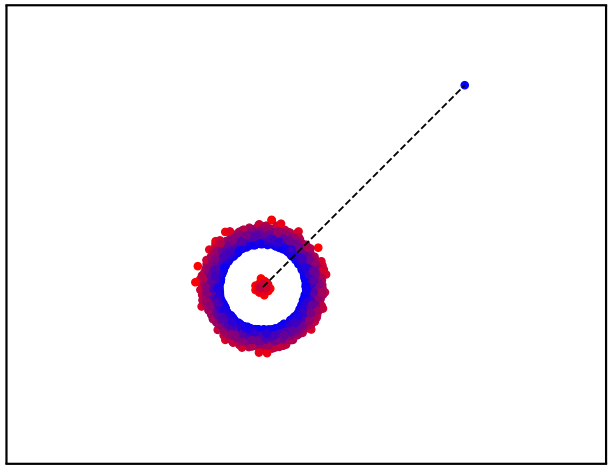

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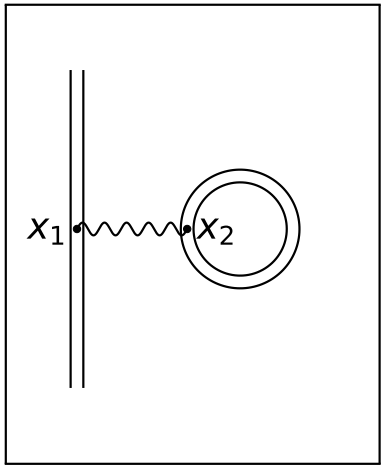

(c) Vacuum polarization

In the presence of an external four-potential

$$A^e(x) = (\phi(\boldsymbol{x})/c, 0) \tag{21}$$

the VP energy-shift experienced by an atomic state $\{E_i, \psi_i\}$ becomes

$$E_i^{\mathrm{VP}} = -e \int d^3x_1 \int d^3x_2 \psi_i^\dagger(\boldsymbol{x}_1)\psi_i(\boldsymbol{x}_1) \frac{1}{4\pi\varepsilon_0 |\boldsymbol{x}_1 - \boldsymbol{x}_2|} \rho^{\mathrm{VP}}(\boldsymbol{x}_2) \tag{22}$$

where the vacuum polarization cloud density can be written as

$$\rho^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e}{2}\left[\sum_{E_i>0} \psi_i^\dagger(\boldsymbol{x})\psi_i(\boldsymbol{x}) - \sum_{E_i<0} \psi_i^\dagger(\boldsymbol{x})\psi_i(\boldsymbol{x})\right] \tag{23}$$

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In the spherical free-particle case, $\mathcal{C}$-symmetry allows to write the $-\kappa$ density as:

$$\rho_{-\kappa}^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi r^2}\sum_{n}\mathrm{sgn}\left(E_{n,-\kappa}\right)\left[P_{n,-\kappa}^2 + Q_{n,-\kappa}^2\right] = -\rho_{\kappa}^{\mathrm{VP}}(\boldsymbol{x}) \tag{27}$$

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This relation shows that opposite κ-sign densities cancel each other out:

$$\rho^{\mathrm{VP}}(\boldsymbol{x}) = \sum_{\kappa=+1,+2\ldots}\left[\rho_{\kappa}^{\mathrm{VP}}(\boldsymbol{x}) + \rho_{-\kappa}^{\mathrm{VP}}(\boldsymbol{x})\right] = 0 \tag{28}$$

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Numerical vacuum polarization density

We shall now use RKB and $\mathcal{C}$-DKB to compute the VP density

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We shall first present RKB and $\mathcal{C}$-DKB computations, and focus on:

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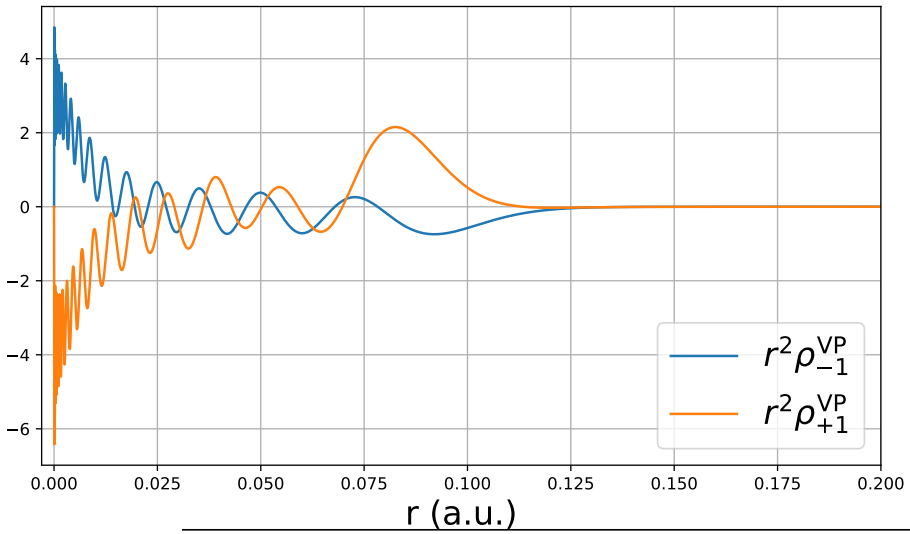
Quantitative computations

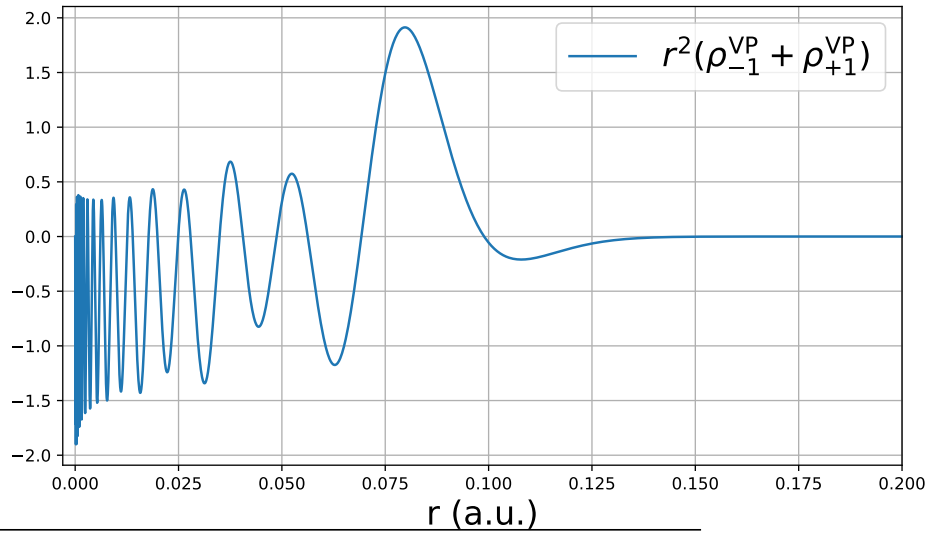
Subtract the VP density that is linear in the nuclear charge (containing the Uehling effect + divergence), and compare our results with the more sophisticated computation.

A sign of $\mathcal{C}$-symmetry violation: VP density with j-basis

We have done two free (Z=0) calculations using uranium j-basis:

- **RKB** ⚠ ($\mathcal{C}$-symmetry is violated):





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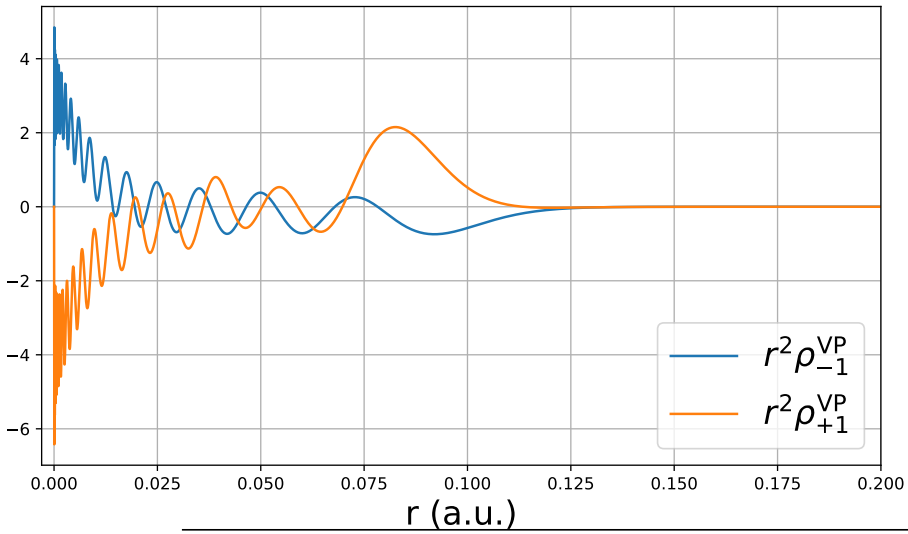

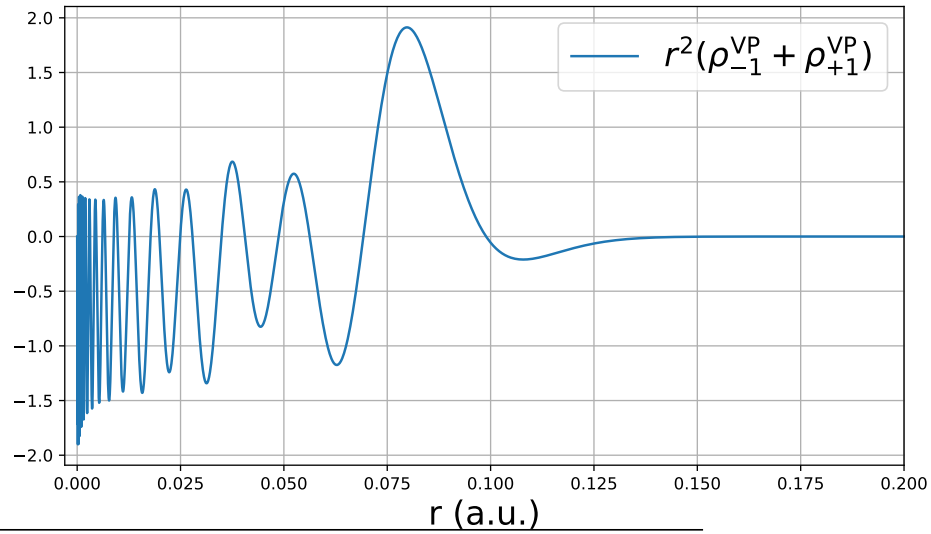

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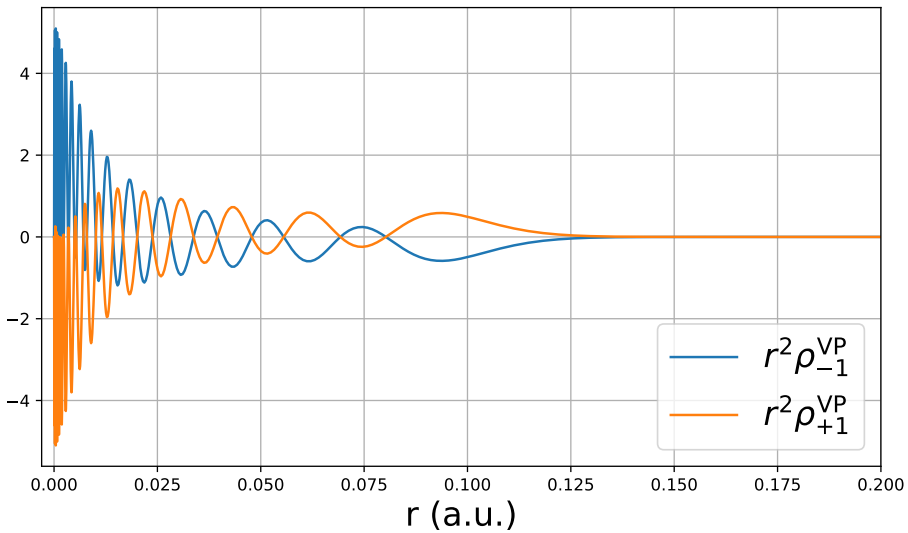

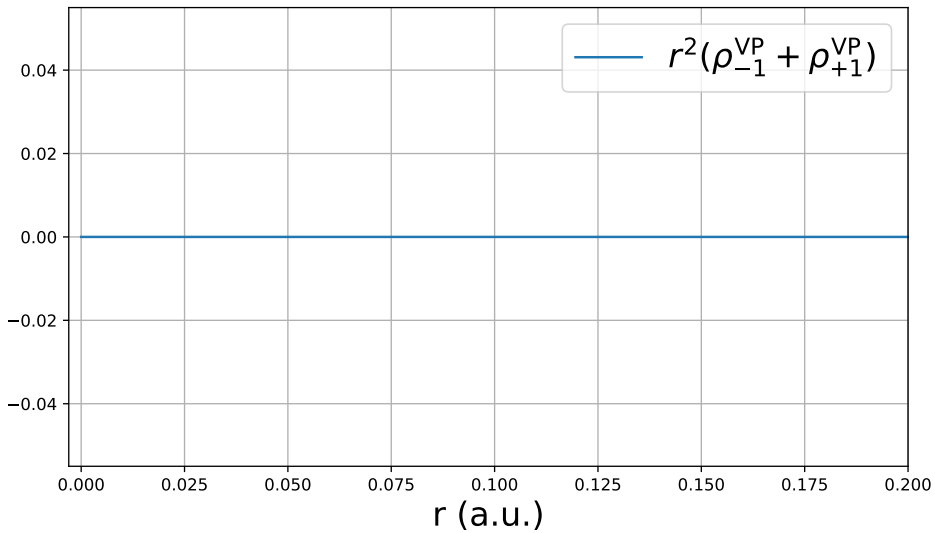

RKB vs $\mathcal{C}$-DKB: 1e uranium atom at large distances

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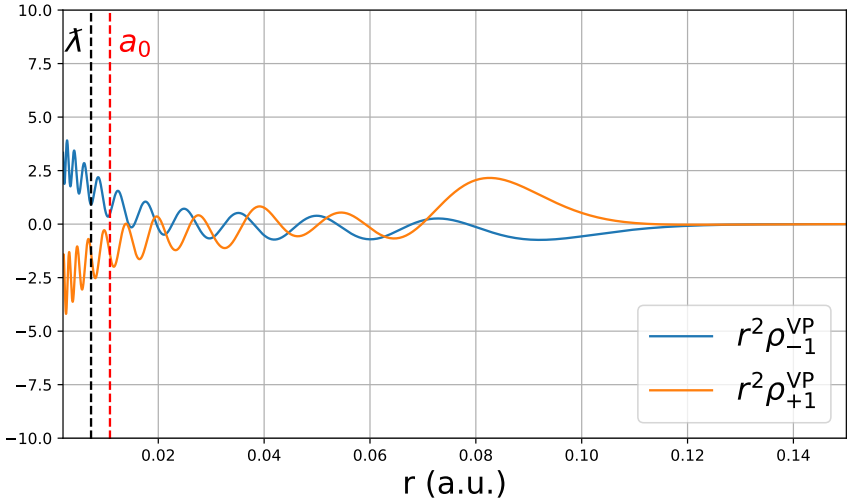

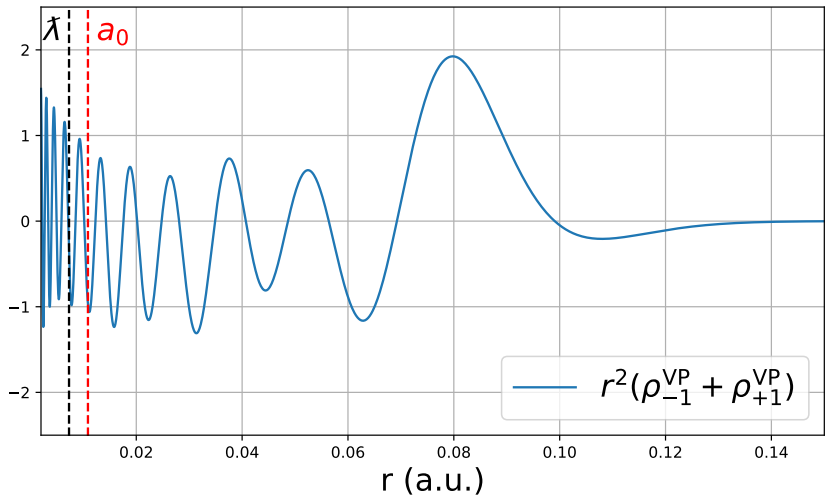

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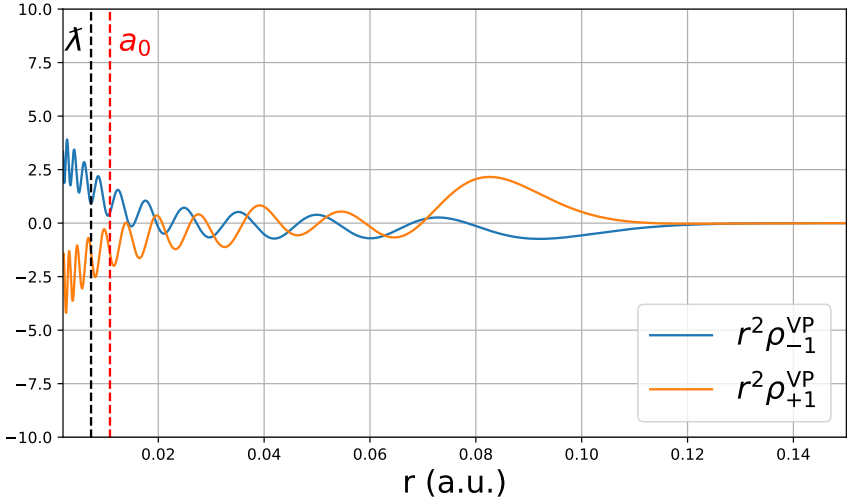
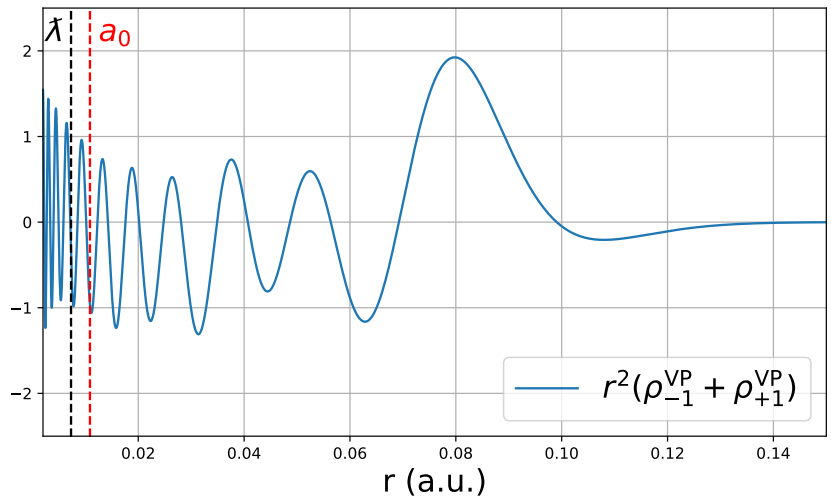
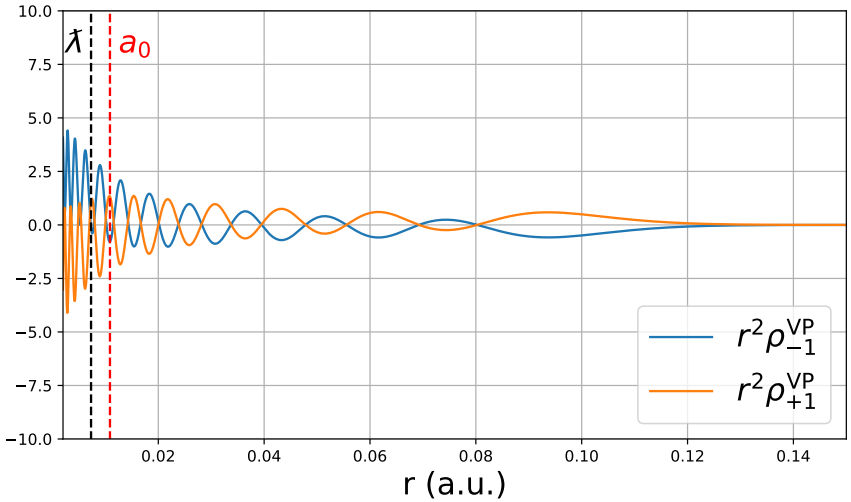
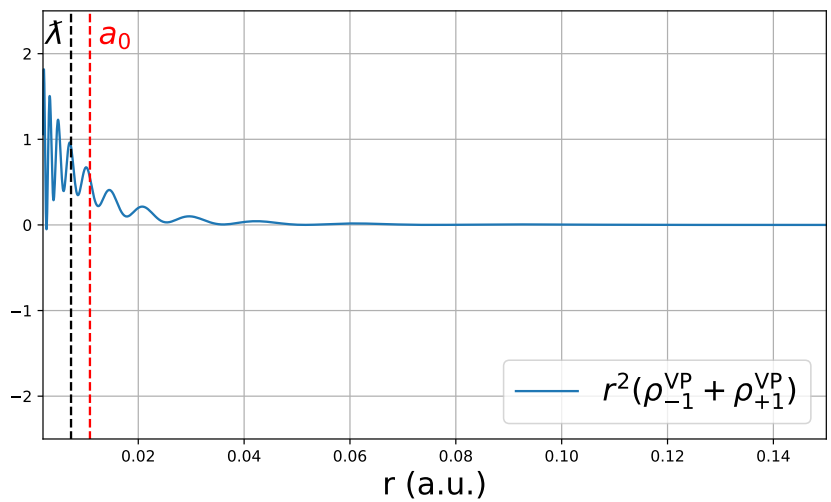




DKB ✔ ($\mathcal{C}$-symmetry is obeyed):





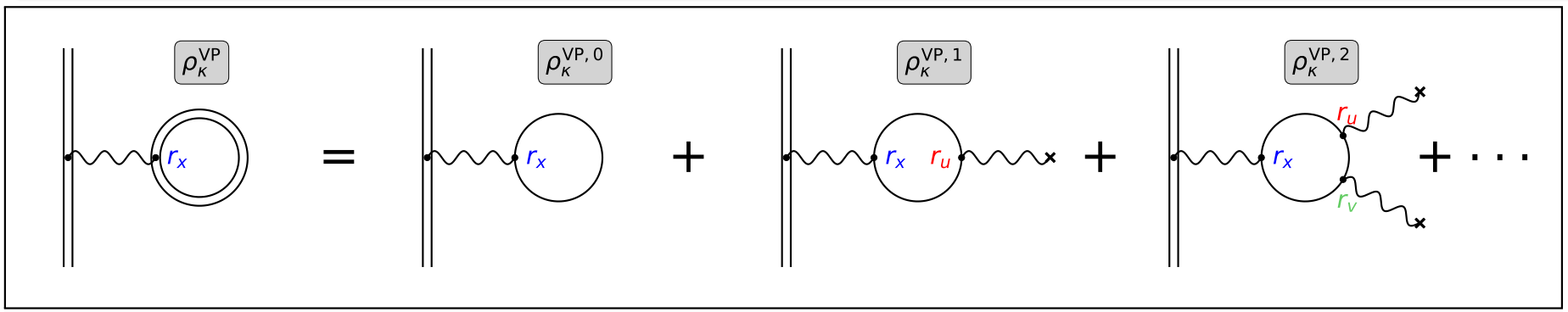
The linear vacuum polarization is divergent!

The total VP density can be expanded in powers of the external scalar potential $\phi(x)$ as

$$\rho_\kappa^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e|\kappa|}{4\pi^2 i}\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa(r_x, r_x; z)\right] = \rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) + \boxed{\rho_\kappa^{\mathrm{VP},1}(\boldsymbol{x})} + \rho_\kappa^{\mathrm{VP},2}(\boldsymbol{x}) + \dots \quad (30)$$

Furry's theorem

Diagrams with free electron loops with odd number of vertices are discarded.



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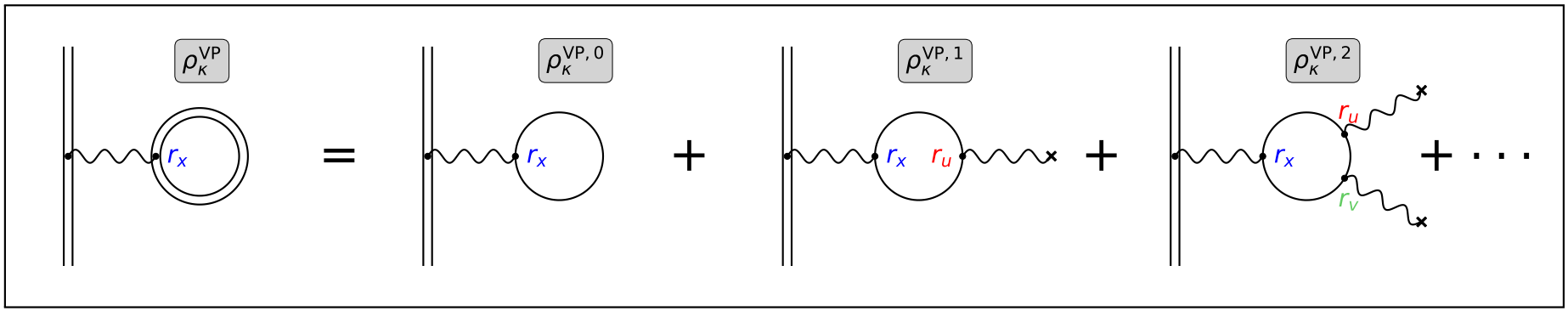

$\rho_\kappa^{\mathrm{VP},1}(\boldsymbol{x})$ (linear in Z) is divergent!

$$\rho^{\mathrm{VP},1}(x) = \int \frac{d^4q}{(2\pi\hbar)^4} e^{-\frac{i}{\hbar}q\cdot x}\Pi^{00}(q)\,\phi(q)\,. \quad (31)$$

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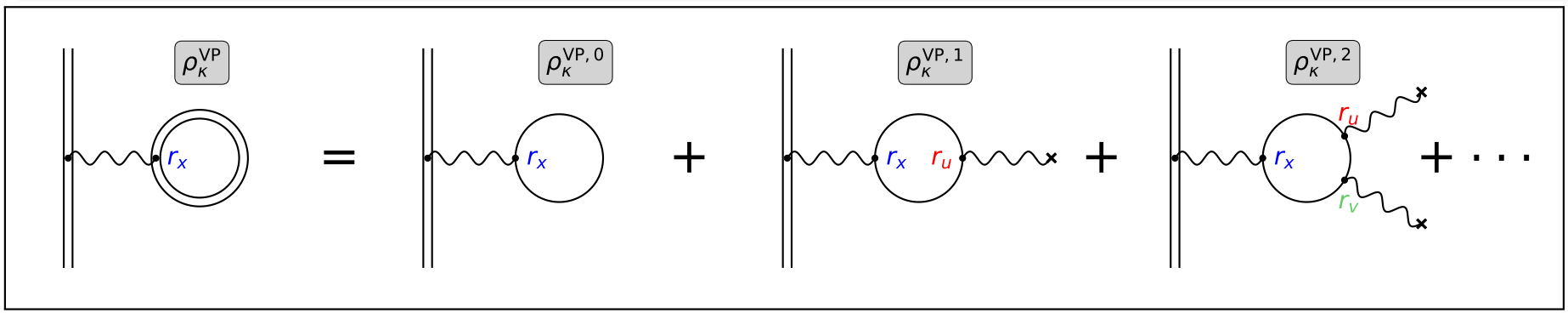

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The source of divergence comes from the polarization tensor (photon self-energy)

$$\Pi^{\mu\nu}(q) = -\frac{i\hbar e^2}{c}\int \frac{d^4p}{(2\pi\hbar)^4}\mathrm{Tr}\left[\gamma^\mu \frac{\not{p}+mc}{p^2-m^2c^2+i\epsilon}\gamma^\nu \frac{\not{p}-\not{q}+mc}{(p-q)^2-m^2c^2+i\epsilon}\right] \sim \Lambda^2 \quad (32)$$

On the infinite: by David Hilbert

In summary, let us return to our main theme and draw some conclusions from all our thinking about the infinite. Our principal result is that the infinite is nowhere to be found in reality. It neither exists in nature nor provides a legitimate basis for rational thought – a remarkable harmony between being and thought. In contrast to the earlier efforts of Frege and Dedekind, we are convinced that certain intuitive concepts and insights are necessary conditions of scientific knowledge, and logic alone is not sufficient. Operating with the infinite can be made certain only by the finitary.

The role that remains for the infinite to play is solely that of an idea – if one means by an idea, in Kant's terminology, a concept of reason which transcends all experience and which completes the concrete as a totality – that of an idea which we may unhesitatingly trust within the framework erected by our theory.

Hilbert, D. On the infinite (1984). In P. Benacerraf and H. Putnam (Eds.), Philosophy of Mathematics: Selected Readings (p183-201). Cambridge University Press.

Subtracting the linear vacuum polarization

The VP density that is linear in Z is divergent. Rinker and Wilets[5] suggested to remove the linear part through

$$\rho_\kappa^{n\geq 3}(\boldsymbol{x}; Z) = \rho_\kappa^{\mathrm{VP}}(\boldsymbol{x}; Z) - \lim_{\delta\to 0} \frac{Z}{\delta} \rho_\kappa^{\mathrm{VP}}(\boldsymbol{x}; \delta)$$

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[7] Kenneth G Dyall. Basis sets for the $1s^2$ ground states of two-electron rare gas ions

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  1. Point nucleus with:
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     2. 30G basis: 30 even-tempered exponents.

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[5] Rinker Jr, G. A., and L. Wilets. Phys. Rev. A 12.3 (1975): 748.
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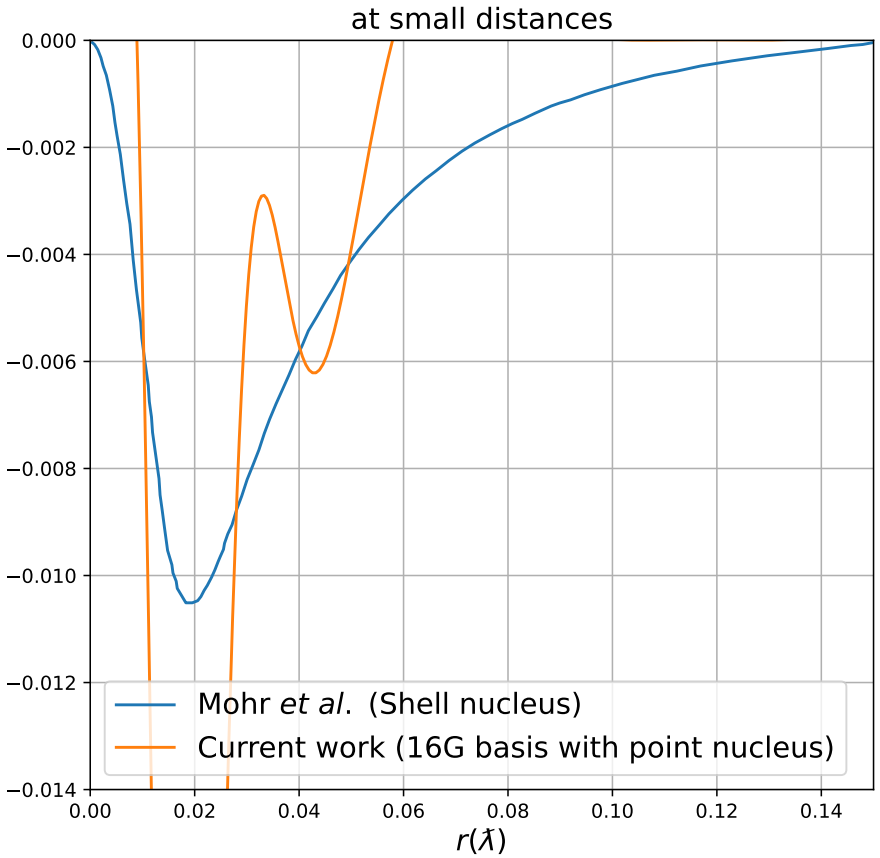
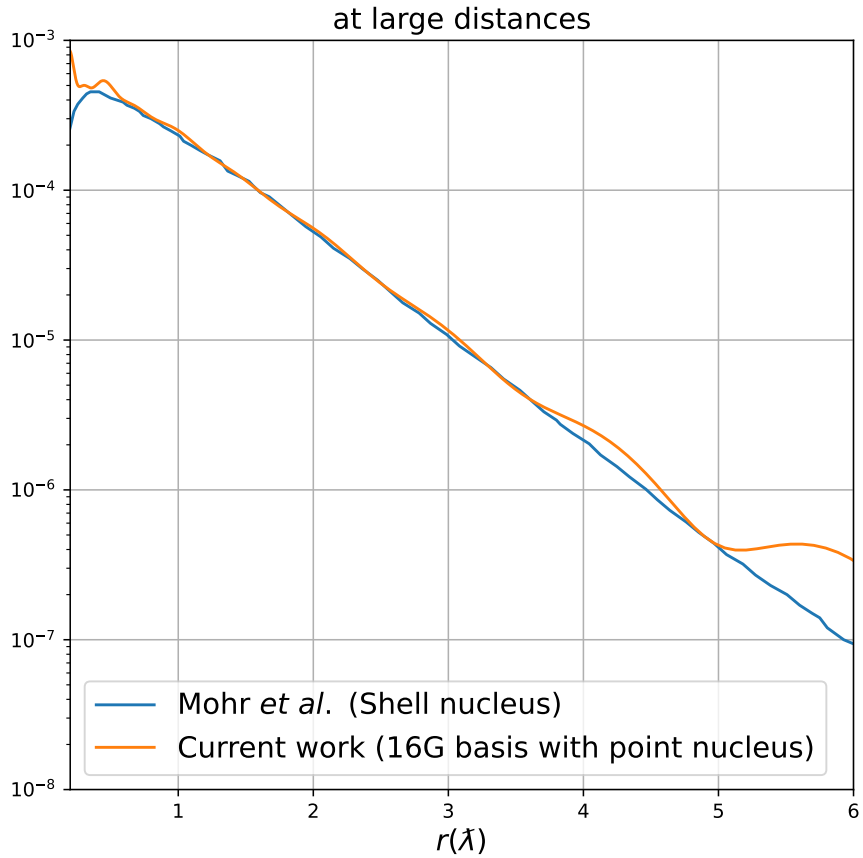
Non-linear VP density: $\mathcal{C}$-DKB + point nucleus + 16G basis

Non-linear vacuum polarization density: $r^2(\rho_{+\kappa}^{\mathrm{VP},n} + \rho_{-\kappa}^{\mathrm{VP},n})$, for $\kappa = 1$ and $n \geq 3$





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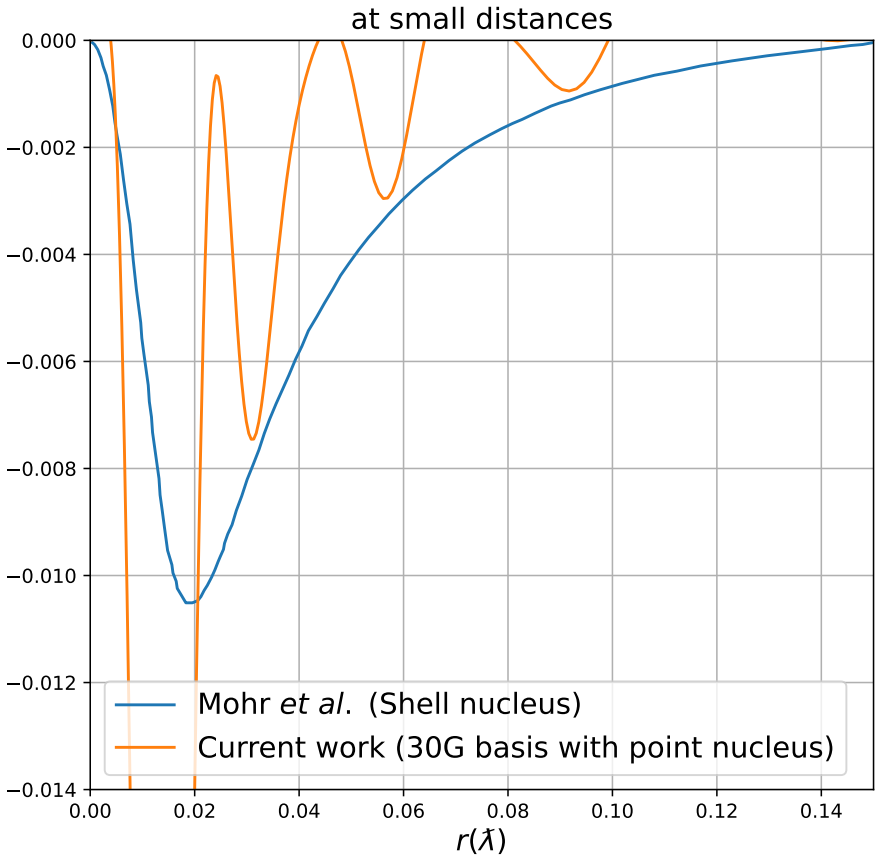

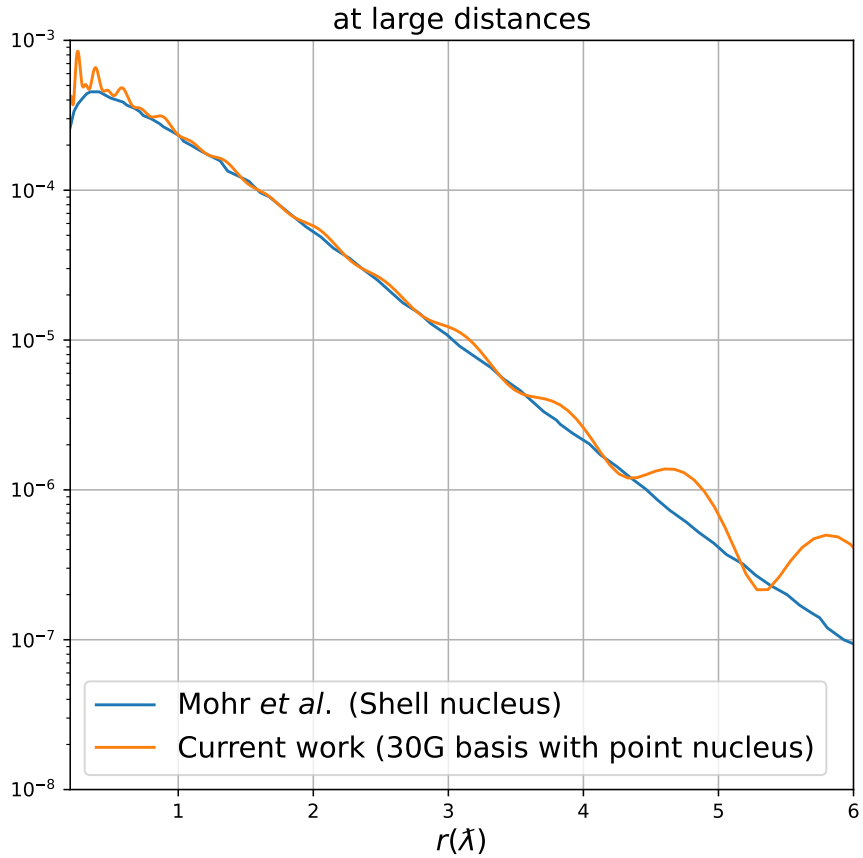

Non-linear VP density: $\mathcal{C}$-DKB + shell nucleus + 16G basis

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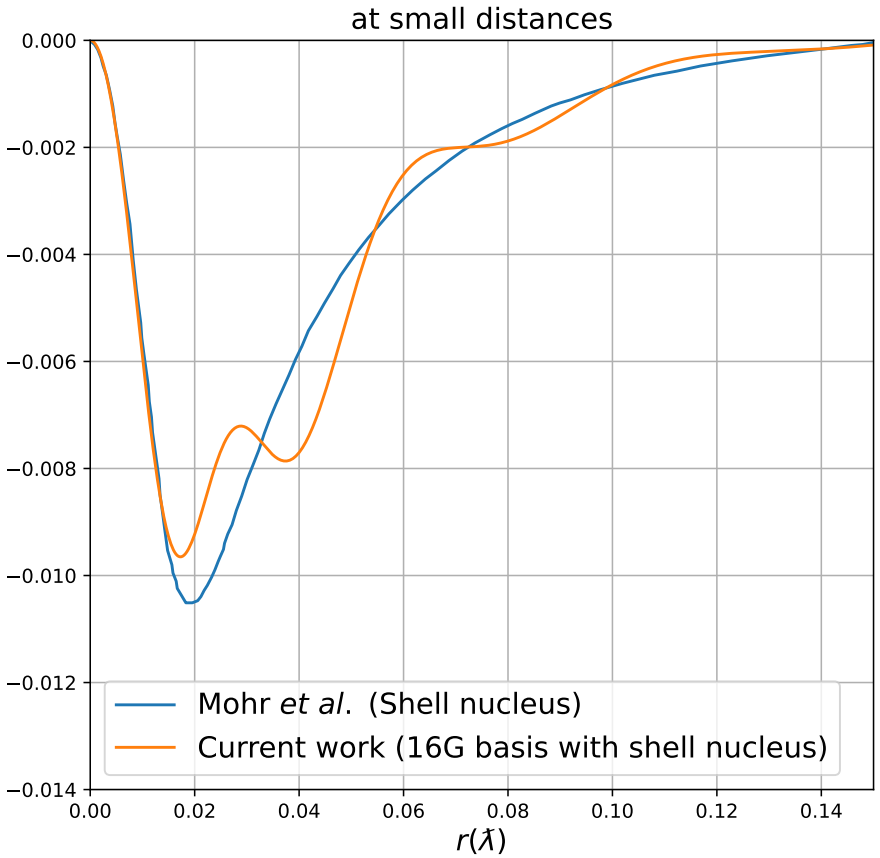

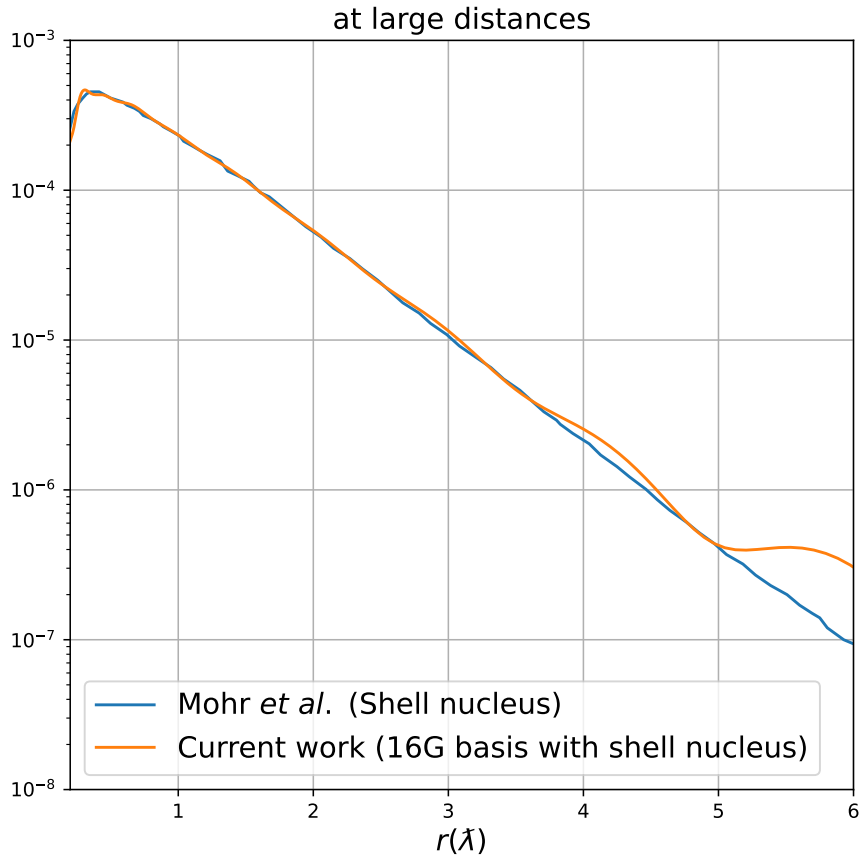

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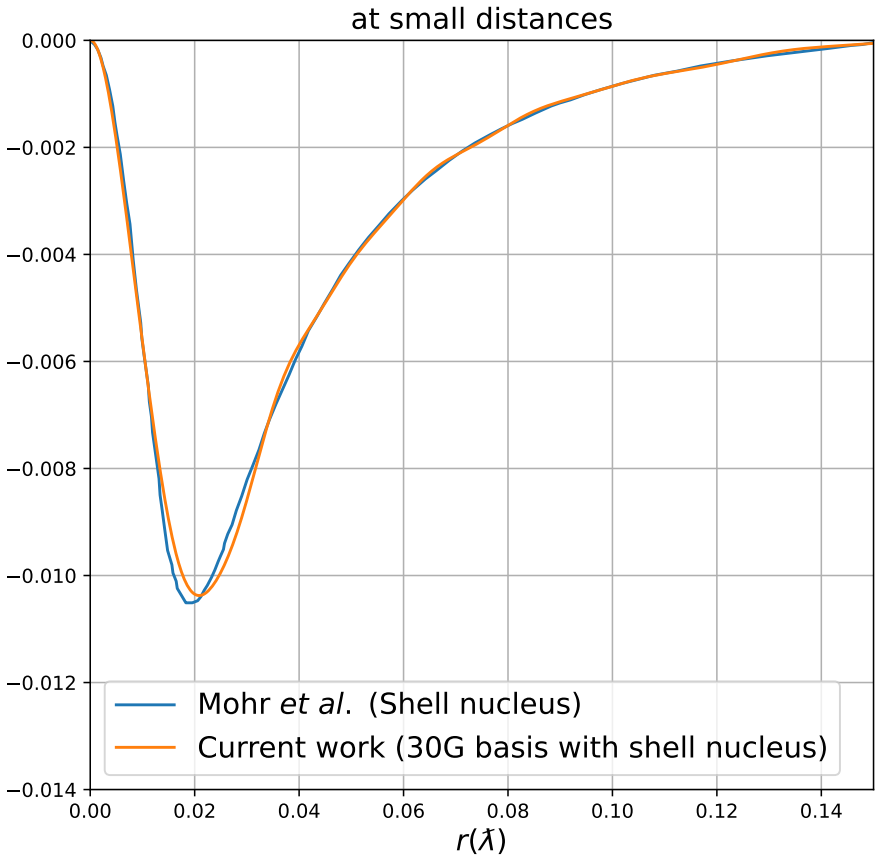

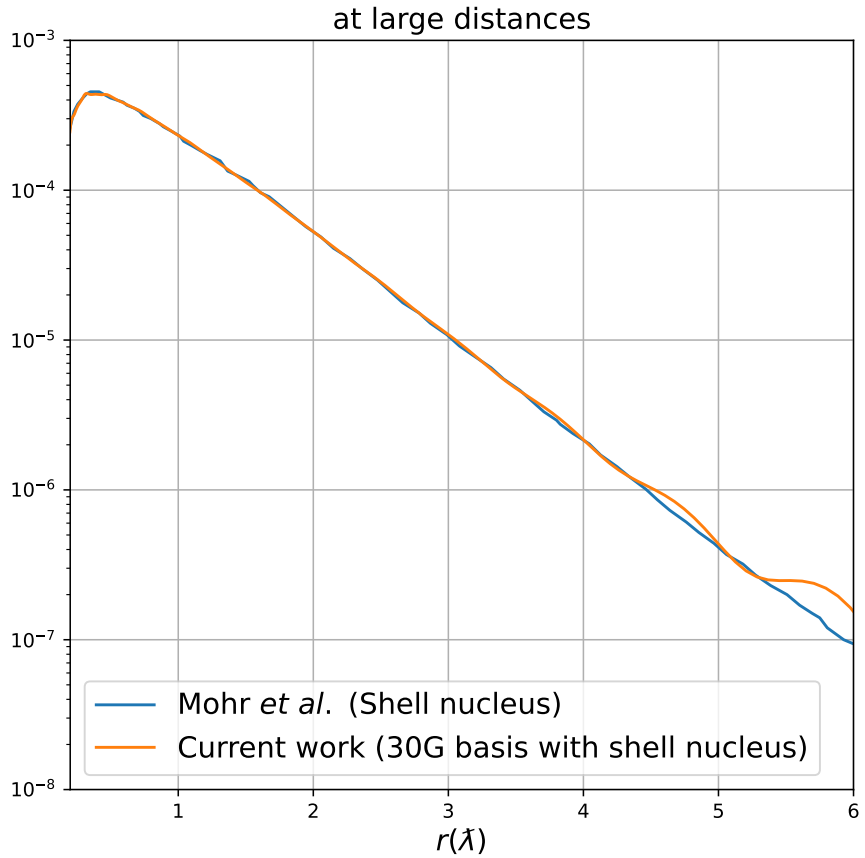

Non-linear VP density in RKB: Gauss nucleus + 16G

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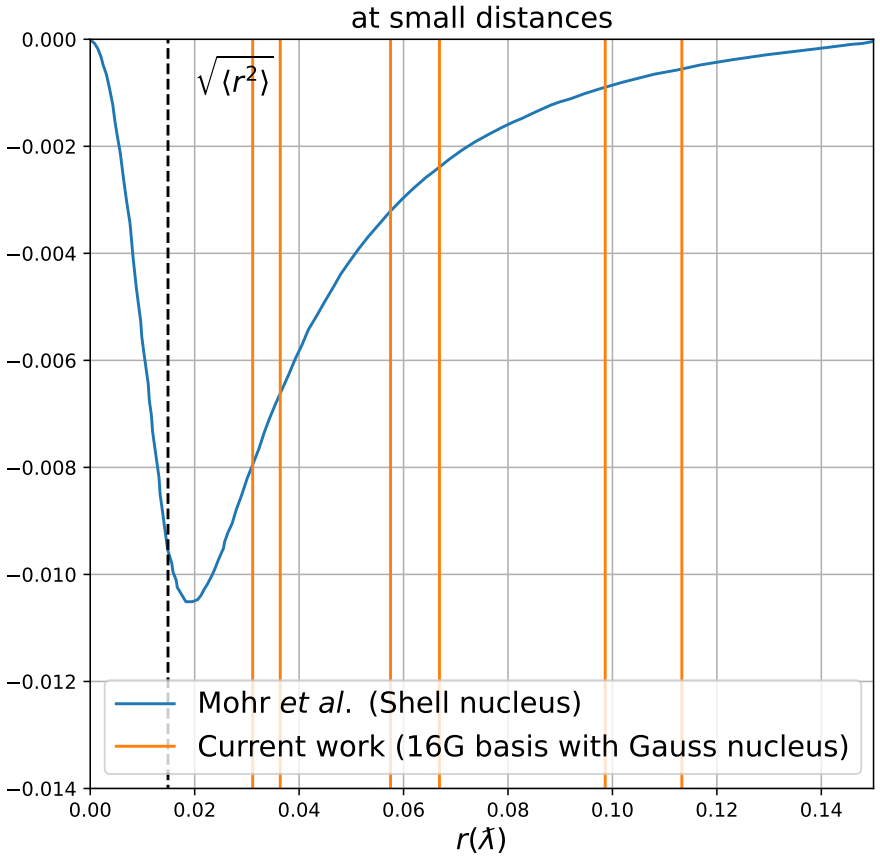

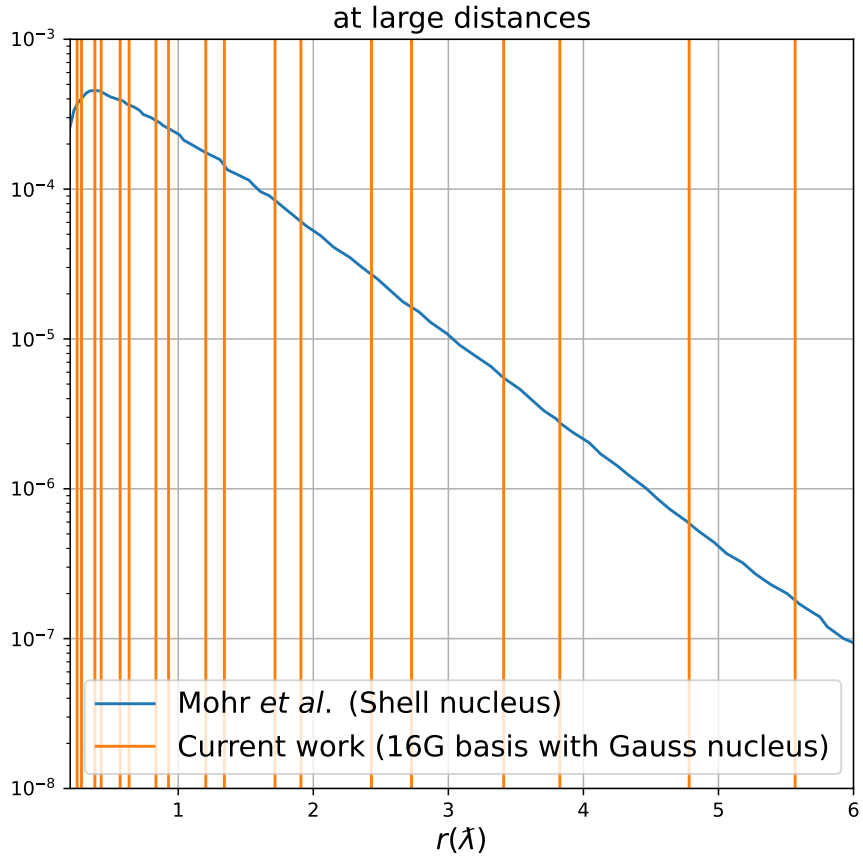

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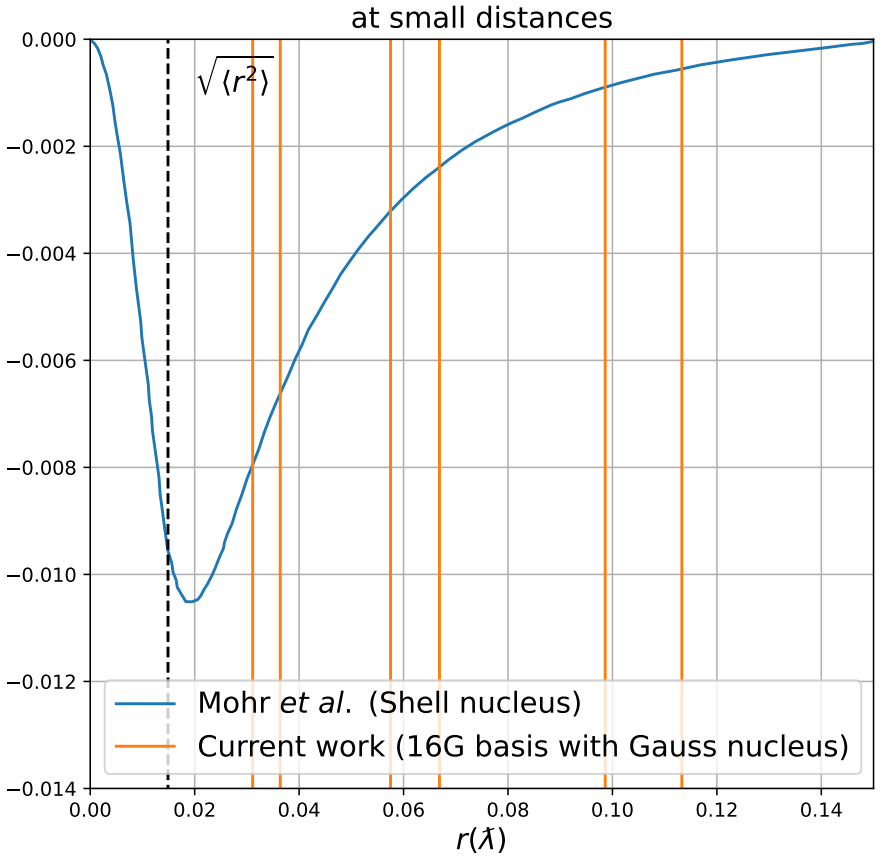

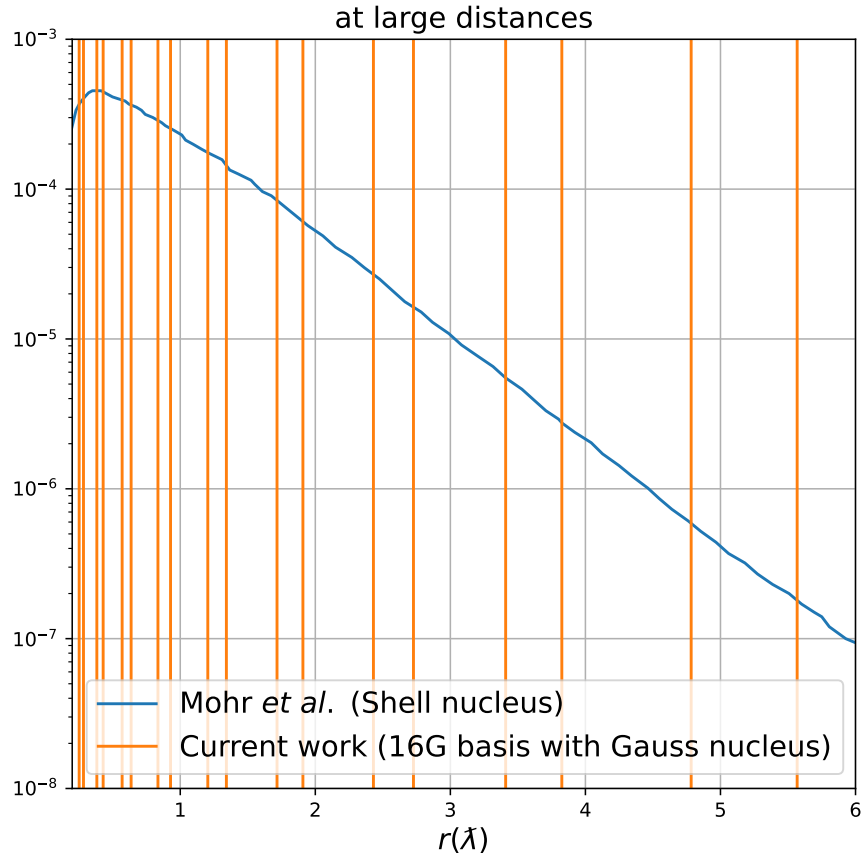

Why?

- RKB favors positive- on negative-energy solutions
- RKB violates the $\mathcal{C}$-symmetry. We thus have:
  $\rho_{\kappa}^{\mathrm{VP},0}, \rho_{\kappa}^{\mathrm{VP},2}, \rho_{\kappa}^{\mathrm{VP},4}, \ldots \neq 0$

Vacuum polarization density: $(Z\alpha)$-expansion

The VP density is related to the Dirac-Coulomb Green's function by:

$$\rho^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e}{4\pi^2 i} \sum_{\kappa} |\kappa| \int_{C_F} dz \, \mathrm{Tr}\left[G_\kappa\left(r_x, r_x; z\right)\right] \quad , \tag{33}$$

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This Green's function satisfies the following Dirac equation:

$$\sum_{\kappa}\begin{bmatrix} +mc^2 - e\phi(r_x) - z & -\hbar c\left[\frac{\partial}{\partial r_x} + \frac{1-\kappa}{r_x}\right] \\ \hbar c\left[\frac{\partial}{\partial r_x} + \frac{1+\kappa}{r_x}\right] & -mc^2 - e\phi(r_x) - z \end{bmatrix} G_\kappa(r_x, r_y; z) = \frac{\delta(r_x - r_y)}{r_x r_y}\mathbb{1}_2, \tag{34}$$

and can be written as:

$$G_\kappa(r_x, r_y; z) = \sum_n \frac{\psi_{n,\kappa}(r_x)\,\psi^\dagger_{n,\kappa}(r_y)}{E_{n,\kappa} - z} = \sum_n \frac{1}{E_{n,\kappa} - z}\begin{bmatrix} G^{LL}_{n,\kappa}(r_x, r_y) & G^{LS}_{n,\kappa}(r_x, r_y) \\ G^{SL}_{n,\kappa}(r_x, r_y) & G^{SS}_{\kappa}(r_x, r_y) \end{bmatrix}, \tag{35}$$

$$G^{\alpha\beta}_{n,\kappa}(r_x, r_y) = R^\alpha_{n,\kappa}(r_x)\,R^\beta_{n,\kappa}(r_y), \qquad \alpha, \beta = L, S. \tag{36}$$

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The total Green's function can be expanded as:

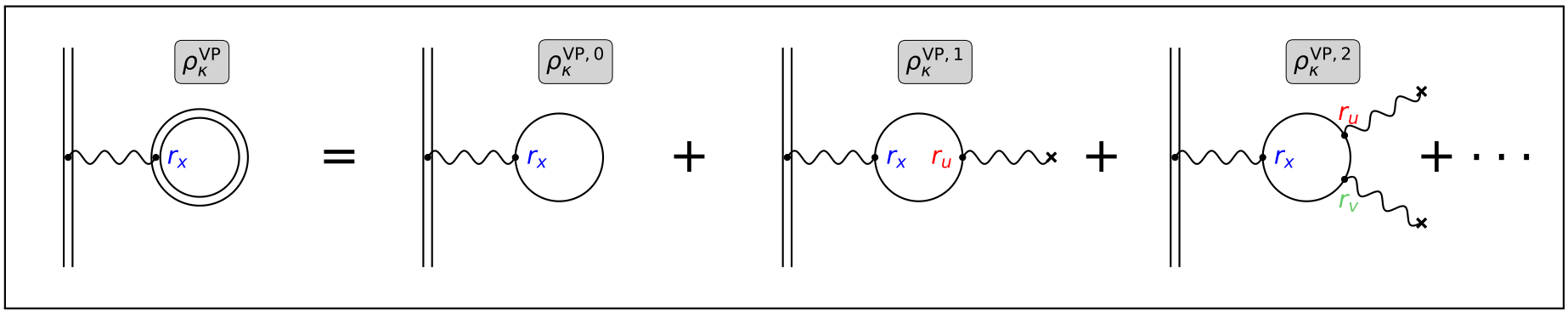
$$\begin{aligned} G_\kappa(r_x, r_y; z) &= G^0_\kappa(r_x, r_y; z) + e\int_0^\infty r_u^2 dr_u\, G^0_\kappa(r_x, r_u; z)\,\phi(r_u)\,G^0_\kappa(r_u, r_y; z) \\ &+ e^2\int_0^\infty r_u^2 dr_u \int_0^\infty r_v^2 dr_v\, G^0_\kappa(r_x, r_u; z)\,\phi(r_u)\,G^0_\kappa(r_u, r_v; z)\,\phi(r_v)\,G^0_\kappa(r_v, r_y; z) + \mathcal{O}(e^6), \end{aligned} \tag{37}$$

where $G^0_\kappa(r_x, r_y; z) = \lim_{Z\to 0} G_\kappa(r_x, r_y; z)$.

VP density: $(Z\alpha)$-expansion

The full vacuum polarization density can be thus written as a sum:

$$\rho_\kappa^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi^2 i}\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa(r_x, r_x; z)\right] = \rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) + \rho_\kappa^{\mathrm{VP},1}(\boldsymbol{x}) + \rho_\kappa^{\mathrm{VP},2}(\boldsymbol{x}) + \ldots \quad (38)$$



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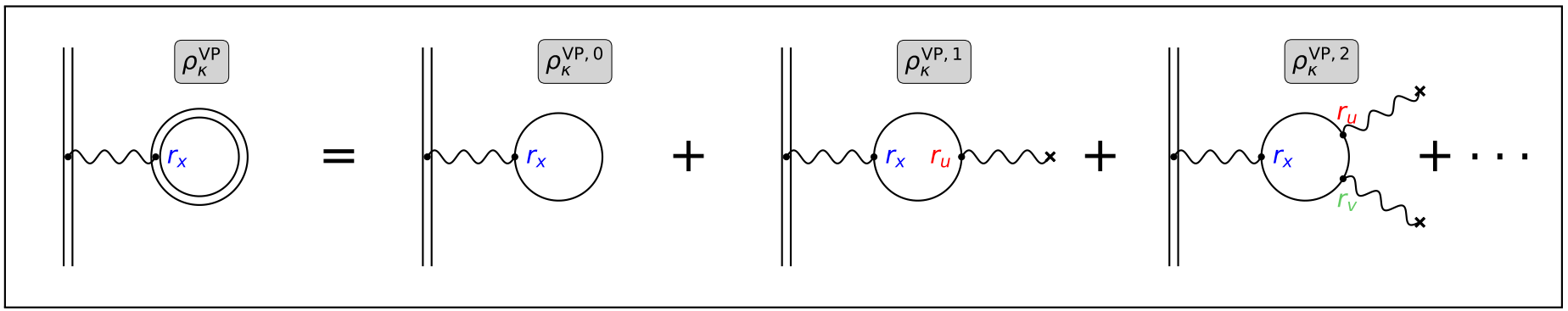

The associated individual VP densities are given by:

$$\rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi^2 i}\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa^0(r_x, r_x; z)\right] \quad (39)$$

$$\rho_\kappa^{\mathrm{VP},1}(\boldsymbol{x}) = \frac{e^2\,|\kappa|}{4\pi^2 i}\int_0^\infty r_u^2 dr_u \phi(r_u)\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa^0(r_x, r_u; z)\,G_\kappa^0(r_u, r_x; z)\right] \quad (40)$$

$$\vdots \quad (41)$$

We shall use the numerical free Green's function expression

$$G_\kappa^0(r_x, r_y; z) = \sum_{i=1}^{n_\kappa}\frac{\varphi_{\kappa,i}(r_x)\,\varphi_{\kappa,i}^\dagger(r_y)}{E_{\kappa,i} - z} \quad (42)$$

to derive the n-potential VP density expression: $\rho_\kappa^{\mathrm{VP},n}$.

$(Z\alpha)^n$ VP density in the finite basis

The n-potential VP density:

$$\rho^n_\kappa(\boldsymbol{x}) = \frac{e^{n+1}\,|\kappa|}{4\pi^2 i}\int_0^\infty r_1^2 dr_1 \phi(r_1)\ldots\int_0^\infty r_n^2 dr_n \phi(r_n) \times \int_{C_F} dz\,\mathrm{Tr}\left[G^0_\kappa(r_x, r_1; z)\, G^0_\kappa(r_1, r_2; z)\ldots G^0_\kappa(r_{n-1}, r_n; z)\, G^0_\kappa(r_n, r_x; z)\right], \tag{43}$$

can be written as

$$\rho^n_\kappa(\boldsymbol{x}) = \frac{e^{n+1}\,|\kappa|}{4\pi^2 r_x i}\sum_{\alpha_1,\ldots,\alpha_{n+1}} s^\kappa_{\alpha_{n+1}\alpha_1}(r_x) \times V^\kappa_{\alpha_1\alpha_2} V^\kappa_{\alpha_2\alpha_3}\ldots V^\kappa_{\alpha_{n-1}\alpha_n} V^\kappa_{\alpha_n\alpha_{n+1}} \boxed{I(n,\kappa)} \tag{44}$$

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where $V^\kappa_{\alpha\beta}$ and $s^\kappa_{\beta\alpha}(r)$ are given by

$$V^\kappa_{\alpha\beta} = \int_0^\infty dr\,\phi(r)\,\varphi^\dagger_{\alpha,\kappa}(r)\,\varphi_{\beta,\kappa}(r). \tag{45}$$

$$s^\kappa_{\beta\alpha}(r) = \varphi^\dagger_{\beta,\kappa}(r)\,\varphi_{\alpha,\kappa}(r). \tag{46}$$

$(Z\alpha)^n$ VP density in the finite basis

The n-potential VP density:

$$\rho^n_\kappa(\boldsymbol{x}) = \frac{e^{n+1}|\kappa|}{4\pi^2 i}\int_0^\infty r_1^2 dr_1 \phi(r_1)\ldots\int_0^\infty r_n^2 dr_n \phi(r_n) \times \int_{C_F} dz\,\mathrm{Tr}\left[G^0_\kappa(r_x, r_1; z)\, G^0_\kappa(r_1, r_2; z)\ldots G^0_\kappa(r_{n-1}, r_n; z)\, G^0_\kappa(r_n, r_x; z)\right], \tag{43}$$

can be written as

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where $V^\kappa_{\alpha\beta}$ and $s^\kappa_{\beta\alpha}(r)$ are given by

$$V^\kappa_{\alpha\beta} = \int_0^\infty dr\,\phi(r)\,\varphi^\dagger_{\alpha,\kappa}(r)\,\varphi_{\beta,\kappa}(r). \tag{45}$$

$$s^\kappa_{\beta\alpha}(r) = \varphi^\dagger_{\beta,\kappa}(r)\,\varphi_{\alpha,\kappa}(r). \tag{46}$$

We are thus left with the evaluation of the contour integral

$$I(n,\kappa) = \int_{C_F} dz\,\frac{1}{E_{\alpha_1,\kappa} - z}\ldots\frac{1}{E_{\alpha_{n+1},\kappa} - z} = ? \tag{47}$$

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$\{\varphi_{\alpha,\kappa}(r), E_{\alpha,\kappa}\}$ are the eigensolutions of the free radial Dirac equation.

$(Z\alpha)^n$ VP density contour integral

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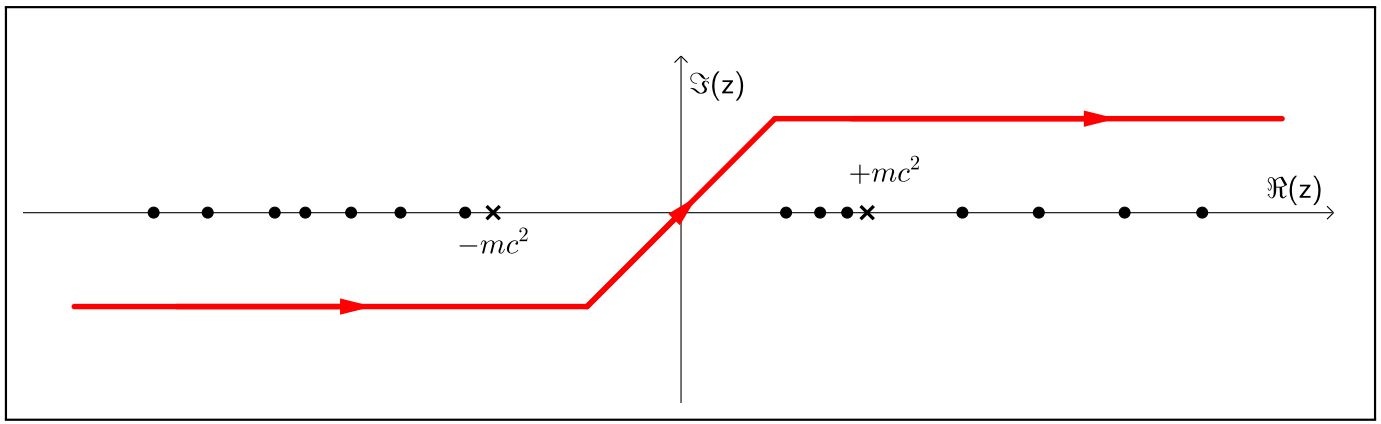

Figure: Dirac eigenvalues (black dots), and Feynman contour (C_F: red path).

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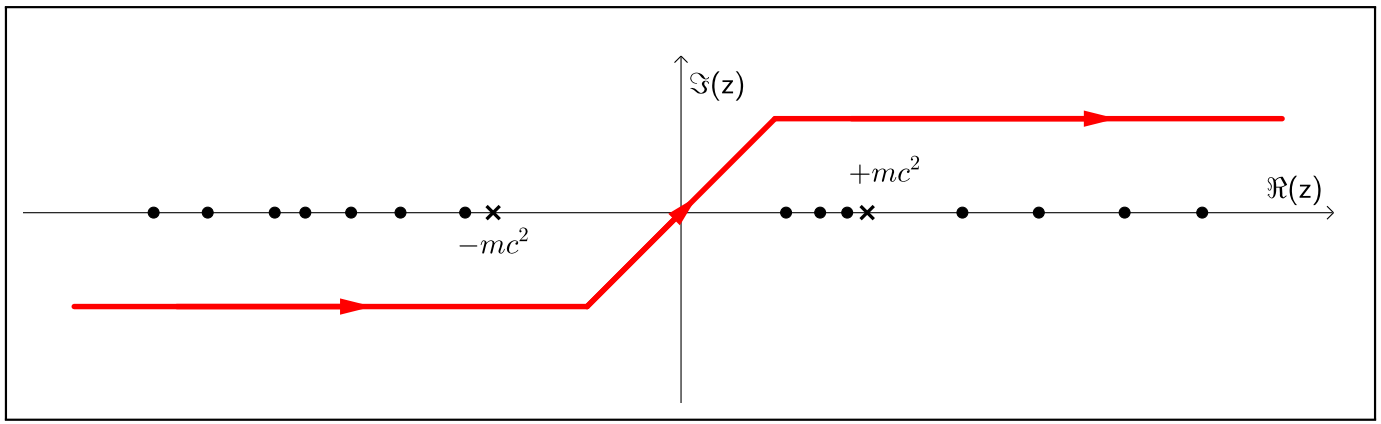

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After a lengthy calculation, we find

$$\int_{C_F} dz \frac{1}{E_1 - z} \cdots \frac{1}{E_{n+1} - z} = \frac{(-1)^n \, i\pi \sum_{i=1}^{n+1} (-1)^{i+1} \operatorname{sgn}(E_i) \prod_{j\neq i} \prod_{k>j, k\neq i} (E_j - E_k)}{\prod_{l=1}^{n} \prod_{m>l} (E_l - E_m)}$$

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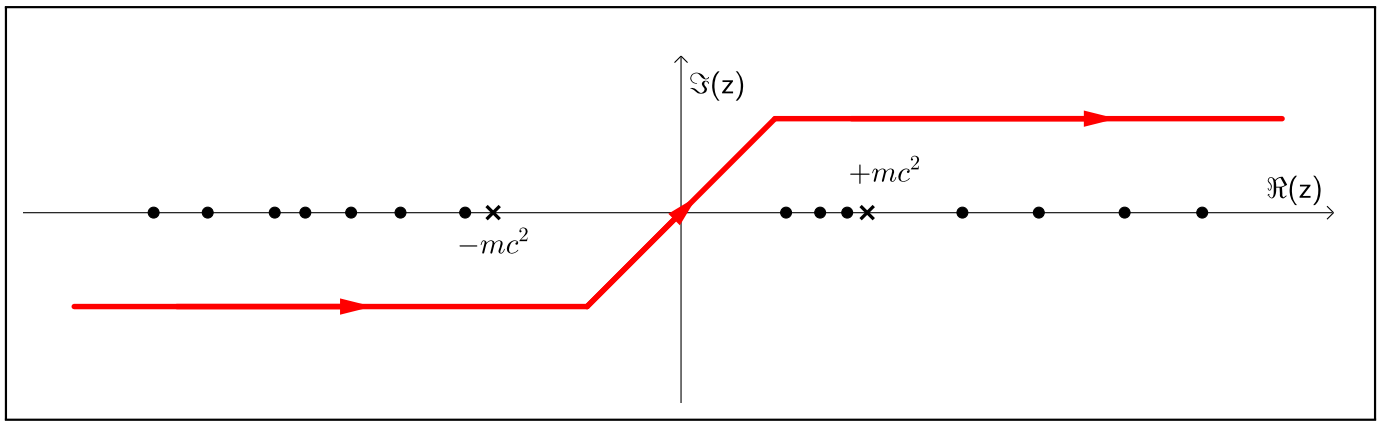

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We now have the exact expression of the $(Z\alpha)^n$ VP density!

Furry's theorem in the $\mathcal{C}$-symmetric finite basis

The n-potential VP densities associated with $\pm\kappa$ are:

$$\rho^{n}_{+\kappa}(\boldsymbol{x}) = \frac{e^{n+1}\,|\kappa|}{4\pi^2 r_x i} \sum_{\alpha_1,\ldots,\alpha_{n+1}} s^{+\kappa}_{\alpha_{n+1},\alpha_1}(r_x)\, V^{+\kappa}_{\alpha_1\alpha_2}\ldots V^{+\kappa}_{\alpha_n\alpha_{n+1}}\, I(n,+\kappa) \tag{49}$$

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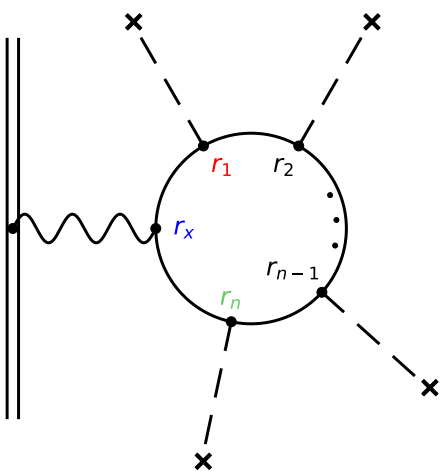

[8] Furry, Wendell H. "A symmetry theorem in the positron theory." Phys. Rev. 51.2 (1937): 125.

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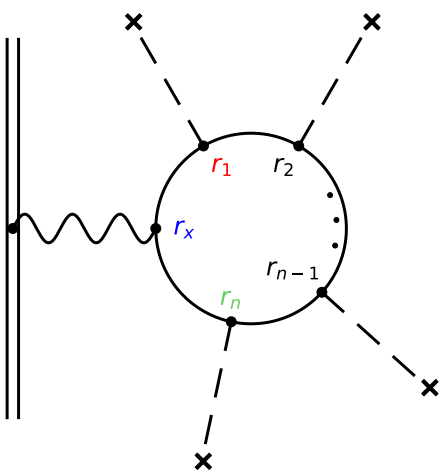

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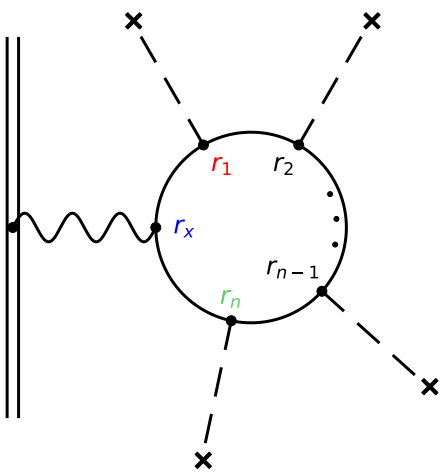

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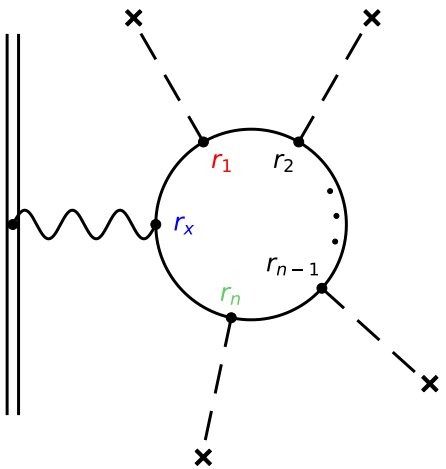

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Two things to know:

1. In a $\mathcal{C}$-symmetric basis, even orders of VP density vanish (as in reality).
2. One needs to calculate one κ sign VP density.

[8] Furry, Wendell H. "A symmetry theorem in the positron theory." Phys. Rev. 51.2 (1937): 125.

Conclusions

1. Kinetic balances and $\mathcal{C}$-symmetry:
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2. The use of non-$\mathcal{C}$-symmetric basis yields non-physical VP results.
1. The use of a $\mathcal{C}$-symmetric basis leads to a VP density that is
   1. In line with Furry's theorem
   2. Vanishing at relatively shorter distances
   3. In good agreement with the complicated many-potential (WK) density

Perspectives

Next goals

1. Compute individual odd-order VP densities $\rho_\kappa^n(\boldsymbol{x})$ using freshly derived results and check their convergence to the total $\rho^{\mathrm{VP}}(\boldsymbol{x})$ (ongoing).
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Far future goals

1. Extend our machinery to more sophisticated (correlated) methods.
2. Extend the basis-set-computed e^2 VP and SE to e^n-orders with $n > 2$.

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Q: How to get rid of your divergences?

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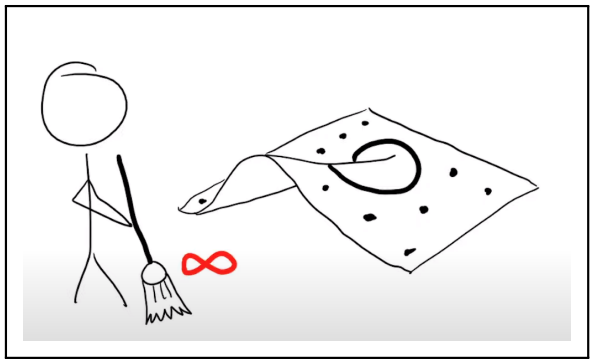

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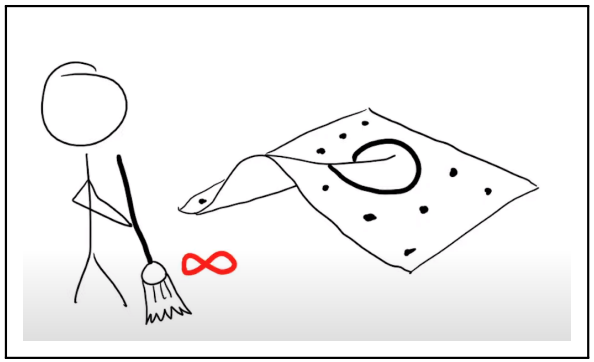

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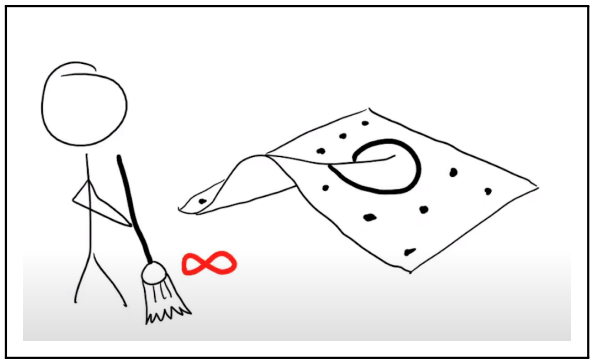
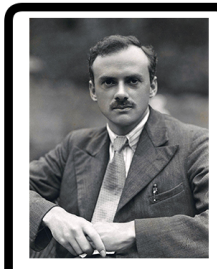


3. Make Dirac angry

> Hence most physicists are very satisfied with the situation. They say: "Quantum electrodynamics is a good theory, and we do not have to worry about it any more." I must say that I am very dissatisfied with the situation, because this so-called "good theory" does involve neglecting infinities which appear in its equations, neglecting them in an arbitrary way. This is just not sensible mathematics. Sensible mathematics involves neglecting a quantity when it turns out to be small—not neglecting it just because it is infinitely great and you do not want it!



Angry Dirac!

Dirac, P. A. M. "Directions in physics. Lectures delivered during a visit to Australia and New Zealand, August/September 1975." (1978).

B1: Gaussian bases with RKB

The spherical Gaussian basis functions are:

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- ℓ-basis: Same exponents for same ℓ-functions.
- j-basis: Same exponents for same j-functions.

	κ	ℓ-basis	j-basis
$s_{\frac{1}{2}}$	-1	●	●
$p_{\frac{1}{2}}$	$+1$	●	●
$p_{\frac{3}{2}}$	-2	●	●
$d_{\frac{3}{2}}$	$+2$	●	●
$d_{\frac{5}{2}}$	-3	●	●
⋮	⋮	⋮	⋮

Table: Same color means same list of exponents

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κ	ℓ	j	ζ^L	ζ^S
-1	0	$\frac{1}{2}$	●	●
+1	1	$\frac{1}{2}$	●	●
-2	1	$\frac{3}{2}$	●	●
+2	2	$\frac{3}{2}$	●	●
-3	2	$\frac{5}{2}$	●	●
⋮			⋮	⋮

(a) Exponents in $\mathcal{C}$-DKB

κ	ℓ	j	ζ^L	ζ^S
-1	0	$\frac{1}{2}$	●	●
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⋮			⋮	⋮

(b) Exponents in ℓ-bases

κ	ℓ	j	ζ^L	ζ^S
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-2	1	$\frac{3}{2}$	●	●
+2	2	$\frac{3}{2}$	●	●
-3	2	$\frac{5}{2}$	●	●
⋮			⋮	⋮

(c) Exponents in j-bases

B2: Uranium exponents

i	16G (7z basis)
1	5.66530865E+07
2	1.50715339E+07
3	5.14926020E+06
4	1.95346438E+06
5	8.11107677E+05
6	3.55863972E+05
7	1.63626745E+05
8	7.76952979E+04
9	3.78943130E+04
10	1.88681659E+04
11	9.56625072E+03
12	4.92635288E+03
13	2.57221011E+03
14	1.35785927E+03
15	7.19791611E+02
16	3.73653024E+02

i	30G	⋮	⋮
1	5.6653086E+07	16	1.1844662E+05
2	3.7547139E+07	17	7.8501137E+04
3	2.4884569E+07	18	5.2027052E+04
4	1.6492382E+07	19	3.4481210E+04
5	1.0930415E+07	20	2.2852608E+04
6	7.2441918E+06	21	1.5145689E+01
7	4.8011272E+06	22	1.0037887E+04
8	3.1819730E+06	23	6.6526640E+03
9	2.1088698E+06	24	4.4090890E+03
10	1.3976648E+06	25	2.9221475E+03
11	9.2630991E+05	26	1.9366690E+03
12	6.1391689E+05	27	1.2835379E+03
13	4.0687673E+05	28	8.5067164E+02
14	2.6965975E+05	29	5.6378722E+02
15	1.7871846E+05	30	3.7365302E+02

B3: Kinetic balances

The radial Dirac equation can be written as:

$$Q_{n,\kappa} = \frac{\hbar}{mc} \frac{1}{1 + \frac{e\varphi + E_{n,\kappa}}{mc^2}} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{n,\kappa} \tag{57}$$

$$P_{n,\kappa} = \frac{\hbar}{mc} \frac{1}{1 - \frac{e\varphi + E_{n,\kappa}}{mc^2}} \left[\frac{d}{dr} - \frac{\kappa}{r} \right] Q_{n,\kappa}. \tag{58}$$

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Atomic Balance (AB):

$$Q_\kappa^{\mathrm{AB}} = \frac{c\hbar}{2mc^2 + e\varphi} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_\kappa$$

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Atomic Balance (AB):

$$Q_\kappa^{\mathrm{AB}} = \frac{c\hbar}{2mc^2 + e\varphi} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_\kappa$$

Restricted Kinetic Balance (RKB):

$$Q_\kappa^{\mathrm{RKB}} = \frac{\hbar}{2mc} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_\kappa$$

B3: Kinetic balances

The radial Dirac equation can be written as:

$$Q_{n,\kappa} = \frac{\hbar}{mc} \frac{1}{1 + \frac{e\varphi + E_{n,\kappa}}{mc^2}} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{n,\kappa} \tag{57}$$

$$P_{n,\kappa} = \frac{\hbar}{mc} \frac{1}{1 - \frac{e\varphi + E_{n,\kappa}}{mc^2}} \left[\frac{d}{dr} - \frac{\kappa}{r} \right] Q_{n,\kappa}. \tag{58}$$

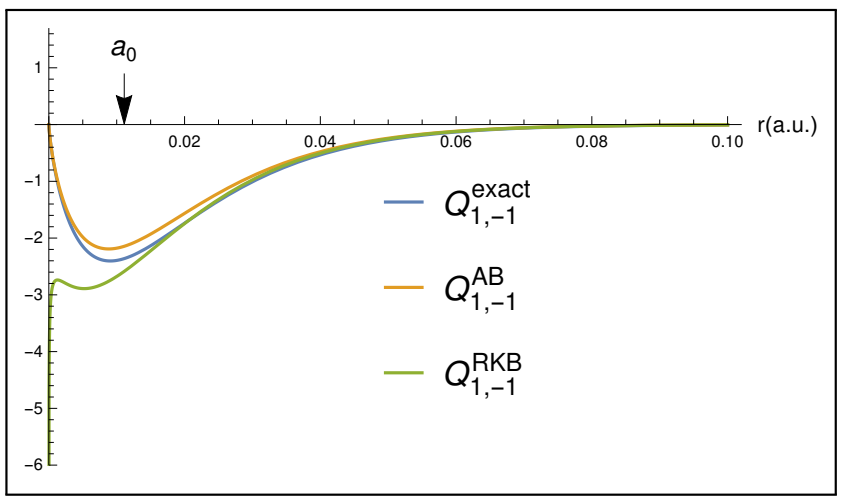

Figure: AB and RKB approxs of the 1e radon ground state small component.

Atomic Balance (AB):

$$Q^{\text{AB}}_{\kappa} = \frac{c\hbar}{2mc^2 + e\varphi} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{\kappa}$$

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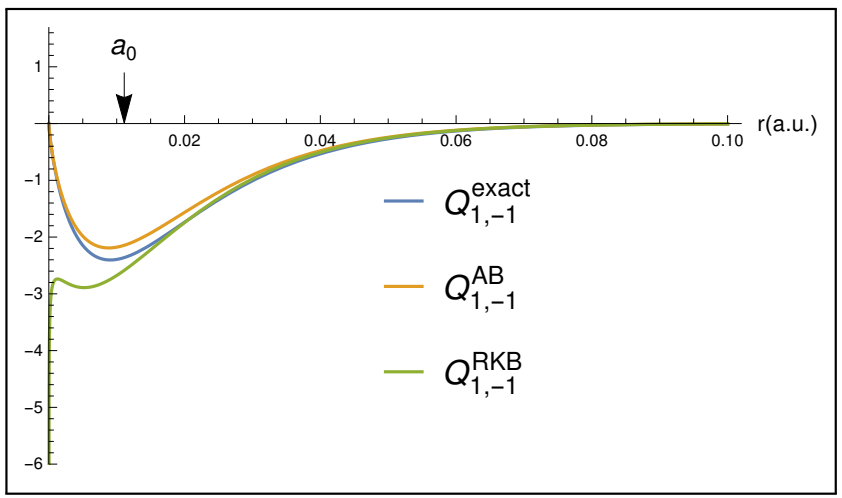

Figure: AB and RKB approxs of the 1e radon ground state small component.

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$$Q^{\text{AB}}_{\kappa} = \frac{c\hbar}{2mc^2 + e\varphi} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{\kappa}$$

Restricted Kinetic Balance (RKB):

$$Q^{\text{RKB}}_{\kappa} = \frac{\hbar}{2mc} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{\kappa}$$

Inverse Kinetic Balance (IKB):

$$P^{\text{IKB}}_{n,\kappa} = \frac{\hbar}{2mc} \left[\frac{d}{dr} - \frac{\kappa}{r} \right] Q_{n,\kappa}$$

B4: Vacuum polarization density: (αZ)-expansion

The VP density is related to the Dirac-Coulomb Green's function by:

$$\rho^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e}{4\pi^2 i}\sum_{\kappa}|\kappa|\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa(r_x, r_x; z)\right] \quad , \tag{59}$$

This Green's function satisfies the following Dirac equation:

$$\sum_{\kappa}\begin{bmatrix} +mc^2 - e\phi(r_x) - z & -\hbar c\left[\frac{\partial}{\partial r_x} + \frac{1-\kappa}{r_x}\right] \\ \hbar c\left[\frac{\partial}{\partial r_x} + \frac{1+\kappa}{r_x}\right] & -mc^2 - e\phi(r_x) - z \end{bmatrix} G_\kappa(r_x, r_y; z) = \frac{\delta(r_x - r_y)}{r_x r_y}\mathbb{1}_2, \tag{60}$$

and can be written as:

$$G_\kappa(r_x, r_y; z) = \sum_n \frac{\psi_{n,\kappa}(r_x)\,\psi^\dagger_{n,\kappa}(r_y)}{E_{n,\kappa} - z}$$

Using the well-known identity:

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A}B\frac{1}{A} + \frac{1}{A}B\frac{1}{A}B\frac{1}{A} + \ldots, \tag{61}$$

the total Green's function can be expanded as:

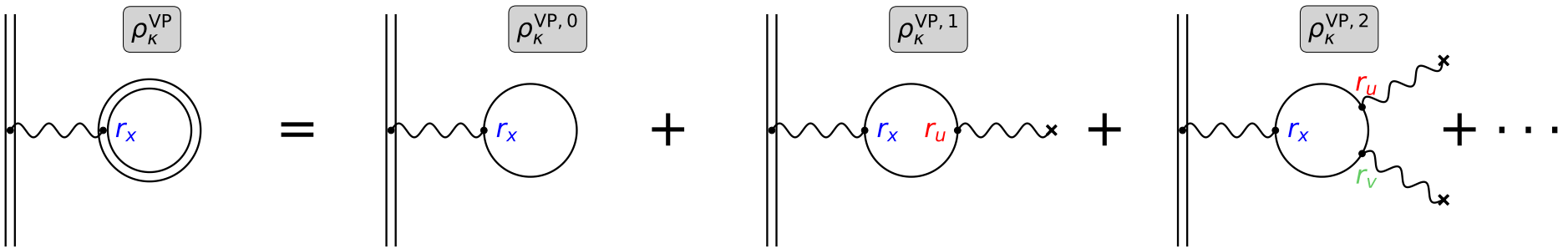
$$G_\kappa = G^0_\kappa + G^0_\kappa e\phi G^0_\kappa \quad + \ldots \tag{62}$$

We shall now plug this result in the first equation.

B5: VP density: (αZ)-expansion in the finite basis problem

The full vacuum polarization density can be thus written as a sum:

$$\rho_\kappa^{\mathrm{VP}}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi^2 i}\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa(r_x, r_x; z)\right] = \rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) + \rho_\kappa^{\mathrm{VP},1}(\boldsymbol{x}) + \rho_\kappa^{\mathrm{VP},2}(\boldsymbol{x}) + \ldots \quad (63)$$



Individual VP densities are given by:

$$\rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi^2 i}\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa^0(r_x, r_x; z)\right] \quad (64)$$

$$\rho_\kappa^{\mathrm{VP},1}(\boldsymbol{x}) = \frac{e^2\,|\kappa|}{4\pi^2 i}\int_0^\infty r_u^2 dr_u \phi(r_u)\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa^0(r_x, r_u; z)\,G_\kappa^0(r_u, r_x; z)\right] \quad (65)$$

$$\vdots$$

Green's functions G_κ and G_κ^0 are constructed from numerical solutions through:

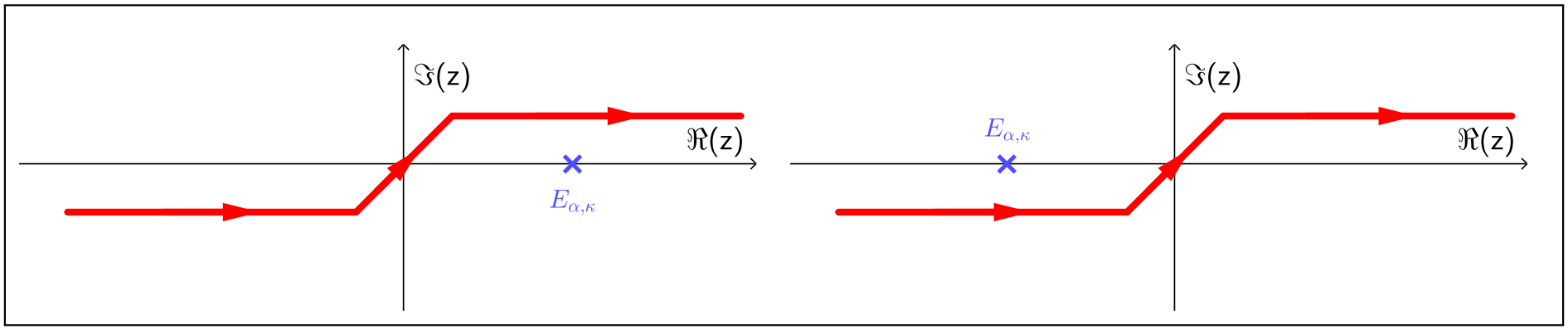
$$G_\kappa(r_x, r_y; z) = \sum_{n=1}^{n_\kappa}\frac{\psi_{n,\kappa}(r_x)\,\psi_{n,\kappa}^\dagger(r_y)}{E_{n,\kappa} - z}, \qquad G_\kappa^0(r_x, r_y; z) = \sum_{n=1}^{n_\kappa}\frac{\varphi_{n,\kappa}(r_x)\,\varphi_{n,\kappa}^\dagger(r_y)}{E_{n,\kappa}^0 - z},$$

B6: VP density in the finite basis

The zero-potential VP density:

$$\rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi^2 i}\int_{C_F} dz\,\mathrm{Tr}\left[G_\kappa^0(r_x, r_x; z)\right] = \frac{e\,|\kappa|}{4\pi^2 i}\sum_\alpha \varphi_{\alpha,\kappa}^\dagger(r_x)\,\varphi_{\alpha,\kappa}(r_x)\int_{C_F}\frac{dz}{E_{\alpha,\kappa}^0 - z}$$

The two scenarios of $E_{\alpha,\kappa}$ are represented in the following figures:



Using Cauchy's integral formula (residue theorem), one can show that (backup slides):

$$\int_{C_F} dz\,\frac{1}{E_{\alpha,\kappa}^0 - z} = i\pi\,\mathrm{sgn}\left(E_{\alpha,\kappa}^0\right) \tag{66}$$

This leads to the following result:

$$\rho_\kappa^{\mathrm{VP},0}(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi}\sum_\alpha \mathrm{sgn}\left(E_{\alpha,\kappa}^0\right)\varphi_{\alpha,\kappa}^\dagger(r_x)\,\varphi_{\alpha,\kappa}(r_x)\,, \tag{67}$$

B7: $(\alpha Z)^{n=1}$ VP density in the finite basis

The one-potential VP density:

$$\rho_{\kappa}^{\mathrm{VP},1}(\boldsymbol{x}) = \frac{e^2\,|\kappa|}{4\pi^2 i}\int_0^{\infty} r_u^2 dr_u \phi(r_u) \int_{C_F} dz\,\mathrm{Tr}\left[G_{\kappa}^0(r_x, r_u; z)\, G_{\kappa}^0(r_u, r_x; z)\right] \tag{68}$$

The two Green's functions expansions contribute with two denominators, integrating to (backup slides):

$$\int_{C_F} dz\,\frac{1}{E_{\alpha,\kappa}^0 - z}\,\frac{1}{E_{\beta,\kappa}^0 - z} = \pi i\,\frac{1-\mathrm{sgn}\left(E_{\alpha,\kappa}^0 E_{\beta,\kappa}^0\right)}{\left|E_{\alpha,\kappa}^0\right| + \left|E_{\beta,\kappa}^0\right|}, \tag{69}$$

Integrating over the red variable r_u gives the following 1-potential VP density:

$$\rho_{\kappa}^{\mathrm{VP},1}(\boldsymbol{x}) = \frac{e^2\,|\kappa|}{4\pi}\sum_{\alpha,\beta} s_{\beta,\alpha}^{\kappa}(r_x)\, V_{\alpha,\beta}^{\kappa}\,\frac{1-\mathrm{sgn}\left(E_{\alpha,\kappa}^0 E_{\beta,\kappa}^0\right)}{\left|E_{\alpha,\kappa}^0\right| + \left|E_{\beta,\kappa}^0\right|} \tag{70}$$

where $V_{\alpha,\beta}^{\kappa}$ and $s_{\beta,\alpha}^{\kappa}(r)$ are given by:

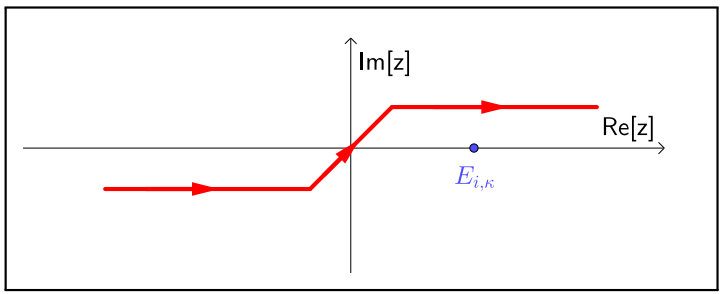
$$V_{\alpha,\beta}^{\kappa} = \int_0^{\infty} r^2 dr\,\phi(r)\,\varphi_{\alpha,\kappa}^{\dagger}(r)\,\varphi_{\beta,\kappa}(r)\,. \tag{71}$$

$$s_{\beta,\alpha}^{\kappa}(r) = \varphi_{\beta,\kappa}^{\dagger}(r)\,\varphi_{\alpha,\kappa}(r)\,. \tag{72}$$

B8: Contour integrations 1

The one-pole integral: $$\int_{C_F} dz \frac{1}{E_{i,\kappa} - z} = ? \tag{73}$$

Positive pole case



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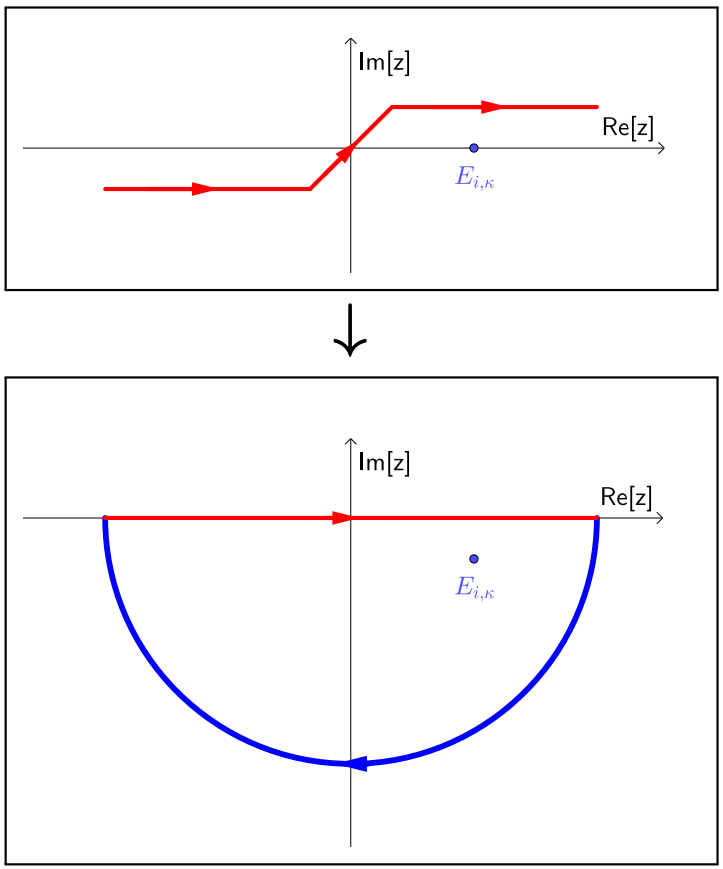

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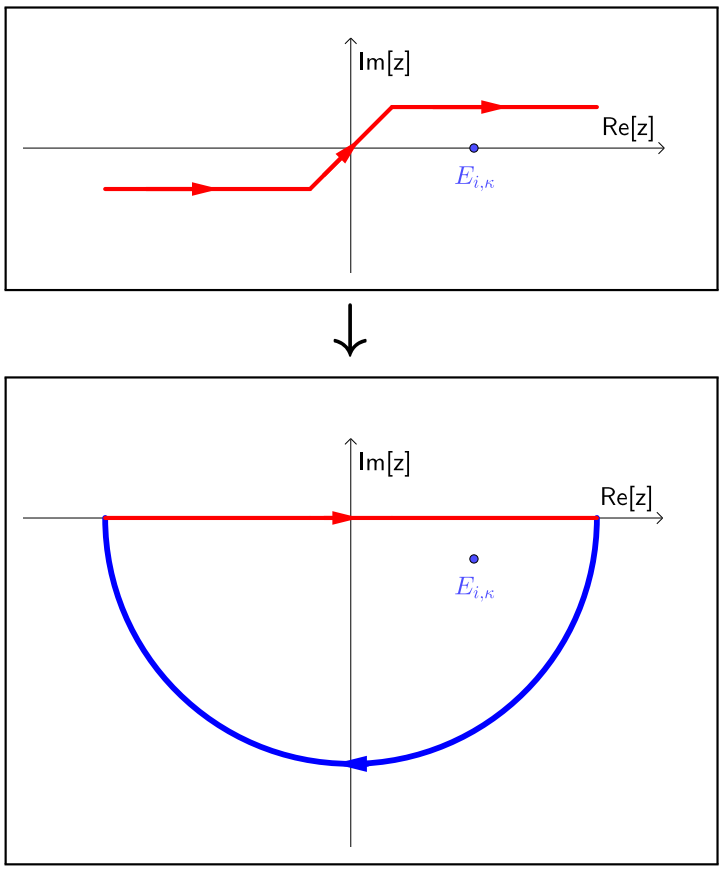
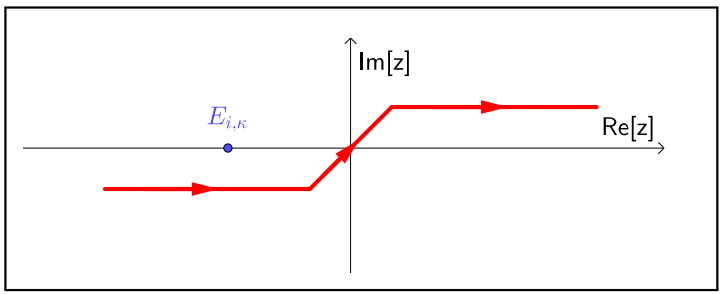


Negative pole case



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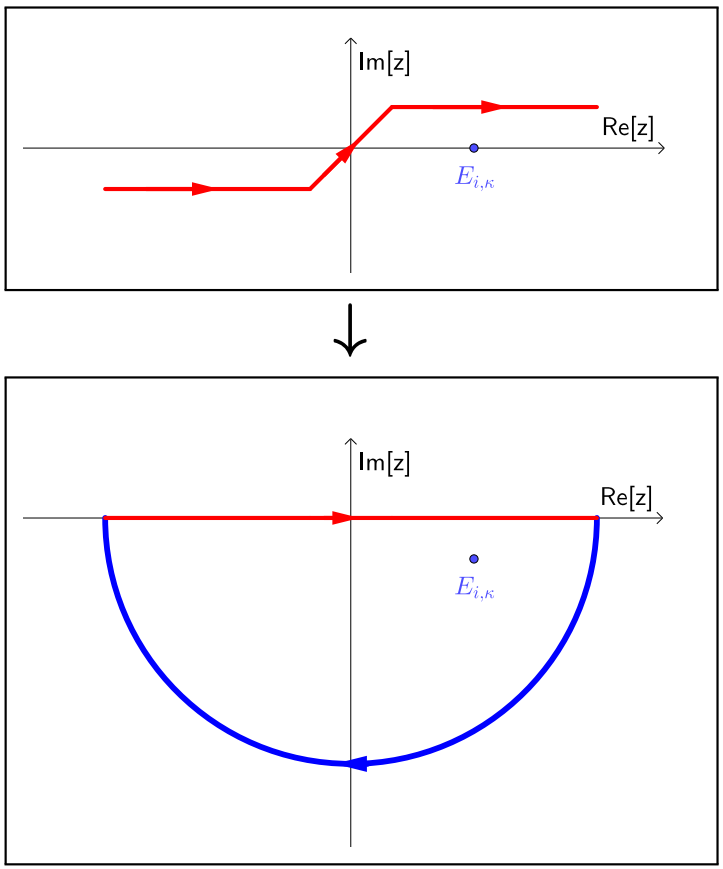
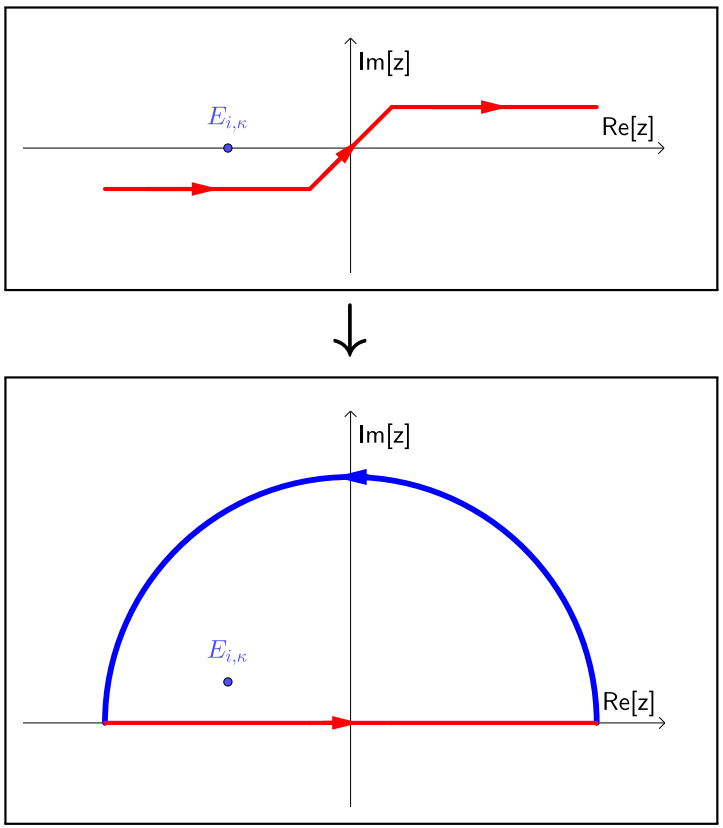


Negative pole case



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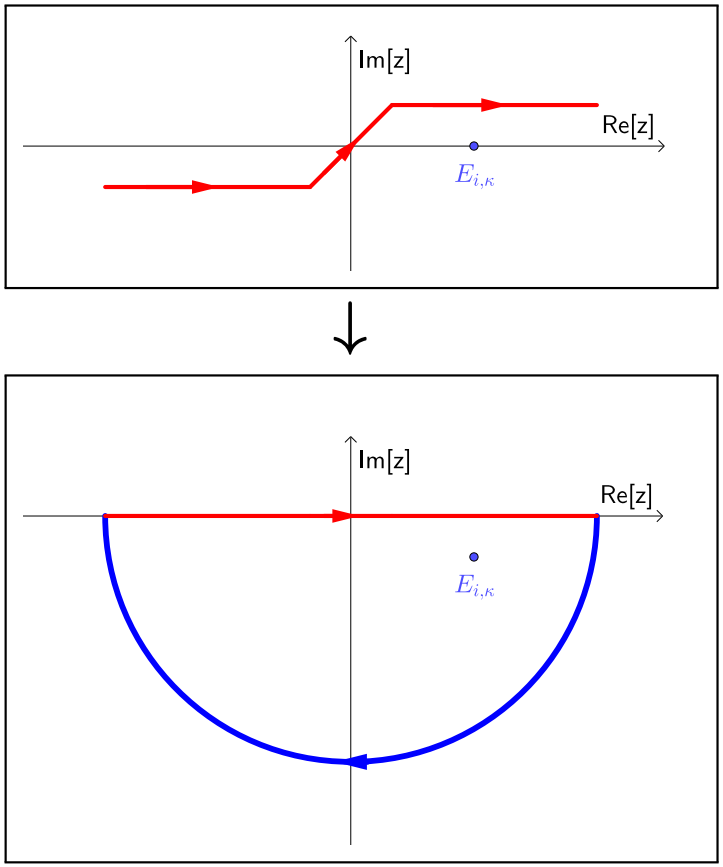
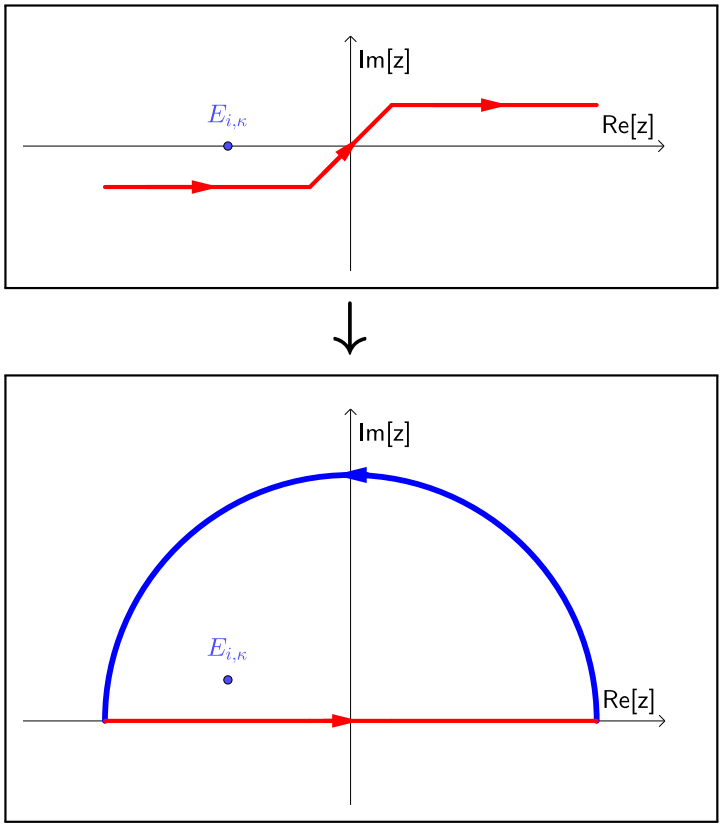


Negative pole case



The final result is:

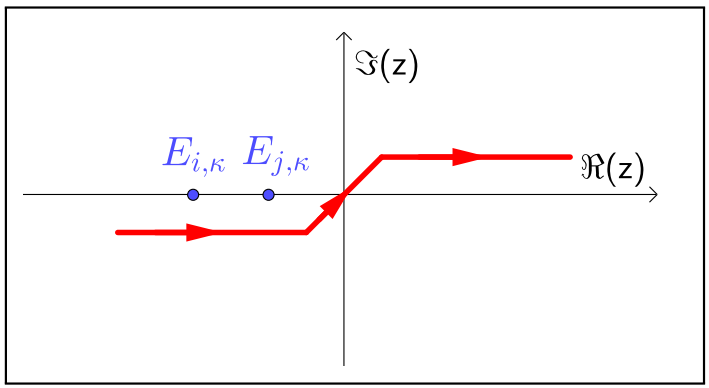
$$\int_{C_F} dz \frac{1}{E_{i,\kappa} - z} = i\pi \mathrm{sgn}\left(E_{i,\kappa}\right) \tag{74}$$

B9: Contour integrations 2

The two-pole integral:

$$\int_{C_F} dz \frac{1}{E_{i,\kappa} - z} \frac{1}{E_{j,\kappa} - z} = ? \tag{75}$$

Same energy signs



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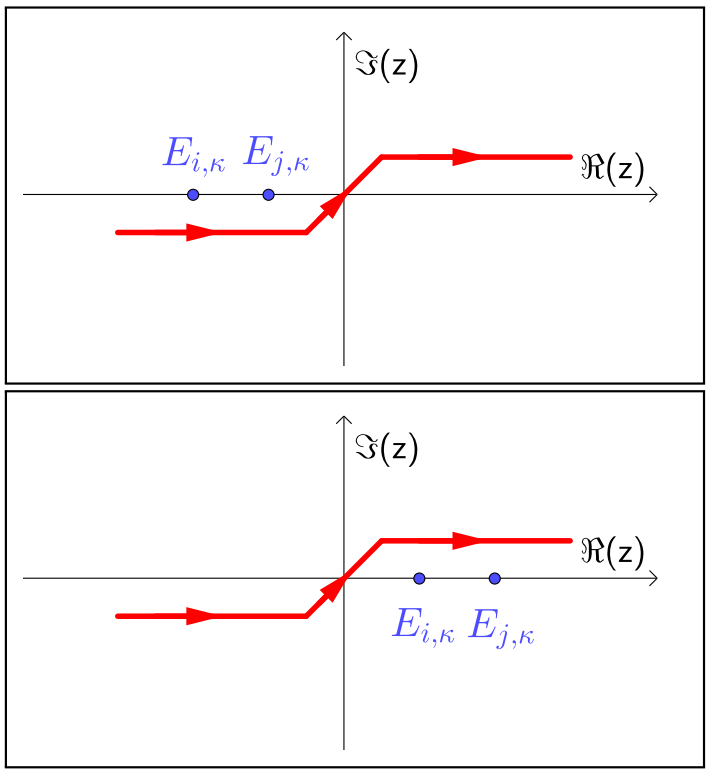

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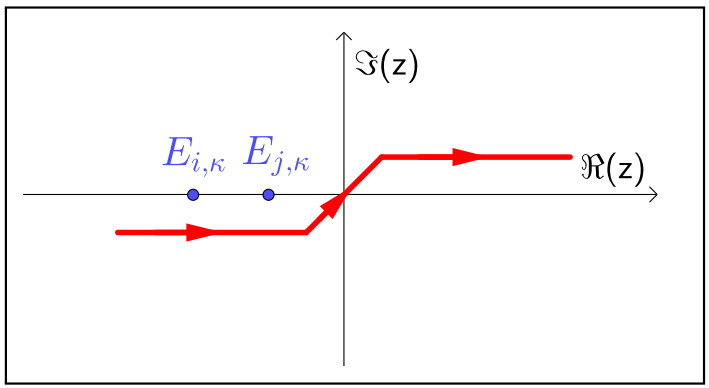
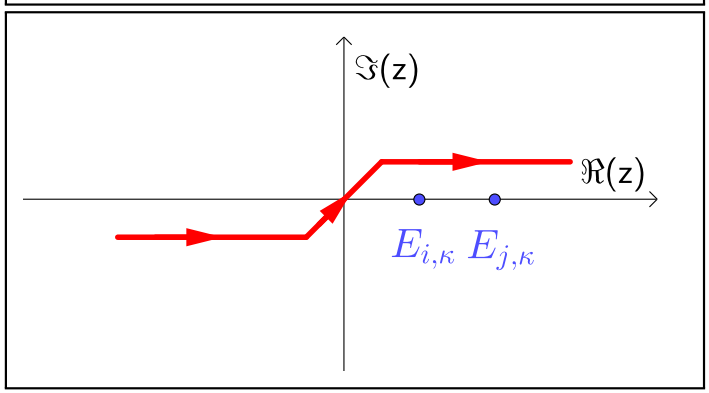
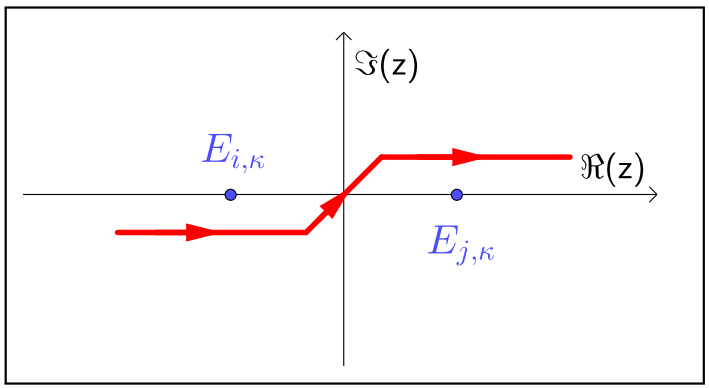




Opposite energy signs



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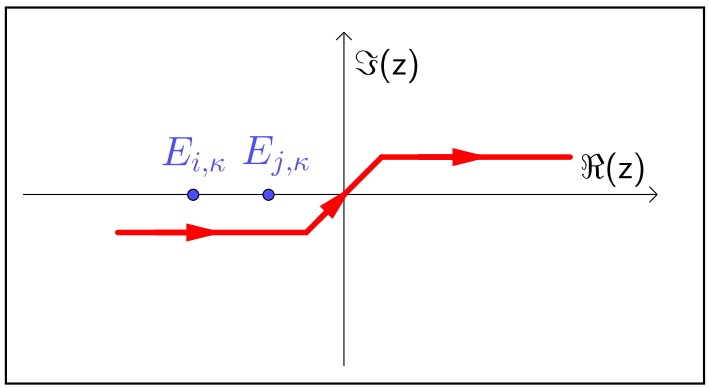
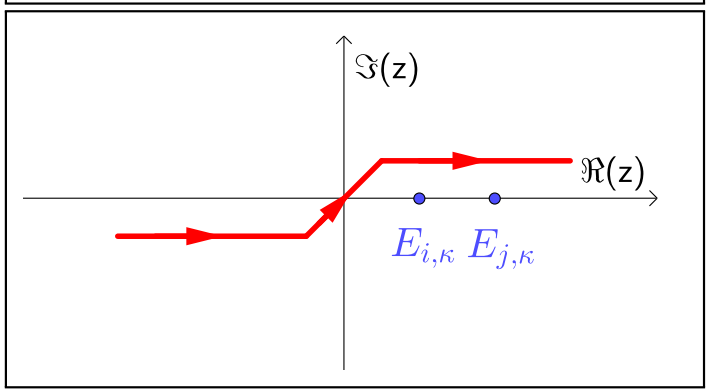
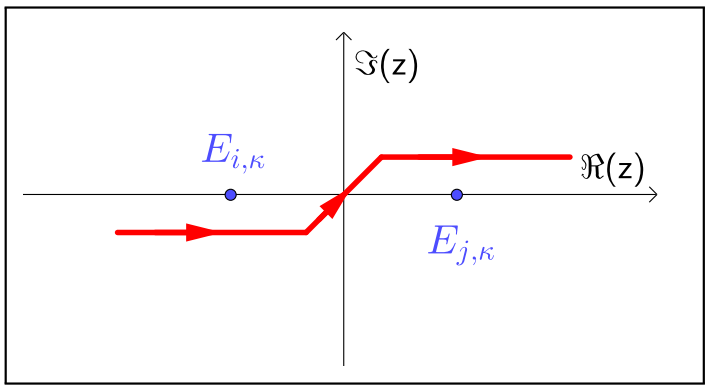
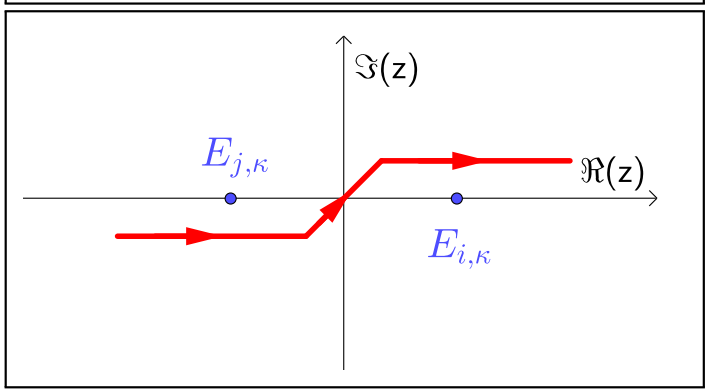
Same energy signs





Opposite energy signs





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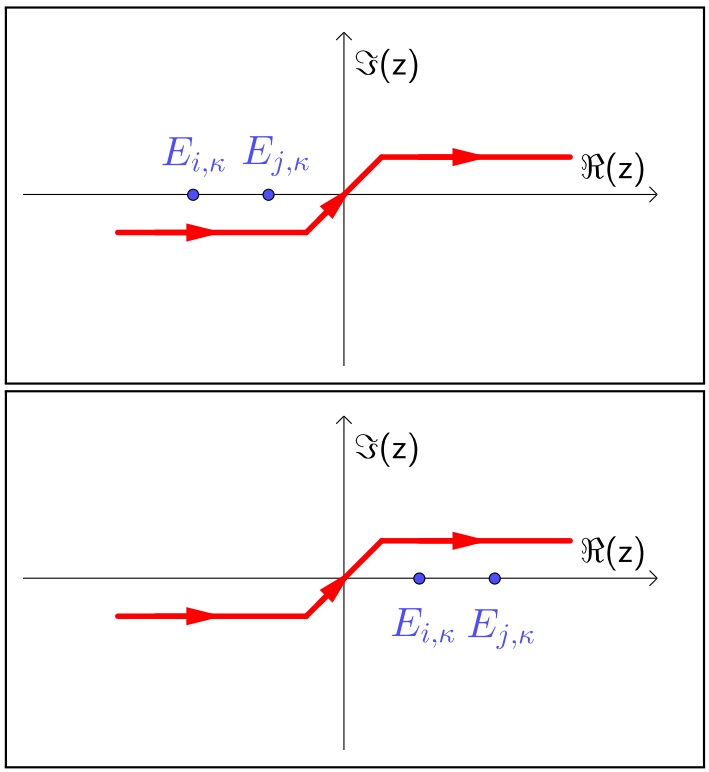
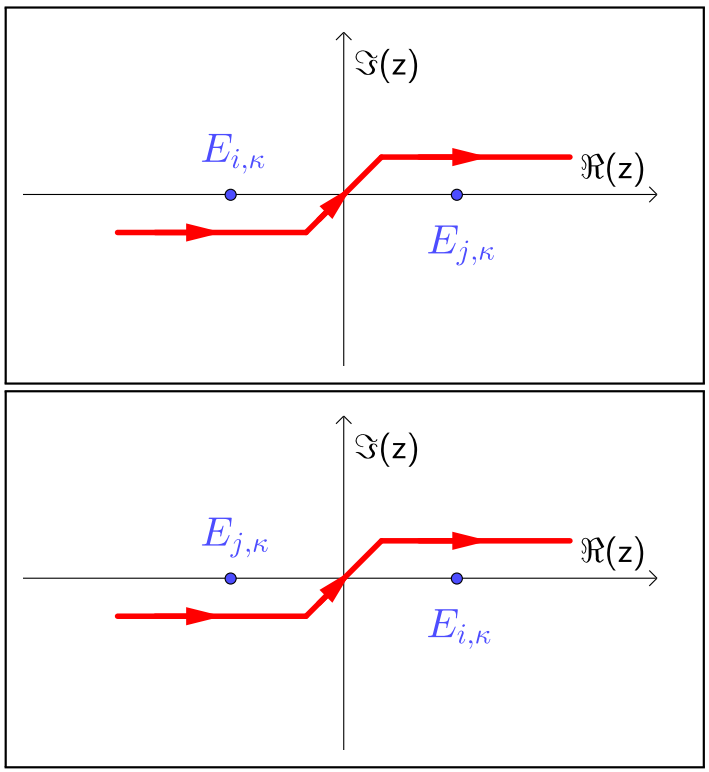


Opposite energy signs

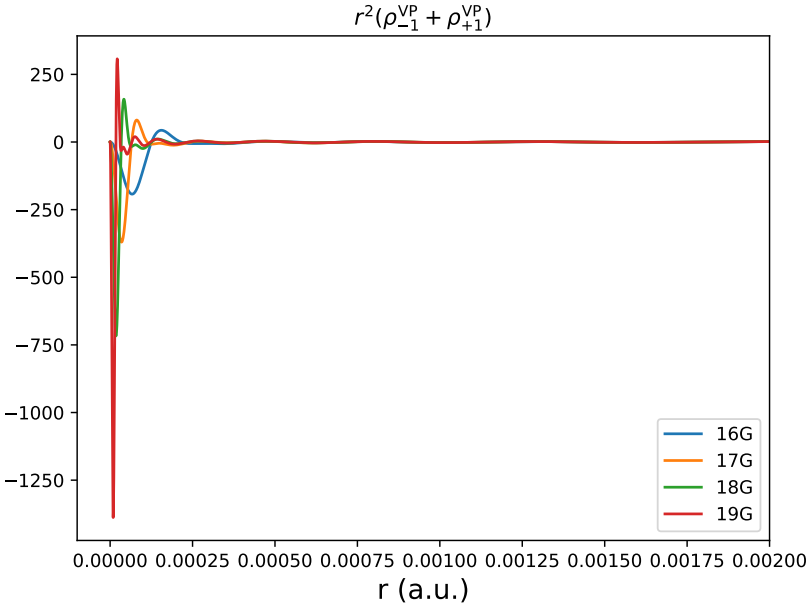


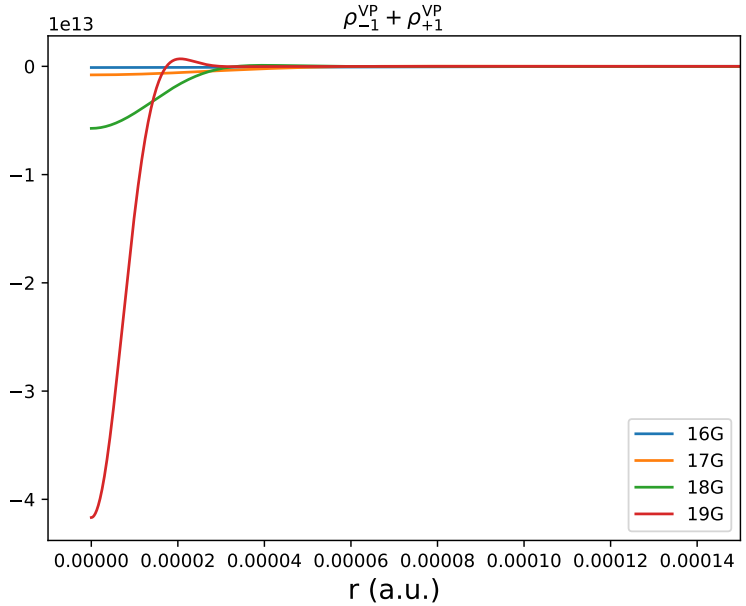
The final result is:

$$\int_{C_F} dz \frac{1}{E_{i,\kappa} - z} \frac{1}{E_{j,\kappa} - z} = i\pi \frac{1 - \mathrm{sgn}\left(E_{i,\kappa} E_{j,\kappa}\right)}{|E_{i,\kappa}| + |E_{j,\kappa}|} \tag{76}$$

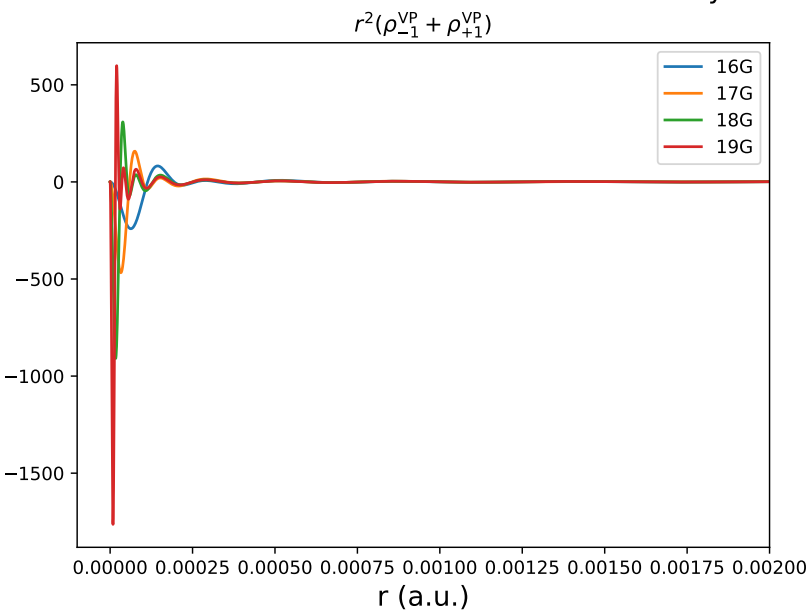
B10: VP divergence with Z=92 point nucleus

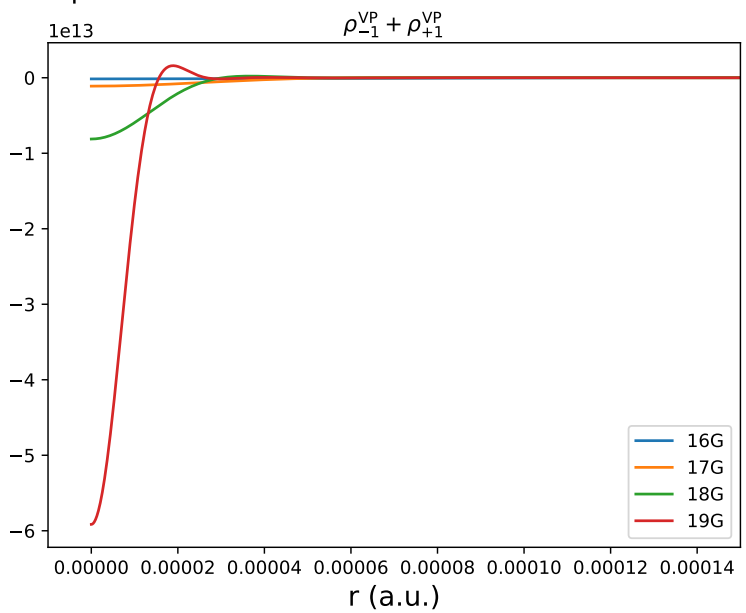
RKB VP density for Z=92 with point nucleus





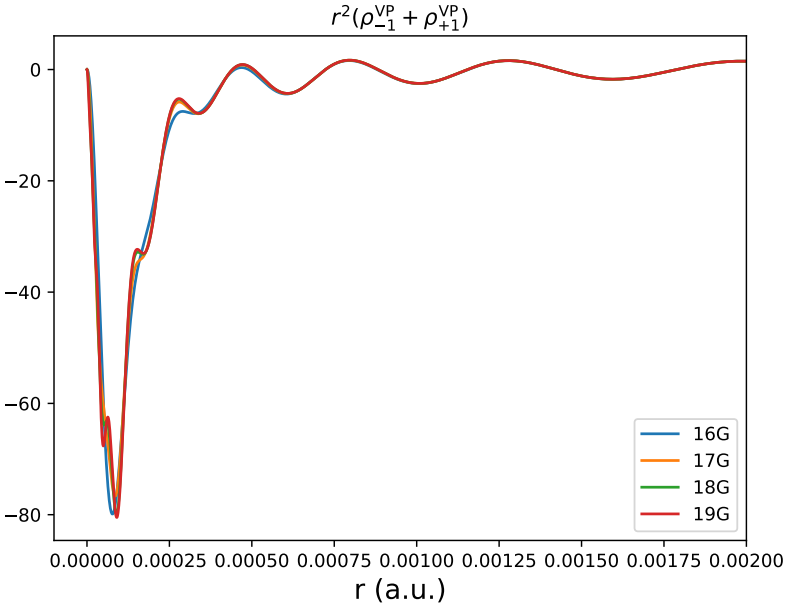
DKB VP density for Z=92 with point nucleus

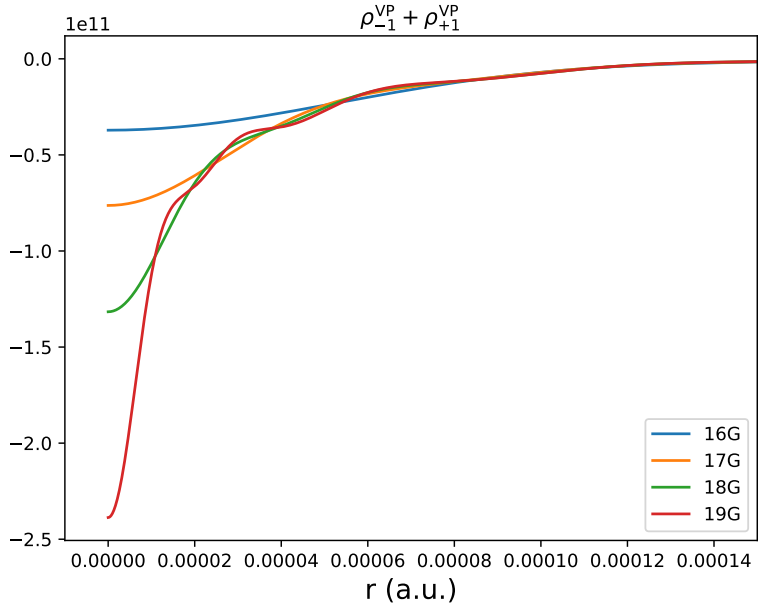




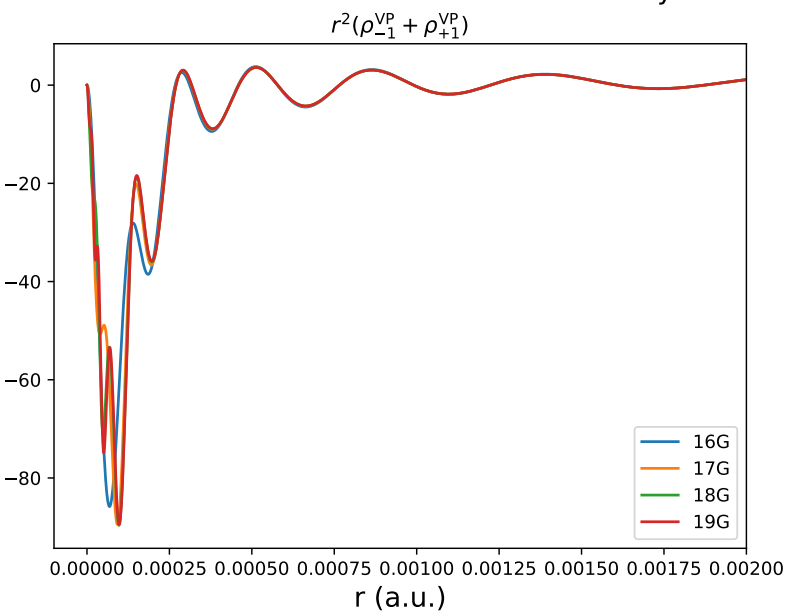
B11: VP divergence with Z=92 Gauss nucleus

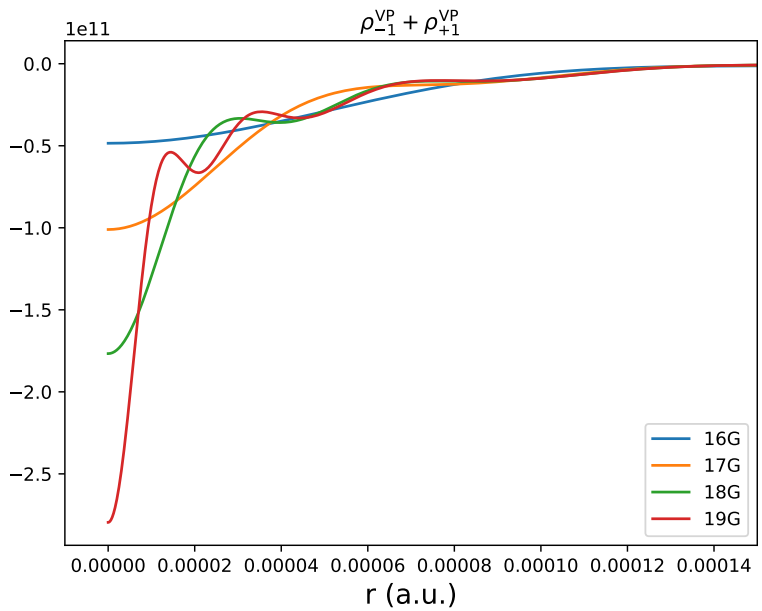
RKB VP density for Z=92 with Gaussian nucleus





DKB VP density for Z=92 with Gaussian nucleus





B12: $\alpha(Z\alpha)$ effective VP potential

In the point-nucleus problem, the Uehling potential is found to be

$$\varphi_{\text{Ueh.}}^{\text{point}}(\boldsymbol{x}) = \frac{2\alpha}{3\pi}\boxed{\frac{Ze}{4\pi\epsilon_0 r_x}}K_1\left(\frac{2}{\bar{\lambda}}r_x\right) \tag{77}$$

$$K_1(x) = \int_1^\infty d\zeta e^{-x\zeta}\left(\frac{1}{\zeta^2}+\frac{1}{2\zeta^4}\right)\sqrt{\zeta^2-1} \tag{78}$$

For a general nucleus, with an arbitrary normalized nuclear distribution $\rho^{\text{nuc.}}(\boldsymbol{x})$, this potential becomes

$$\varphi_{\text{Ueh.}}^{\text{nuc.}}(\boldsymbol{x}) = \int d^3y \rho^{\text{nuc.}}(\boldsymbol{x}-\boldsymbol{y})\varphi_{\text{Ueh.}}^{\text{point}}(\boldsymbol{y}) \tag{79}$$

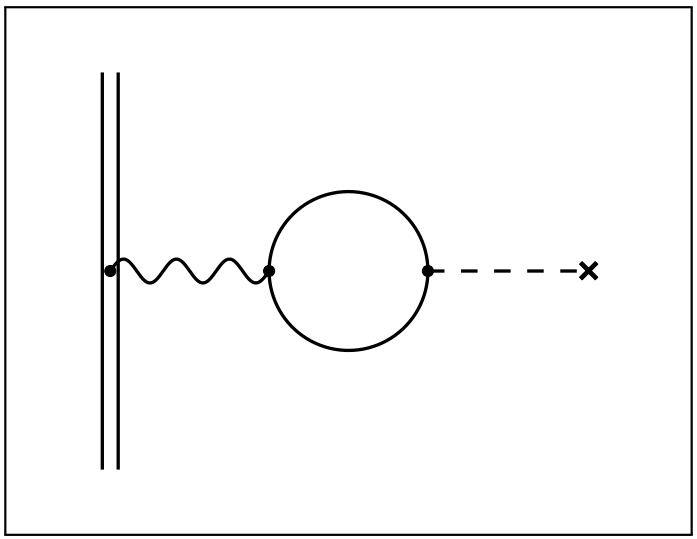


Figure: The $\alpha(Z\alpha)$ vacuum polarization process (Uehling)

B13: $\alpha\,(Z\alpha)^3$ effective VP potential

The first non-linear vacuum polarization potential is given by

$$\varphi_{\mathrm{WK}}^{\mathrm{point}}(\boldsymbol{x}) = -\alpha\,(Z\alpha)^2 \boxed{\frac{Ze}{4\pi\epsilon_0 r_x}} \int_0^\infty \mathrm{d}t \mathrm{e}^{-2tr_x} \frac{1}{t^4}$$
$$\times \left\{ -\frac{1}{12}\pi^2 \sqrt{t^2-1}\theta(t-1) + \int_0^t \mathrm{d}x \sqrt{t^2-x^2} f(x) \right\}$$

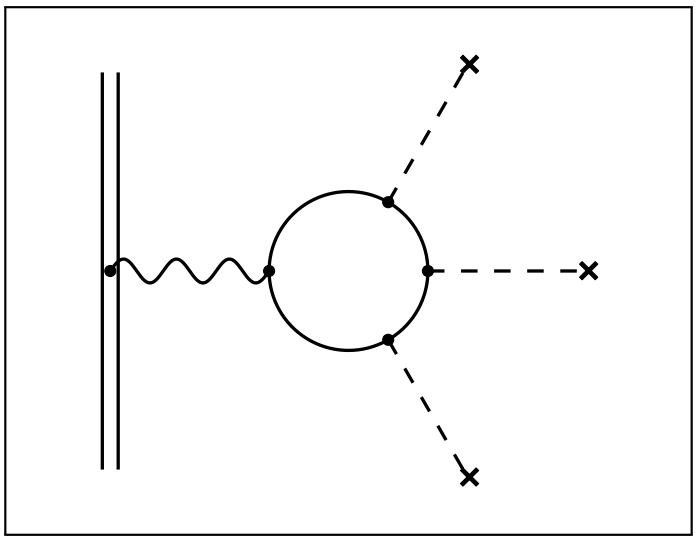


Figure: The $\alpha\,(Z\alpha)^3$ vacuum polarization process (Wichmann and Kroll).

B14: $\alpha\,(Z\alpha)^3$ effective VP potential

Functions $f\,(x)$ and $\psi\,(x)$ are given by

$$f(x) = -2x\psi\left(x^2\right) - x\log^2\left(1-x^2\right) + \frac{1-x^2}{x^2}\log\left(1-x^2\right)\log\frac{1+x}{1-x} + \frac{1-x^2}{4x}\log^2\frac{1+x}{1-x}$$
$$+ \frac{2-x^2}{x\left(1-x^2\right)}\log\left(1-x^2\right) + \frac{3-2x^2}{1-x^2}\log\frac{1+x}{1-x} - 3x, \quad x<1$$

$$f(x) = \frac{1}{x^2}\psi\left(\frac{1}{x^2}\right) - \frac{3x^2+1}{2x}\left[\psi\left(\frac{1}{x}\right) - \psi\left(-\frac{1}{x}\right)\right] - \frac{2x^2-1}{2x^2}\left[\log^2\left(1-\frac{1}{x^2}\right)\right.$$
$$\left. + \log^2\frac{x+1}{x-1}\right] - (2x-1)\log\left(1-\frac{1}{x^2}\right)\log\frac{x+1}{x-1} + \frac{3x^2+1}{4x}\log^2\frac{x+1}{x-1}$$
$$- 2\log x\log\left(1-\frac{1}{x^2}\right) - \frac{3x^2+1}{2x}\log x\log\frac{x+1}{x-1} + \left[5 - \frac{x\left(3x^2-2\right)}{x^2-1}\right]$$
$$\times\log\left(1-\frac{1}{x^2}\right) + \left[\frac{3x^2+2}{x} - \frac{3x^2-2}{x^2-1}\right]\log\frac{x+1}{x-1} + 3\log x - 3, \quad x>1,$$

$$\psi\,(x) = -\int_0^x \mathrm{d}x'\,\frac{\log\left(1-x'\right)}{x'} = \sum_{n=1}^{\infty}\frac{x^n}{n^2}, \quad -1\leqslant x\leqslant 1$$