On the variational inclusion of vacuum polarization in 4-component relativstic molecular calculations

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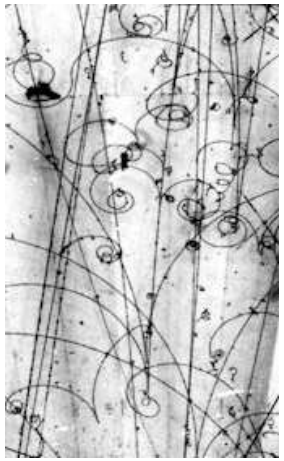
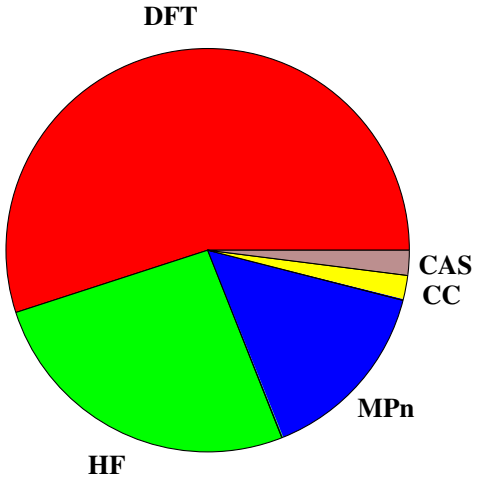


Density Functional Theory



S. Grimme,

Nachrichten aus der Chemie,

49 (2001) 340

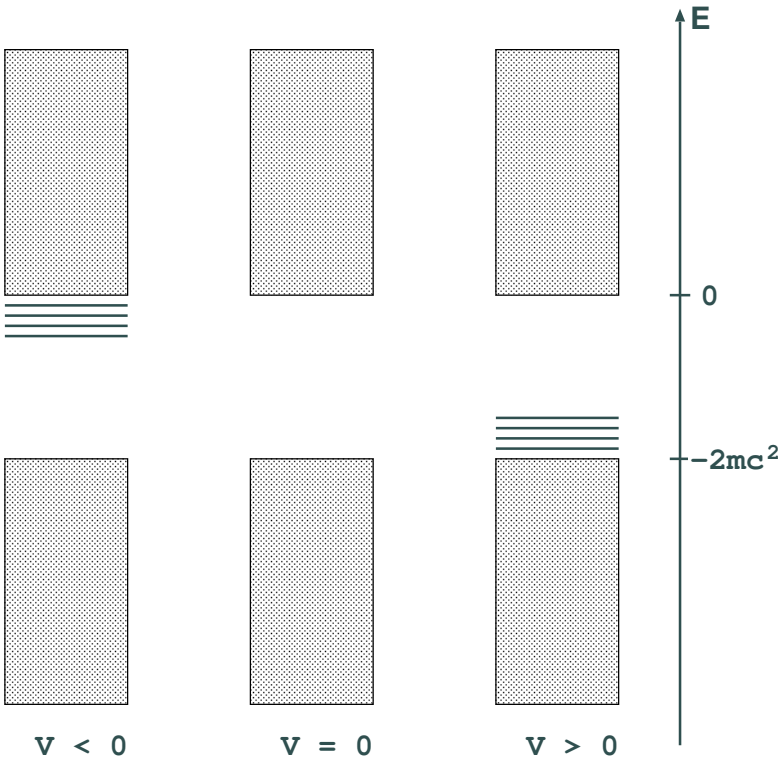
- ✔ Currently the most popular electronic structure method:
  The energy is a functional of the charge density only.

- ✔ Rigourous foundation: Hohenberg-Kohn theorem
  P. Hohenberg and W. Kohn, Phys. Rev. B **136** (1964) 864
  - the simple proof requires a minimisation principle

- ✔ Practical implementation: Kohn-Sham approach
  W. Kohn and L. J. Sham, Phys. Rev. A **140** (1965) 1133

- ✔ Extension to relativity: QED framework
  A. K. Rajagopal and J. Callaway, Phys. Rev. B **7** (1973) 1912
  - vacuum polarisation is enough...

Spectrum of the Dirac equation



Negative-energy orbitals:

- QED: filled ("Dirac sea")
  $\Rightarrow$ minimisation principle

- standard approach: empty
  (orthonormal complement allowing the complete relaxation of the electronic wave function)
  $\Rightarrow$ min-max-principle

  J. D. Talman, Phys. Rev. Lett. **57** (1986) 1091

Second quantization formalism

✔ Einstein summation convention employed throughout

✔ Field operators

$$\Psi(1) = \varphi_p(\mathbf{r}_1)\, a_p = \widetilde{\varphi}_p(\mathbf{r}_1)\, \widetilde{a}_p$$

✔ Second-quantized Hamiltonian

$$\begin{aligned} \hat{H} &= \int \Psi^\dagger(1)\hat{h}(1)\Psi(1)d\tau_1 + \frac{1}{2}\int\int \Psi^\dagger(1)\Psi^\dagger(2)\ \underbrace{\hat{g}(1,2)}_{\text{Coulomb term}}\ \Psi(2)\Psi(1)d\tau_1 d\tau_2 \\ &= h_{pq}a_p^\dagger a_q + \frac{1}{4}\mathcal{L}_{pq,rs}a_p^\dagger a_r^\dagger a_s a_q \end{aligned}$$

✔ Anti-symmetrized two-electron integrals

$$\mathcal{L}_{pq,rs} = (pq\,|\,rs) - (ps\,|\,rq) = \mathcal{L}_{rs,pq} = -\mathcal{L}_{ps,rq}$$

Hartree-Fock method

✔ Starting from a selected orbital set $\{\varphi_q\}$,
Slater determinants (Hilbert space) map into occupation-number vectors (Fock space)

$$|\Phi\rangle = a_1^\dagger a_2^\dagger \dots a_N^\dagger |0\rangle$$

which are eigenfunctions of the number operator $\hat{N} = a_p^\dagger a_p$

✔ The vacuum state

$$a_i |0\rangle = 0; \quad \forall a_i$$

✔ Hartree-Fock variational ansatz

$$\left|\widetilde{\Phi}\right\rangle = \exp\left[-\widehat{\kappa}\right] |\Phi\rangle ; \quad \widehat{\kappa} = \kappa_{pq} a_p^\dagger a_q; \quad \kappa_{pq} = -\kappa_{qp}^*$$

✔ $\left[\widehat{\kappa}, \widehat{N}\right] = 0 \quad \Rightarrow \quad$ The orbital rotation operator conserves particle number.

Orbital rotation

✔ The Hartree-Fock variational ansatz can be re-written as

$$\begin{aligned}\left|\widetilde{\Phi}\right\rangle &= \exp\left[-\widehat{\kappa}\right]|\Phi\rangle = \widehat{U}a_1^\dagger a_2^\dagger \ldots a_N^\dagger |0\rangle \\ &= \widehat{U}a_1^\dagger \widehat{U}^\dagger \widehat{U}a_2^\dagger \widehat{U}^\dagger \widehat{U} \ldots \widehat{U}^\dagger \widehat{U}a_N^\dagger \widehat{U}^\dagger \widehat{U}\,|0\rangle \\ &= \widetilde{a}_1^\dagger \widetilde{a}_2^\dagger \ldots \widetilde{a}_N^\dagger |0\rangle\end{aligned}$$

✔ Transformed creation operators and orbitals

$$\widetilde{a}_p^\dagger = \exp\left[-\widehat{\kappa}\right] a_p^\dagger \exp\left[\widehat{\kappa}\right] = a_q^\dagger U_{qp}; \quad \widetilde{\varphi}_p = \varphi_q U_{qp}^*; \quad U = \exp\left[-\kappa\right].$$

✔ Important: To derive the above we have used

$$\exp\left[-\widehat{\kappa}\right]|0\rangle = \left(1 - \kappa_{pq}a_p^\dagger a_q + \ldots\right)|0\rangle = |0\rangle$$

Towards QED

✔ I will consider QED in the semiclassical limit,
that is without quantization of electromagnetic fields.

✔ Particle-hole formalism

$$\Psi = \varphi_p a_p \quad \rightarrow \quad \Psi = \varphi_p^+ b_p + \varphi_p^- d_p^\dagger$$

- *electron* annihilation operators b_p associated with the positive-energy orbitals φ_p^+
- *positron* creation operators $d_p^\dagger$ describing the creation of positrons whose orbitals are obtained by charge conjugating the associated negative-energy orbitals φ_p^-

The QED Hamiltonian

$$
\begin{aligned}
\hat{H} \quad &= \quad h_{pq}^{++} b_p^\dagger b_q + h_{pq}^{+-} b_p^\dagger d_q^\dagger + h_{pq}^{-+} d_p b_q + h_{pq}^{--} d_p d_q^\dagger \\
&+ \quad \frac{1}{4}\mathcal{L}_{pqrs}^{++++} b_p^\dagger b_r^\dagger b_s b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{+-++} b_p^\dagger b_r^\dagger b_s d_q^\dagger + \frac{1}{4}\mathcal{L}_{pqrs}^{+++-} b_p^\dagger b_r^\dagger d_s^\dagger b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{+-+-} b_p^\dagger b_r^\dagger d_s^\dagger d_q^\dagger \\
&+ \quad \frac{1}{4}\mathcal{L}_{pqrs}^{++-+} b_p^\dagger d_r b_s b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{+--+} b_p^\dagger d_r b_s d_q^\dagger + \frac{1}{4}\mathcal{L}_{pqrs}^{++--} b_p^\dagger d_r d_s^\dagger b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{+---} b_p^\dagger d_r d_s^\dagger d_q^\dagger \\
&+ \quad \frac{1}{4}\mathcal{L}_{pqrs}^{-+++} d_p b_r^\dagger b_s b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{--++} d_p b_r^\dagger b_s d_q^\dagger + \frac{1}{4}\mathcal{L}_{pqrs}^{-++-} d_p b_r^\dagger d_s^\dagger b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{--+-} d_p b_r^\dagger d_s^\dagger d_q^\dagger \\
&+ \quad \frac{1}{4}\mathcal{L}_{pqrs}^{-+-+} d_p d_r b_s b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{---+} d_p d_r b_s d_q^\dagger + \frac{1}{4}\mathcal{L}_{pqrs}^{-+--} d_p d_r d_s^\dagger b_q + \frac{1}{4}\mathcal{L}_{pqrs}^{----} d_p d_r d_s^\dagger d_q^\dagger
\end{aligned}
$$

✔ The QED Hamiltonian couples occupation-number vectors with different particle number, but conserves charge.

Hartree-Fock theory in semiclassical QED

✔ Reference occupation-number vector (bound electronic states)

$$|\Phi\rangle = b_1^\dagger b_2^\dagger \ldots b_n^\dagger |0\rangle$$

✔ QED vacuum state

$$(b_p |0\rangle = 0, \quad \forall b_p) \quad \text{and} \quad (d_p |0\rangle = 0, \quad \forall d_p)$$

✔ Variational Hartree-Fock *ansatz*

$$\left|\widetilde{\Phi}\right\rangle = \exp\left[-\widehat{\kappa}\right] |\Phi\rangle$$

✔ The $\widehat{\kappa}$ single replacement operator

$$\widehat{\kappa} = \underbrace{\kappa_{pq}^{++} b_p^\dagger b_q}_{\widehat{\kappa}^{++}} + \underbrace{\kappa_{pq}^{+-} b_p^\dagger d_q^\dagger}_{\widehat{\kappa}^{+-}} + \underbrace{\kappa_{pq}^{-+} d_p b_q}_{\widehat{\kappa}^{-+}} + \underbrace{\kappa_{pq}^{--} d_p d_q^\dagger}_{\widehat{\kappa}^{--}}$$

Number and charge operators

✔ Number operators

$$\hat{N}^e = b_p^\dagger b_p \quad \text{and} \quad \hat{N}^p = d_p^\dagger d_p$$

- the $\hat{\kappa}$ operator commutes with neither number operator

$$\left[\hat{\kappa}, \hat{N}^e\right] = \left[\hat{\kappa}, \hat{N}^p\right] = \hat{\kappa}^{-+} - \hat{\kappa}^{+-}$$

✔ Charge operator

$$\hat{Q} = e\left(\hat{N}^p - \hat{N}^e\right)$$

- The orbital rotation operator of QED conserves charge but *not* the particle number:

$$\left[\hat{\kappa}, \widehat{Q}\right] = 0$$

Vacuum polarization

✔ Using the unitarity of the orbital rotation operator we may now rewrite the HF ansatz as

$$\left|\widetilde{\Phi}\right\rangle = \exp\left[-\widehat{\kappa}\right]|\Phi\rangle = \widetilde{b}_1^\dagger \widetilde{b}_2^\dagger \ldots \widetilde{b}_n^\dagger \left|\widetilde{0}\right\rangle$$

✔ Transformed creation operators

$$\widetilde{b}_p^\dagger = \exp\left[-\widehat{\kappa}\right] b_p^\dagger \exp\left[\widehat{\kappa}\right] = b_q^\dagger U_{qp}; \quad U = \exp\left[-\kappa\right]$$

✔ The dressed vacuum

$$\begin{aligned}\left|\widetilde{0}\right\rangle &= \exp\left[-\widehat{\kappa}\right]|0\rangle = \\ &= \left\{1 - \kappa_{pq}^{++} b_p^\dagger b_q - \kappa_{pq}^{+-} b_p^\dagger d_q^\dagger - \kappa_{pq}^{-+} d_p b_q - \kappa_{pq}^{--} d_p d_q + O(\kappa^2)\right\}|0\rangle \neq |0\rangle\end{aligned}$$

Energy renormalization

- If we evaluate the expectation value of the QED Hamiltonian with respect to the reference determinant we obtain the standard expression, but with *all* the negative-energy orbitals included amongst the occupied orbitals, thus leading to an infinite negative energy. In order to avoid working with infinite energies renormalization procedures are introduced in QED. In the present case the infinite negative energy is avoided by writing the Hamiltonian on *reordered* form, that is all creation operators are shifted to the left and all annihilation operators are shifted to the right as if they anticommuted.
  Note that this is not the same as charge renormalization.

- The reordered QED Hamiltonian

$$\begin{aligned}\hat{H} &= \int N\left[\Psi^\dagger(1)\hat{h}(1)\Psi(1)d\tau_1\right] \\ &+ \frac{1}{2}\int\int N\left[\Psi^\dagger(1)\Psi^\dagger(2)\hat{g}(1,2)\Psi(2)\Psi(1)\right]d\tau_1 d\tau_2\end{aligned}$$

Reordering

✔ One-electron part

$$N\left[\Psi^{\dagger}(1)\Psi(2)\right] = \Psi^{\dagger}(1)\Psi(2) - \left\langle 0^{(ref)} \left| \Psi^{\dagger}(1)\Psi(2) \right| 0^{(ref)} \right\rangle$$

- normal ordering of a one-electron operator corresponds to the subtraction of its reference vacuum expectation value

✔ Two-electron part

$$\begin{aligned} N\left[\Psi^{\dagger}(1)\Psi^{\dagger}(2)\Psi(3)\Psi(4)\right] &= \Psi^{\dagger}(1)\Psi^{\dagger}(2)\Psi(3)\Psi(4) \\ &- N\left[\Psi^{\dagger}(1)\Psi(4)\right]\Psi^{\dagger}(2)\Psi(3) - N\left[\Psi^{\dagger}(2)\Psi(3)\right]\Psi^{\dagger}(1)\Psi(4) \\ &+ N\left[\Psi^{\dagger}(1)\Psi(3)\right]\Psi^{\dagger}(2)\Psi(4) + N\left[\Psi^{\dagger}(2)\Psi(4)\right]\Psi^{\dagger}(1)\Psi(3) \\ &- \left\langle 0^{(ref)} \left| \Psi^{\dagger}(1)\Psi^{\dagger}(2)\Psi(3)\Psi(4) \right| 0^{(ref\ )} \right\rangle \end{aligned}$$

✔ The bare vacuum expectation value of the reordered Hamiltonian is zero.

Reducing complexity

✔ With the introduction of reordering more complexity is added and manipulations involving the reordered Hamiltonian become extremely tedious. In order to simplify the ensuing manipulations it is therefore advantageous to not use the particle-hole formalism and instead explicitly define the bare vacuum as filled with all the negative-energy solutions of the free-particle Dirac equation

$$\left|0^{(ref\ )}\right\rangle = a^{\dagger}_{[-1]}a^{\dagger}_{[-2]}\ldots a^{\dagger}_{[-\infty]}\left|\mathrm{empty}\right\rangle$$

- The empty state $|\mathrm{empty}\rangle$ now corresponds to the vacuum of the standard approach to 4-component relativistic molecular theory.

✔ Reordered QED Hamiltonian

$$\hat{H} = \left\{h_{pq} - \Gamma_{pq}\left[\varphi^{-}_{[i]}\right]\right\}a^{\dagger}_{p}a_{q} + \frac{1}{4}\mathcal{L}_{pqrs}a^{\dagger}_{p}a^{\dagger}_{r}a_{s}a_{q} - h^{--}_{[ii]} + \frac{1}{2}\mathcal{L}^{----}_{[iijj]}$$

- we use *square brackets* (e.g. $h^{--}_{[pq]}$) around indices referring to the negative-energy solutions of the *free-particle* Dirac equation.
- compare with I. Lindgren and J. Morrison: *Atomic Many-Body Theory*, Springer, New York 1982

The Hartree-Fock energy

✔ The expectation value of the energy with respect to the current Slater determinant

$$E^{HF} = \left\langle \Phi \left| \hat{H} \right| \Phi \right\rangle = h_{ii} + \frac{1}{2}\Gamma_{ii}\left[\varphi_j\right]; \quad \Gamma_{pq}\left[\varphi_i\right] = \mathcal{L}_{pqii}$$

- Mean-field potential $\Gamma\left[\varphi_i\right]$ involving summation over the orbital set $\{\varphi_i\}$.

✔ AO-basis

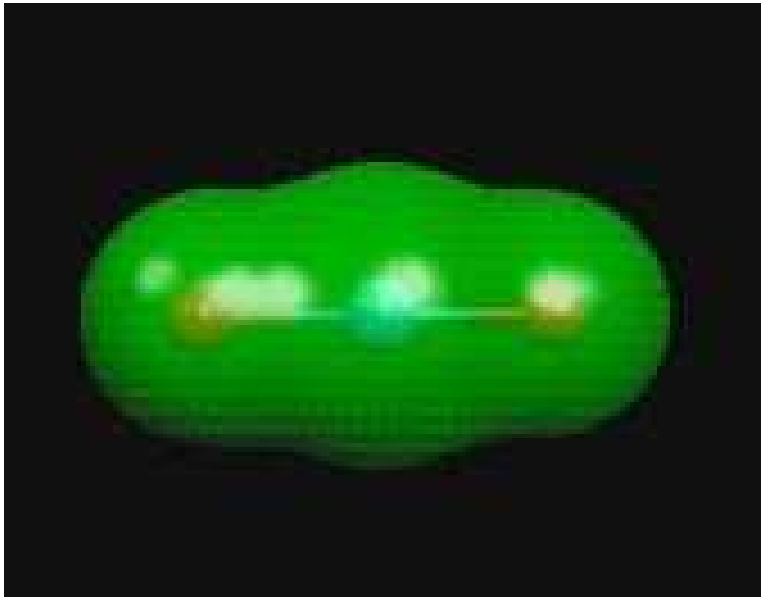
$$\varphi_p = \chi_\mu c_{\mu p} \quad \Rightarrow E = D_{\mu\nu}h_{\nu\mu} + \frac{1}{2}D_{\mu\nu}\mathcal{L}_{\nu\mu\lambda\kappa}D_{\kappa\lambda}$$

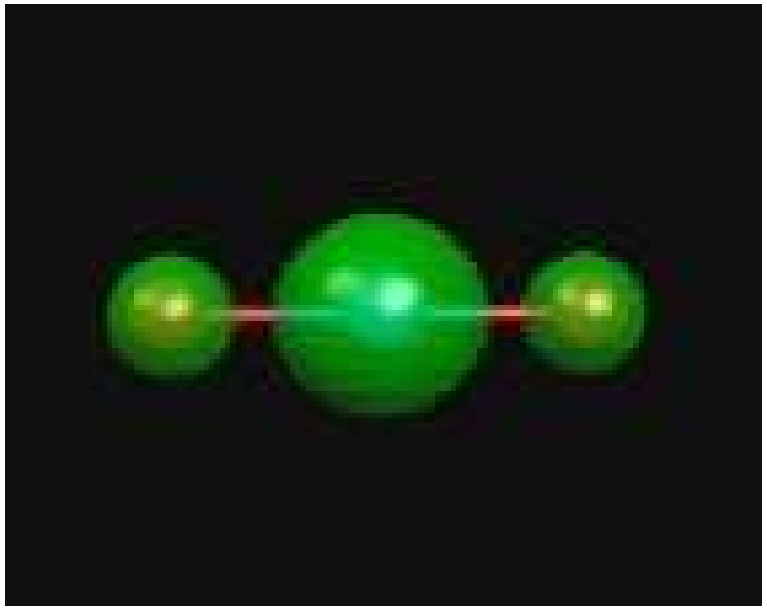
- AO-density matrix $D_{\lambda\kappa} = c_{\lambda i}c^*_{\kappa i}$

✔ Introducing vacuum polarisation

$$D^{HF}_{\lambda\kappa} \rightarrow D^{\mathrm{QED}}_{\kappa\lambda} = D^{HF}_{\kappa\lambda} + D^{\mathrm{VP}}_{\kappa\lambda}; \quad D^{\mathrm{VP}}_{\kappa\lambda} = \sum_i^{(-)} \left(c_{\kappa i}c^*_{\kappa i} - c_{\kappa[i]}c^*_{\kappa[i]} \right)$$

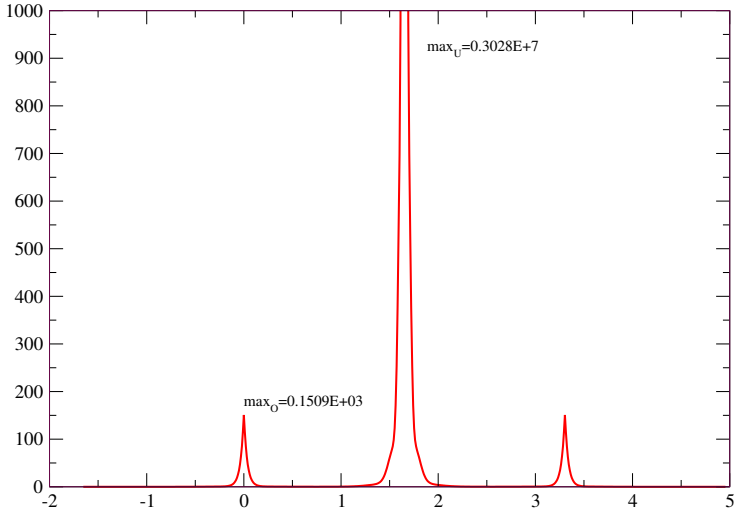
Densities





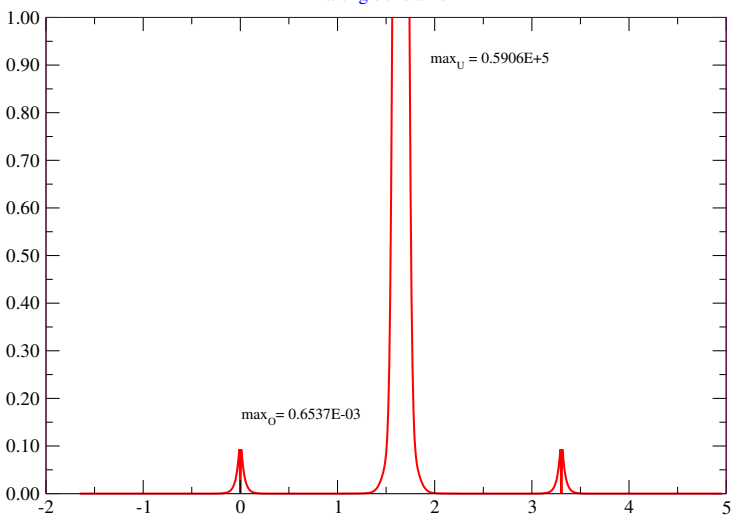
Large component density of uranyl

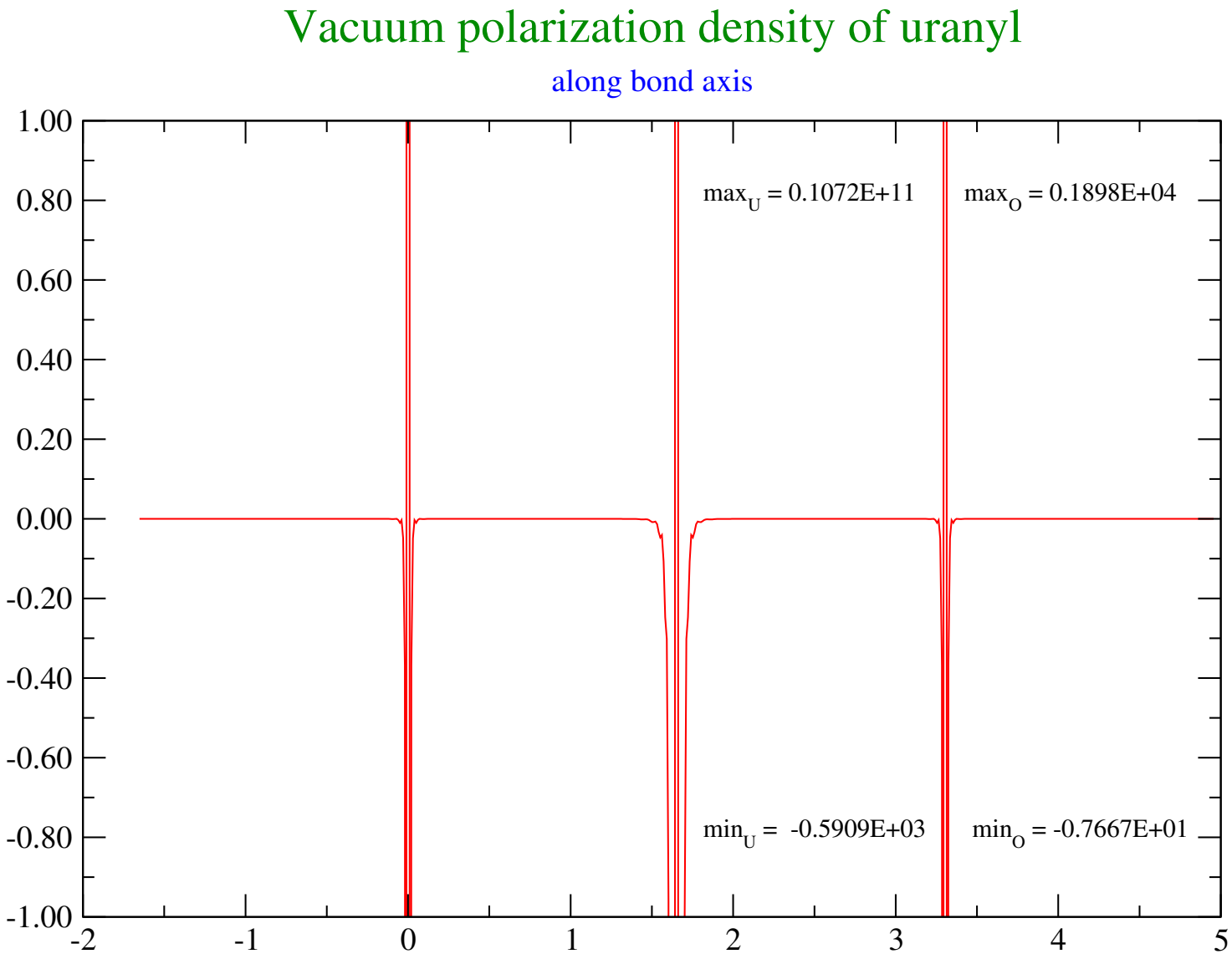
along bond axis



Small component density of uranyl

along bond axis





Note that we plot the probability density $n^{VP}(1)$; charge density $\rho^{VP}(1) = -en^{VP}(1)$.

Vacuum polarisation density

J. J. Sakurai, *Advanced Quantum mechanics*, Wesley 1967:

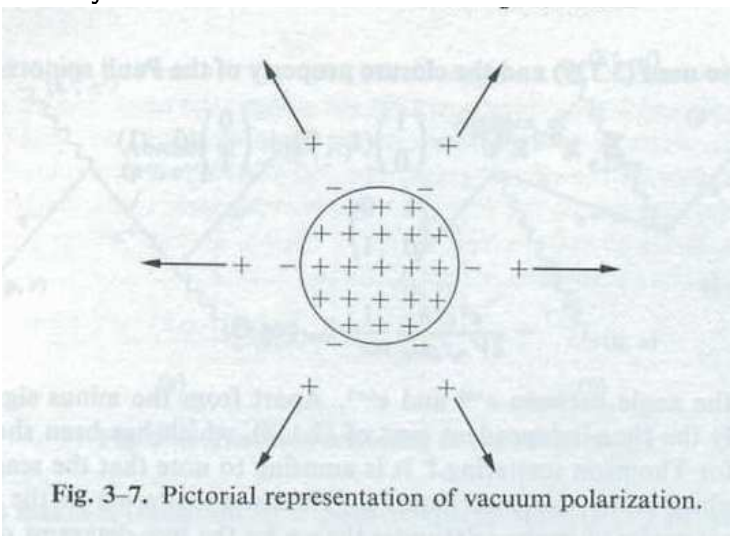


Fig. 3–7. Pictorial representation of vacuum polarization.

W. Greiner and J. Reinhardt: *Quantum Electrodynamics,* Springer 1994:

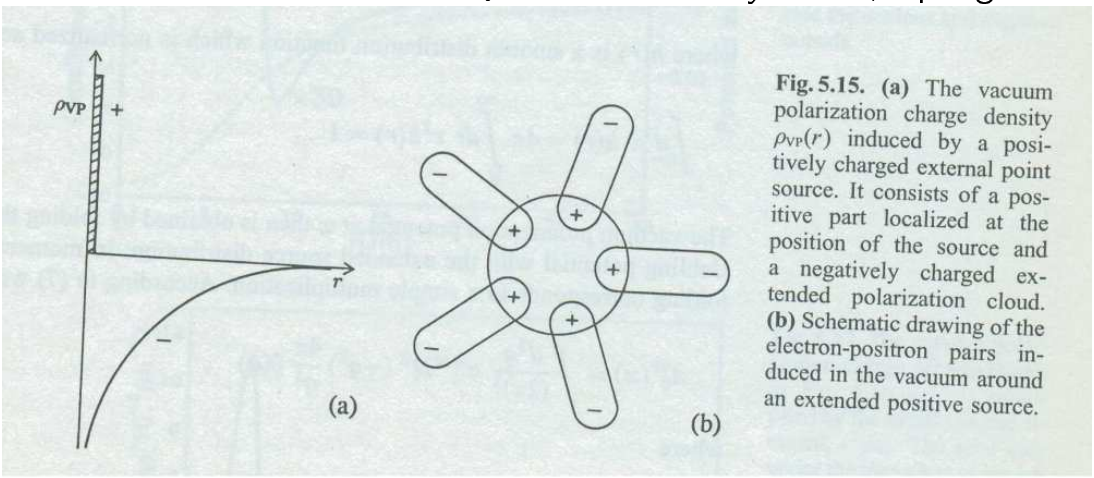


Fig. 5.15. **(a)** The vacuum polarization charge density $\rho_{VP}(r)$ induced by a positively charged external point source. It consists of a positive part localized at the position of the source and a negatively charged extended polarization cloud. **(b)** Schematic drawing of the electron-positron pairs induced in the vacuum around an extended positive source.

Which text book is right ???

So what about the Uehling potential ?

✔ We expand the HF energy

$$E^{HF+VP} = E^{HF} + D^{\rm VP}_{\mu\nu} h_{\nu\mu} + D^{\rm HF}_{\mu\nu} \mathcal{L}_{\nu\mu\lambda\kappa} D^{\rm VP}_{\kappa\lambda} + \frac{1}{2} D^{\rm VP}_{\mu\nu} \mathcal{L}_{\nu\mu\lambda\kappa} D^{\rm VP}_{\kappa\lambda}$$

✔ Consider the energy difference $E_1 - E_2$ between two states in the same orbital basis. Assume $D^{\rm VP}_1 = D^{\rm VP}_2$:

$$\begin{aligned}
\Delta E^{HF+VP} &= E^{HF+VP}_2 - E^{HF+VP}_1 \\
&= \Delta E^{HF} + (D_2 - D_1)^{\rm HF}_{\mu\nu} \mathcal{L}_{\nu\mu\lambda\kappa} D^{\rm VP}_{\kappa\lambda} \\
&= \Delta E^{HF} + \int \rho_2(1) \phi^{VP}(1) d1 - \int \rho_1(1) \phi^{VP}(1) d1 + \Delta(\text{exchange})
\end{aligned}$$

where

$$\phi^{VP}(1) = \int \frac{\rho^{VP}(2)}{r_{12}} d1$$

Charge renormalisation

- Modified electron-nucleus interaction

$$
\begin{aligned}
E &= \int \rho_e(1)\left[\phi_{nuc}(1)+\phi^{VP}(1)\right]d1 \\
&= -Ze^2\int\int n_e(1)D'_F(1-2)n_{nuc}(2)d1d2 \\
&= -Ze^2\int n_e(1)\frac{1}{(2\pi)^3}\int e^{iq\cdot x}\left[1-\frac{e^2}{3\pi}\ln\frac{\Lambda^2}{m^2}+\Pi^R(-\mathbf{q}^2)+\ldots\right]\frac{4\pi}{q^2}dqd1
\end{aligned}
$$

- The logarithmic divergence is absorbed with the bare electron charge

$$
e \rightarrow e_{\text{bare}} = e_R\left(1-\frac{e^2}{3\pi}\ln\frac{\Lambda^2}{m^2}\right)^{-1/2}
$$

Vacuum polarisation density

✔ In this work: $\rho^{VP} = \left[\rho_e^{(-)} - \rho_0^{(-)}\right]$

✔ Often in the literature: $\rho^{VP} = \frac{1}{2}\left[\rho_e^{(-)} - \rho_e^{(+)}\right]$
e.g. E. H. Wichmann and N. M. Kroll, Phys. Rev. **101**(1956) 843

✔ The charge density can be related using charge conjugation symmetry:

$$\mathcal{C} = U_C \mathcal{K}_0, \quad U_C = i\beta\alpha_y$$

notably

$$\begin{aligned} n_e^{(-)} + n_e^{(+)} &= n_0^{(-)} + n_0^{(+)} \\ n_0^{(-)} &= \sum_{(-)k} \psi_k^\dagger(\mathbf{r})\psi_k(\mathbf{r}) = \sum_{(+)k} \left(\mathcal{C}\psi_k(r)\right)^\dagger \left(\mathcal{C}\psi_k(r)\right) = n_0^{(+)} \end{aligned}$$

✔ By the same argument

$$\rho^{VP} = \frac{1}{2}\left[\rho_e^{(-)} - \rho_e^{(+)}\right] = \frac{1}{2}\left[\rho_e^{(-)} + \rho_p^{(-)}\right]$$

Basis set requirements

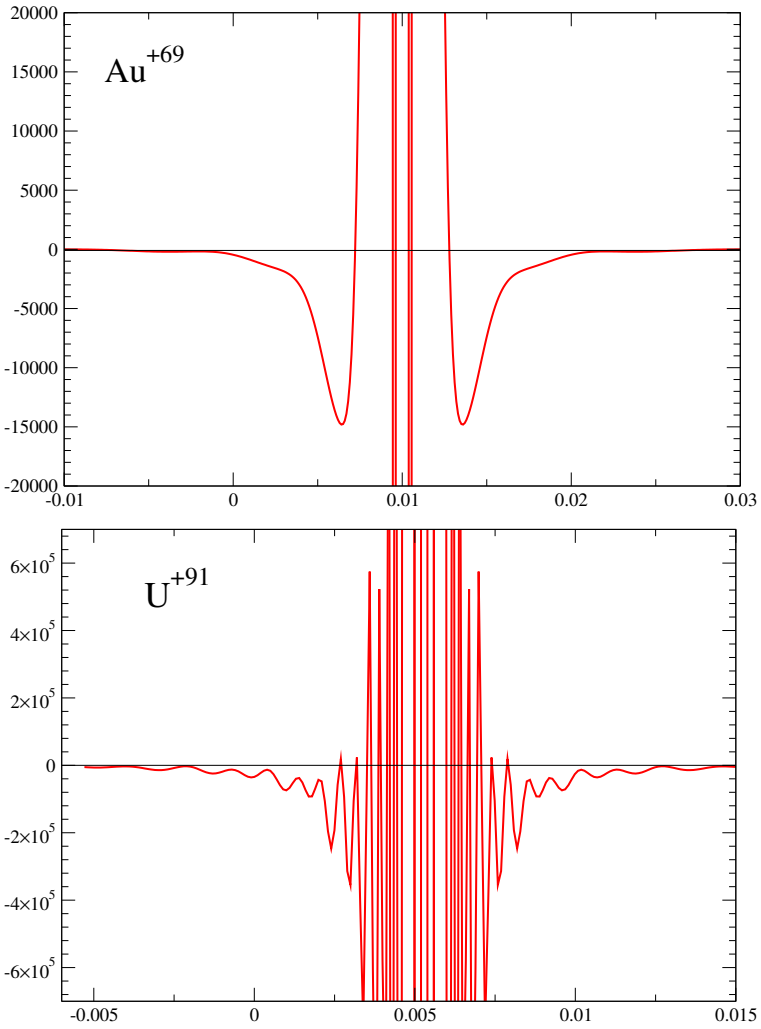
A one-electron system: U^{+91}. Even-tempered basis $\alpha\beta^{N-1}$; $\alpha = 0.00059$; $\beta = 2.05$

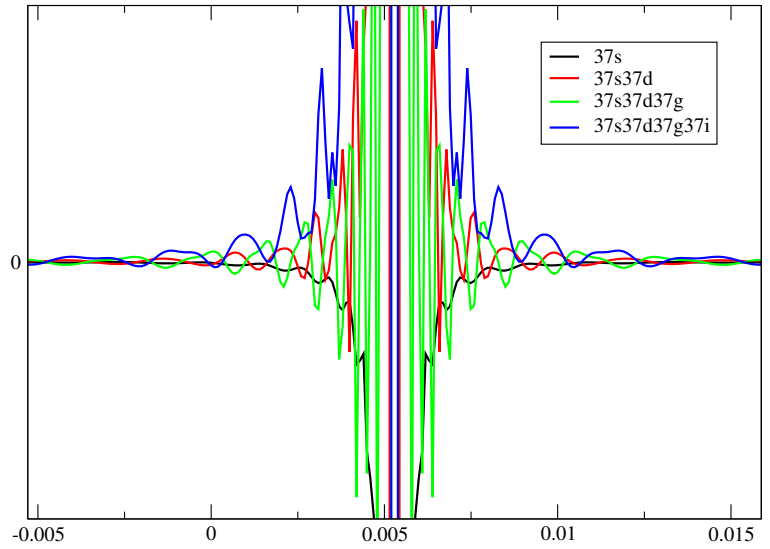
	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$\epsilon_{2s} - \epsilon_{2p}$
Dirac equation	**-4861.197895**	**-1257.395849**	**-1257.395849**	**0.0000**
Dyall_QZ	-4860.335621	-1257.231361	-1257.382703	0.1513
37s37p	-4860.688239	-1257.298511	-1257.385610	0.0871
38s38p	-4860.898540	-1257.338620	-1257.389797	0.0512
39s39p	-4861.022036	-1257.362184	-1257.392247	0.0301
40s40p	-4861.094575	-1257.376016	-1257.393686	0.0177
41s41p	-4861.137188	-1257.384146	-1257.394530	0.0104
42s42p	-4861.162223	-1257.388919	-1257.395025	0.0061
43s43p	-4861.176930	-1257.391725	-1257.395316	0.0036
44s44p	-4861.185571	-1257.393372	-1257.395487	0.0021
45s45p	-4861.190646	-1257.394340	-1257.395587	0.0012
46s46p	-4861.193628	-1257.394909	-1257.395646	0.0007
47s47p	-4861.195379	-1257.395243	-1257.395681	0.0004
47s47p+onepol	-4841.500874	-1254.193066	-1255.430932	1.2379
47s47p+gauss	-4854.158891	-1256.058566	-1257.239387	1.1808

Perturbational vs. variational calculations

		$2s_{1/2}$	$2p_{1/2}$	$\Delta(2s-2p)$
Dirac equation		**-1257.395849**	**-1257.395849**	**0.000000**
standard		-1257.229224	-1257.366880	0.137657
perturbative, -K		-1255.106862	-1256.054236	0.947373
perturbative, +K		-1255.147644	-1256.255674	1.108030
state-specific	orbital energy	-1255.149943	-1256.258773	1.108830
	total energy	-115851.819824	-115852.928229	1.108406
	$E^{(1)}$	-115808.626548	-115808.766011	0.139464
	$E^{(2)}$	-43.1932742	-44.162218	0.968944

A can of worms





Free-particle vacuum polarisation

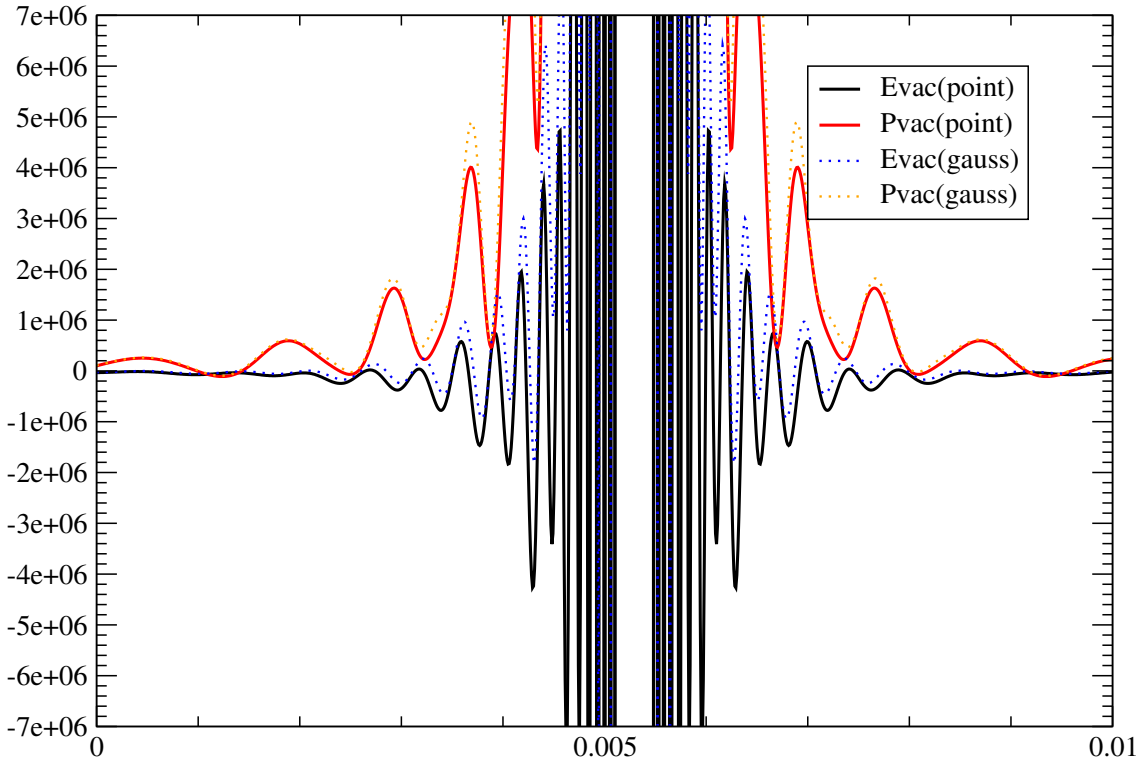
$$n_0^{VP} = n_0^{(-)} - n_0^{(+)}$$

(supposed to be zero...)

A possible solution

✔ The vacuum polarisation can be constructed from positive-energy solutions only

$$n_e^{(-)} + n_e^{(+)} = n_0^{(-)} + n_0^{(+)} \quad \Rightarrow \quad n_e^{(-)} - n_0^{(-)} = n_0^{(+)} - n_e^{(+)} \quad \text{!!!}$$



✔ Are 2-component relativistic calculations including vacuum polarisation possible ???

Conclusions

- ✔ The variational inclusion of vacuum polarisation in 4-component relativistic theory provides a minimisation principle,
- ✔ ... but introduces divergences well-known from quantum field theory.
- ✔ A redefinition of the vacuum polarisation suggests that 2-component relativistic calculations including vacuum polarisation may be possible !
- ✔ A preliminary version of the theory is published in:
  T. Saue and L. Visscher: "Four-component electronic structure methods for molecules"
  in S. Wilson and U. Kaldor (eds.),
  Theoretical Chemistry and Physics of Heavy and Superheavy Elements, Kluwer 2003

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A Coastal Voyage of Current Density Functional Theory

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