On the Scott conjectures for large Coulomb systems

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Mathematical Results of Many-Body Quantum Systems
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Relativistic descriptions I

$$C_{c,Z} := \sqrt{-c^2\Delta + c^4} - c^2 - \frac{Z}{|x|} \quad \text{in } L^2(\mathbb{R}^3 : \mathbb{C}^q)$$

$$D_{c,Z} := -ic\underline{\alpha} \cdot \nabla + c^2\beta - \frac{Z}{|x|} \quad \text{in } L^2(\mathbb{R}^3 : \mathbb{C}^4)$$

with $\underline{\alpha} \cdot \nabla = \sum_{j=1}^3 \alpha_j \partial_{x_j}$, $\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$, and $\beta = \mathrm{diag}(1, 1, -1, -1)$.

For $\gamma := Z/c$ observe $C_{c,Z} \cong c^2 C_{1,\gamma} =: c^2 C_\gamma$ and $D_{c,Z} \cong c^2 D_{1,\gamma} =: c^2 D_\gamma$.

- $C_{c,Z}$ bounded from below if and only if $\gamma \leq \gamma_C := 2/\pi$.
- There is a "physically distinguished" self-adjoint extension of $D_{c,Z}$ if and only if $\gamma \leq 1$.

Relativistic descriptions II

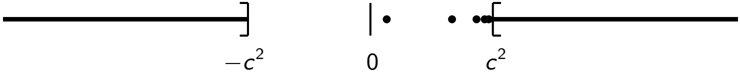
- Description of Z electrons using $C_{c,Z}$ with $\gamma \leq \gamma_C$:

$$H_{C,c,Z} = \sum_{\nu=1}^{Z} (C_{c,Z})_\nu + \sum_{1 \leq \nu < \mu \leq Z} \frac{1}{|x_\nu - x_\mu|} \quad \text{in} \quad \bigwedge_{\nu=1}^{Z} L^2(\mathbb{R}^3 : \mathbb{C}^q).$$

- Extension of $D_{c,Z}$ to a self-adjoint multi-particle operator (Oelker ('19)) possible, **but** the spectrum occupies $\mathbb{R}$ and all eigenvalues (if not already turned into resonances) are embedded:

Brown–Ravenhall disease / continuum dissolution

$\sigma(D_{c,Z})$



Relativistic descriptions III

In Dirac's spirit, Brown–Ravenhall ('51) and Furry–Oppenheimer ('34) proposed to consider $D_{c,Z}$ only in

$$\Lambda_{c,\zeta}(L^2(\mathbb{R}^3:\mathbb{C}^4)) := \mathbb{1}_{(0,\infty)}\left(-ic\underline{\alpha}\cdot\nabla + c^2\beta - \frac{\zeta}{|x|}\right)(L^2(\mathbb{R}^3:\mathbb{C}^4))$$

with $\zeta \in \{0, Z\}$.

For $\psi \in \bigwedge_{\nu=1}^{Z} \Lambda_{c,\zeta}\mathcal{S}(\mathbb{R}^3:\mathbb{C}^4)$ with $\zeta \in \{0, Z\}$ the many-particle energy

$$\left\langle \psi, \left(\sum_{\nu=1}^{Z}\left(D_{c,Z} - c^2\right)_\nu + \sum_{1\leq\nu<\mu\leq Z}\frac{1}{|x_\nu - x_\mu|}\right)\psi\right\rangle$$

is bounded from below if

- $\gamma \leq \gamma_B := 2/(\pi/2 + 2\pi)$ when $\zeta = 0$ (Evans–Perry–Siedentop ('96)),
- $\gamma \leq \gamma_F := 1$ when $\zeta = Z$.

Resulting self-adjoint operators are denoted by

$$H_{B,c,Z} \text{ (when } \zeta = 0,\ \gamma \leq \gamma_B) \quad \text{and} \quad H_{F,c,Z} \text{ (when } \zeta = Z,\ \gamma \leq \gamma_F).$$

Quantities of interest

Let $\# \in \{C, B, F\}$.

- Ground state energy

$$E_{\#,c}(Z) := \inf \operatorname{spec}(H_{\#,c,Z}).$$

- One-particle density of a ground state $\psi \in \bigwedge_{\nu=1}^{Z} L^2(\mathbb{R}^3 : \mathbb{C}^q)$ of $H_{\#,c,Z}$

$$\rho_{\#}(x) := Z \sum_{\sigma=1}^{q} \int_{\Gamma^{Z-1}} |\psi(x,\sigma; y_2, ... y_Z)|^2 \, dy_2 ... dy_Z, \quad x \in \mathbb{R}^3.$$

  Here $\Gamma := \mathbb{R}^3 \times \{1, 2, ..., q\}$ with product measure dy.

- Consider $Z, c \to \infty$ simultaneously with fixed $\gamma = \frac{Z}{c}$ (Schwinger ('80)).

- Predictions for $E_{\#,c}(Z)$ become increasingly accurate as $C \to B \to F$.
  Chemical accuracy for $\# = F$.

Thomas–Fermi theory

$$\mathcal{E}_Z^{\mathrm{TF}}(\rho) := \int_{\mathbb{R}^3} \left(\frac{3}{5} \gamma_{\mathrm{TF}} \rho^{5/3}(x) - \frac{Z}{|x|} \rho(x) \right) dx + D(\rho, \rho)$$

with $\gamma_{\mathrm{TF}} := (6\pi^2/q)^{2/3}/2$ and $D(\rho,\sigma) = 2^{-1} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho(x)\sigma(y)|x-y|^{-1}\, dx\, dy$.

Natural domain: $\mathcal{I} = \{0 \leq \rho \in L^{5/3}(\mathbb{R}^3) : \ D(\rho,\rho) < \infty\}$.

Theorem 1 (Lieb–Simon ('77))

- *$\mathcal{E}_Z^{\mathrm{TF}}$ has a unique minimizer $\rho^{\mathrm{TF}}(Z,\cdot) \in \mathcal{I}$ with $\int \rho^{\mathrm{TF}}(Z,x)\, dx = Z$. Write $E^{\mathrm{TF}}(Z) := \mathcal{E}_Z^{\mathrm{TF}}(\rho^{\mathrm{TF}}(Z,\cdot)) = E^{\mathrm{TF}}(1) \cdot Z^{7/3}$.*
- *Scaling:*

$$\rho^{\mathrm{TF}}(Z,x) = Z^2 \rho^{\mathrm{TF}}(1, Z^{1/3} x).$$

- *Singularity at TF nucleus:*

$$\rho^{\mathrm{TF}}(Z,x) = \left(\frac{Z}{\gamma_{\mathrm{TF}}} \right)^{\frac{3}{2}} |x|^{-3/2} + o_{|x|\to 0}(|x|^{-1/2}).$$

Electrons on the TF scale behave non-relativistically.

(Lieb–Simon ('77), Sørensen ('05), Cassanas–Siedentop ('06), Handrek–Siedentop ('15), M.–Siedentop ('19), M. ('19))

Effects close to the nucleus

Scott ('52): describe the few but innermost electrons using $-\frac{1}{2}\Delta - \frac{Z}{|x|}$:

$$E_{\mathrm{Bohr,non-rel}}(Z) = E^{\mathrm{TF}}_{\mathrm{Bohr}}(Z) + \frac{q}{4}Z^2 + o(Z^2).$$

Scott conjecture (Scott ('52), Lieb ('80), Simon ('84)):

For non-relativistic atoms with electron-electron interactions, Scott's formula holds with $E^{\mathrm{TF}}_{\mathrm{Bohr}}(Z)$ replaced by $E^{\mathrm{TF}}(Z)$.

Ground state density: TF theory predicts

$$\rho_{\#}(x) \sim Z^2(Z^{1/3}|x|) = Z^{3/2}|x|^{-3/2} \quad \text{for } |x| \lesssim Z^{-1/3}.$$

In particular, $\rho_{\#}(Z^{-1}) = \mathcal{O}(Z^3)$.

Strong Scott conjecture (Lieb ('81)):

The ground state density on the length scale Z^{-1} is described by the density of an infinite Bohr atom.

Energy of electrons close to the nucleus

Electrons on the scale Z^{-1} behave relativistically.

The following theorem is due to Frank–Siedentop–Warzel ('08, '09), Solovej–Sørensen–Spitzer ('10), and Handrek–Siedentop ('15).

Theorem 2

Let $\# \in \{C, B, F\}$ and $q = 2$. Then

$$\lim_{Z,c\to\infty} \frac{E_{\#,c}(Z) - \left[E^{\mathrm{TF}}(Z) + \left(\frac{1}{2} - s_\#(\gamma)\right) Z^2\right]}{Z^2} = 0 \quad \textit{for fixed } \frac{Z}{c} < \gamma_\#$$

with the spectral shift

$$[0, \gamma_\#] \ni \gamma \mapsto s_\#(\gamma) := \gamma^{-2} \sum_{n \geq 0} \left(\lambda_n^S(\gamma) - \lambda_n^\#(\gamma)\right) \geq 0$$

between $-\frac{1}{2}\Delta - \frac{\gamma}{|x|}$ and the respective relativistic hydrogen operator.

Inspection of hydrogenic densities I

Let $\psi_n^{\#}$ denote the normalized eigenfunctions of $C_\gamma \otimes 1_{\mathbb{C}^2}$ or D_γ. Define

$$\rho_{\#}^{H}(x) := \sum_{n=0}^{\infty} |\psi_n^{\#}(x)|^2, \quad x \in \mathbb{R}^3, \quad \# \in \{C, F\}.$$

Do the limits $\rho_{\#}^{H}$ even exist? And in which sense?

Introduce

$$\begin{aligned} \sigma_{\gamma,C} &:= \Phi^{-1}(\gamma) \in [0,1] &\quad& \text{for } \gamma \in [0, 2/\pi], \\ \sigma_{\gamma,F} &:= 1 - \sqrt{1-\gamma^2} \in [0,1] && \text{for } \gamma \in [0,1], \end{aligned}$$

where $[0,1] \ni \sigma \mapsto \Phi(\sigma) := (1-\sigma)\tan\frac{\pi\sigma}{2} \in [0, 2/\pi]$ is monotone increasing with $\Phi(0) = 0$ and $\Phi(1) = 2/\pi$.

Remark: $\lim_{|x|\to 0} |x|^{\sigma_{\gamma,F}} \psi_0^F(x) = \mathrm{const}$ (believed to be true also for $\# = C$)

Inspection of hydrogenic densities II

Theorem 3 (Frank–M.–Siedentop–Simon ('20), M.–Siedentop ('22))
Let $\gamma_{C,t} := (1+\sqrt{2})/4$ *and* $\gamma_{F,t} := \sqrt{15}/4$. *Then for* $\# \in \{C, F\}$ *and any* $\varepsilon > 0$ *there are constants* $A_\gamma, A_{\gamma,\varepsilon} > 0$ *such that for all* $x \in \mathbb{R}^3$,

$$\rho_\#^H(x) \leq \begin{cases} A_\gamma |x|^{-3/2} & \text{if } \gamma \in (0, \gamma_{\#,t}), \\ A_{\gamma,\varepsilon}(|x|^{-2\sigma_{\gamma,\#}-\varepsilon}\mathbb{1}_{\{|x|\leq 1\}} + |x|^{-3/2}\mathbb{1}_{\{|x|>1\}}) & \text{if } \gamma \in [\gamma_{\#,t}, \gamma_\#) \end{cases}.$$

Remarks & questions (cf. Heilmann–Lieb ('95)):

(1) $\sigma_{(1+\sqrt{2})/4,C} = \sigma_{\sqrt{15}/4,F} = 3/4$ technical.

(2) Bounds for $|x| < 1$ and $\gamma < \gamma_{\#,t}$ presumably not optimal.

(3) $\lim_{|x|\to 0} |x|^{2\sigma_{\gamma,\#}} \rho_\#^H(x) = \mathrm{const}$?

(4) $\lim_{|x|\to\infty} |x|^{3/2}\rho_\#^H(x) = \lim_{|x|\to 0} |x|^{3/2}\rho^{\mathrm{TF}}(1,x)$?

(5) Monotonicity?

Strong Scott conjecture

Theorem 4 (Frank–M.–Siedentop–Simon ('20), M.–Siedentop ('22))

Let $\varepsilon > 0$ *and* $U \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ *satisfy* $|U(r)| \lesssim r^{-1}\mathbb{1}_{\{r\leq 1\}} + r^{-\frac{3}{2}-\varepsilon}\mathbb{1}_{\{r\geq 1\}}$.
Then for $\# \in \{C, F\}$,

$$\lim_{Z,c\to\infty} \int_{\mathbb{R}^3} c^{-3}\rho_{\#}(c^{-1}x)U(|x|)\,dx = \int_{\mathbb{R}^3} \rho^H_{\#}(x)U(|x|)\,dx \quad \textit{for fixed } \frac{Z}{c} < \gamma_{\#}.$$

Remarks:

- Singularity of U cannot be worse than $|x|^{-1}$ (Kato's inequality).
- $|x|^{-3/2-\varepsilon}$-decay optimal in view of the $|x|^{-3/2}$-decay of $\rho^H_{\#}$.
- Pointwise convergence for $|x|>0$? (cf. Iantchenko–Lieb–Siedentop ('96))

Linear response argument (Chandrasekhar, $q = 1$)

For a ground state $\psi \in \bigwedge_{\nu=1}^{Z} L^2(\mathbb{R}^3)$ of $H_{C,c,Z}$, consider

$$\varrho_{\ell,C}(r) := N r^2 \sum_{m=-\ell}^{\ell} \int_{\mathbb{R}^{3(Z-1)}} \left| \int_{\mathbb{S}^2} \overline{Y_{\ell,m}(\omega)} \psi(r\omega, x_2, ..., x_Z) \right|^2 dx_2 ... dx_Z .$$

For $\lambda \in \mathbb{R}$ sufficiently small, let $H_{C,c,Z,\lambda} := H_{C,c,Z} - \lambda \sum_{\nu=1}^{Z} c^2 U(c|x_\nu|) \Pi_{\ell,\nu}$.
W.l.o.g. $U \geq 0$, and $\lambda > 0$. By the Scott correction,

$$\overline{\lim_{Z\to\infty}} \int_0^\infty c^{-3} \varrho_{\ell,C}(r/c) U(r)\, dr = \frac{1}{2\ell+1} \lim_{\lambda \searrow 0} \overline{\lim_{Z\to\infty}} \operatorname{Tr}\left[\frac{|\psi\rangle\langle\psi|(H_{C,c,Z} - H_{C,c,Z,\lambda})}{\lambda c^2} \right]$$
$$\leq \underline{\lim}_{\lambda\searrow 0} \frac{\operatorname{Tr}(C_{\ell,\gamma} - \lambda U(r))_- - \operatorname{Tr}(C_{\ell,\gamma})_-}{\lambda}$$

with

$$C_{\ell,\gamma} := \sqrt{-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + 1} - 1 - \frac{\gamma}{r} \text{ in } L^2(\mathbb{R}_+, dr).$$

Goal: Interchange $\liminf_{\lambda\searrow 0}$ and Tr to apply the Hellmann–Feynman theorem, **or** compute the derivative!

Hellmann–Feynman theorem for eigenvalue sums

Theorem 5 (Frank–M.–Siedentop–Simon ('20))

Assume that A is self-adjoint with A_- trace class.

Assume that B is non-negative, relatively form bounded with respect to A, and that that there is $1/2 \leq s \leq 1$ such that for some $M > |\inf \operatorname{spec}(A)|$,

(a) $(A+M)^{-s}B(A+M)^{-s}$ *is trace class and*

(b) $\limsup_{\lambda \to 0} \left\|(A+M)^s(A-\lambda B+M)^{-s}\right\| < \infty$ *when $s > 1/2$.*

Then the one-sided derivatives of $\lambda \mapsto S(\lambda) := \operatorname{Tr}(A-\lambda B)_-$ satisfy

$$\operatorname{Tr} B\mathbb{1}_{(-\infty,0)}(A) = D^- S(0) \leq D^+ S(0) = \operatorname{Tr} B\mathbb{1}_{(-\infty,0]}(A).$$

In particular, $S(\lambda)$ is differentiable at $\lambda = 0$, if and only if $B|_{\ker A} = 0$.

Application:

In $L^2(\mathbb{R}_+, dr)$ take $A = C_{\ell,\gamma}$ and $B = U$ with $|U(r)| \lesssim r^{-1}\mathbb{1}_{r<1} + r^{-\frac{3}{2}-\varepsilon}\mathbb{1}_{r>1}$.

Application of generalized Hellmann–Feynman

Decisive inequality (Frank– M.–Siedentop ('21)): Write $|p| := \sqrt{-\Delta}$.
For $0 \leq V \leq \gamma/|x|$ with $\gamma \leq 2/\pi$ and $0 < s < 3/2 - \sigma_{\gamma,C}$, we have

$$|p|^{2s} \sim (|p| - V)^{2s}. \qquad \text{(FMS)}$$

$\Rightarrow (C_{\ell,\gamma} + M)^{2s} \sim (C_{\ell,0} + M)^{2s}$ for $M > |\inf \operatorname{spec}(C_{\ell,\gamma})|$, uniformly in ℓ.

- Comparibility condition (b) in Theorem 5 is immediate.
- Relative trace class condition (a) in Theorem 5:

$$\begin{aligned}
&\|U^{1/2}(C_{\ell,\gamma} + M)^{-s}\|_2^2 \sim \|U^{1/2}(C_{\ell,0} + M)^{-s}\|_2^2 \\
&= \int_0^\infty dr\ U(r) \int_0^\infty dk\ \frac{krJ_{\ell+1/2}(kr)^2}{(\sqrt{k^2+1} - 1 + M)^{2s}} \lesssim \|rU\|_\infty.
\end{aligned}$$

Remark:
Since $(k+1)^{-1} \notin L^1(\mathbb{R}_+, dk)$, we must take $s > 1/2$, no matter what $U(r)$ is.

Strategy for the Furry operator

Main idea: verify the assumptions of the Hellmann–Feynman theorem in terms of F_γ by rolling them back to assumptions in terms of C_γ.
Doable since D_γ (the effective one-particle operator) commutes with Furry projection.

Decisive inequalities:

(1) If $\gamma \in (0,1)$ and $0 < s < \min\{3/2 - \sigma_{\gamma,F}, 1\}$, then

$$\Lambda_\gamma |p|^{2s} \Lambda_\gamma \lesssim_{s,\gamma} (F_\gamma + 1)^{2s}$$

where $\Lambda_\gamma := \mathbb{1}_{(0,\infty)}(D_\gamma)$.

(2) Davis–Sherman inequality ('57):
Let P be an orthogonal projection and $A \geq 0$ be a linear operator. Then

$$(PAP)^{2s} \leq PA^{2s}P, \qquad s \in [1/2, 1].$$

Application: Comparibility condition (b) in Theorem 5. For $U, \lambda \geq 0$,

$$(F_\gamma + 1 - \lambda\Lambda_\gamma U\Lambda_\gamma + \lambda\Lambda_\gamma U\Lambda_\gamma)^{2s} \lesssim (F_\gamma + 1 - \lambda\Lambda_\gamma U\Lambda_\gamma)^{2s} + \lambda^{2s}\Lambda_\gamma \underbrace{U^{2s}}_{\lesssim |p|^{2s}} \Lambda_\gamma$$

Bounds for ρ_C^H I

Let $d_{\ell,C}^H = \mathbb{1}_{(-\infty,0)}(C_{\ell,\gamma})$. Then $\rho_C^H(r) = r^{-2}\sum_{\ell=0}^\infty (2\ell+1)\,\mathrm{Tr}(d_{\ell,C}^H\delta_r)$ for $r>0$.

Suffices to estimate

$$\mathrm{Tr}(d_{\ell,C}^H\delta_r) = \mathrm{Tr}\,ACA^*$$

where

$$A = d_{\ell,C}^H(C_{\ell,\gamma}+a_\ell)^s \quad \text{with} \quad a_\ell = a_\gamma(\ell+1/2)^{-2}$$
$$C = (C_{\ell,\gamma}+a_\ell)^{-s}\delta_r(C_{\ell,\gamma}+a_\ell)^{-s}$$

with $s\in(1/2,1]$. One has $\|A\| \lesssim (\ell+1/2)^{-2s}$.

How to estimate $\mathrm{Tr}\,C = (C_{\ell,\gamma}+a_\ell)^{-2s}(r,r)$ for $r>0$?

Bounds for ρ_C^H II

How to estimate $\mathrm{Tr}\, C = (C_{\ell,\gamma} + a_\ell)^{-2s}(r,r)$ for $r > 0$?

If $\gamma < \ell + \frac{1}{2}$, then $\left(\frac{\gamma}{r}\right)^2 < p_\ell^2$ with $p_\ell = \sqrt{-d_r^2 + \ell(\ell+1)r^{-2}}$ (Hardy)
$\Rightarrow (C_{\ell,\gamma} + a_\ell)^{-2s} \sim (C_{\ell,0} + a_\ell)^{-2s}$ uniformly in ℓ.
$\Rightarrow$ Bounds for $(C_{\ell,0} + a_\ell)^{-2s}(r,r)$ suffice. Could only prove them for $s \leq 3/4$.

If $\gamma \in [1/2, 2/\pi]$:

- For $\ell \geq 1$: Use bounds for $(C_{\ell,0} + a_\ell)^{-2s}(r,r)$ since $\frac{2}{\pi} < \ell + \frac{1}{2}$.
- For $\ell = 0$: (FMS) allows to show $\rho_\#^H(r)\mathbb{1}_{\{r<1\}} \lesssim r^{2s-3}$ for $\gamma \geq \gamma_{\#,t}$.
  Hence, the ε-loss is due to the requirement $s < 3/2 - \sigma_\gamma$.
  For $\gamma \geq \gamma_{\#,t}$, the requirement $s \leq 3/4$ is automatically fulfilled.

Bounds for ρ_C^H III

Alternatively:

- For $\ell \geq 1$: bound $\|(C_{\ell,\gamma}+a_\ell)^{-s} d_{\ell,C}^H (p_\ell^2/2-\gamma/r+a_\ell)^s\|$. Take $s=1/2$ and estimate $(p_\ell^2/2-\gamma/r+a_\ell)^{-1}(r,r)$. (Getting rid of Coulomb is easy)
- For $\ell=0$: estimate $(C_{\ell,\gamma}+a)^{-2s} \sim (p_\ell-\gamma/r+a)^{-2s}$.
Obtain bounds for kernel of RHS using

$$(|p|-\gamma/|x|+a)^{-2s} = \frac{1}{\Gamma(2s)} \int_0^\infty \frac{dt}{t} t^{2s} \mathrm{e}^{-t(|p|-\gamma/|x|+a)}$$

and heat kernel bounds (Bogdan–Grzywny–Jakubowski–Pilarczyk ('19))

$$\exp(-t(|p|-\gamma/|x|))(x,y) \sim \left(1+\frac{t}{|x|}\right)^{\sigma_{\gamma,C}} \left(1+\frac{t}{|y|}\right)^{\sigma_{\gamma,C}} \cdot \frac{t}{(t^2+|x-y|^2)^2}.$$

Leads to

$$\rho_\#^H(x) \lesssim_\gamma \begin{cases} |x|^{-1}\mathbb{1}_{\{|x|\leq 1\}} + |x|^{-3/2}\mathbb{1}_{\{|x|\geq 1\}} & \text{if } \gamma \in (0,\gamma_{\#,e}), \\ |x|^{-2\sigma_{\gamma,\#}}\mathbb{1}_{\{|x|\leq 1\}} + |x|^{-3/2}\mathbb{1}_{\{|x|>1\}} & \text{if } \gamma \in [\gamma_{\#,e},\gamma_\#) \end{cases}$$

with $\gamma_{C,e}=1/2$ and $\gamma_{F,e}=\sqrt{3}/2$.

Some open questions

(1) Previous questions regarding $\rho_{\#}^{H}$. (Power law at $|x| = 0$, asymptotics for $|x| \to \infty$, monotonicity.)

(2) Scott conjectures for no-pair operators where a (not necessary local) mean field χ is taken into account? (Fuzzy operator)

Possible choices for χ are the Thomas–Fermi potential, or Hartree–Fock potentials generated by a set of appropriately chosen orbitals.

Hilbert space: $\Lambda_\chi(L^2(\mathbb{R}^3 : \mathbb{C}^4))$ with $\Lambda_\chi := \mathbb{1}_{(0,\infty)}(D_{c,Z} + \chi)$.

Yet another example for a choice of the vacuum:
Mittleman operator: Define vacuum by P in the set $\mathcal{S}$ of all orthogonal projectors leaving $\mathrm{dom}(D_{c,Z})$ invariant which solves

$$\sup_{P \in \mathcal{S}} \inf_{\substack{-P \le \gamma \le 1-P \\ \gamma P = P\gamma \\ \mathrm{Tr}\,\gamma = N}} \left(\mathrm{Tr}(D_{c,Z}\gamma) + D[\rho_\gamma] - \frac{1}{2} \int \frac{|\gamma(x,y)|^2}{|x-y|} dx\, dy \right).$$

THANK YOU FOR LISTENING!

Comparison of energies I

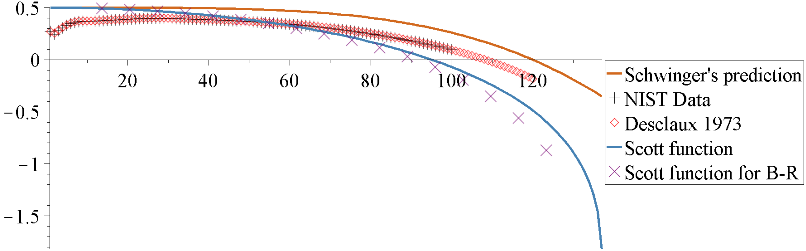


Figure: Plot of the Scott function $1/2 - s_{\#}(Z/137)$ (Handrek–Siedentop ('15))

Comparison of energies II

Graphical representation of

- $(E_{\mathrm{NIST}}(Z) - E^{\mathrm{TF}}(Z))/Z^2$ (measured only to small extent; majority of energies for large Z is extrapolated or computed, i.e., assumptions on underlying approximate mathematically uncontrolled models influence those data. In addition the experimental values obviously also contain other QED effects not contained in the Furry Hamiltonian.)
- $\frac{1}{2} - s_D(Z/137)$ (validity proved only in asymptotic regime $Z, c \to \infty$ with $Z/c < 1$ fixed); observe $\lim_{\gamma\to 1}\left(\frac{1}{2} - s_D(\gamma)\right) \approx -1.91$.
- $\frac{1}{2} - s_B(Z/137)$ (validity proved only in asymptotic regime $Z, c \to \infty$ with $Z/c < \gamma_B$ fixed)
- Schwinger's prediction ('80): γ^4-correction of non-relativistic hydrogen eigenvalues through the second term of the perturbative expansion of the kinetic energy $\langle\psi, \frac{-p^4}{8}\psi\rangle$, the spin-orbit coupling $\langle\psi, \frac{\gamma}{2} S\cdot L\,\frac{1}{|x|^3}\psi\rangle$, and the Darwin term $\langle\psi, \frac{\pi}{2}\gamma\delta(x)\psi\rangle$. This leads to the eigenvalue correction $\delta\lambda_{n,\ell,j} = \frac{\gamma^4}{-2(n+\ell)^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3/4}{n+\ell}\right)$ and the spectral shift $s_{\mathrm{Schwinger}}(\gamma) = \left(\frac{5\pi^2}{24} - \zeta(3)\right)\gamma^2 \approx -0.854\gamma^2$.
- Dirac–Hartree–Fock computations by Desclaux ('73)

Relativistic ground state densities