On the Ultraviolet Limit of the Pauli–Fierz Hamiltonian in LL- and in BHF-Approximation

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Contents

- We consider a free nonrelativistic spinless particle minimally coupled to the quantized radiation field.
- The *Hilbert space* of the model is

$$\mathcal{H} = \mathfrak{h}_{\mathrm{el}} \otimes \mathcal{F}_{\mathrm{ph}} , \quad \mathfrak{h}_{\mathrm{el}} := L^2(\mathbb{R}^3_x) \ \Rightarrow \ \mathcal{H} \simeq L^2(\mathbb{R}^3_x; \mathcal{F}_{\mathrm{ph}}) ,$$

$$\mathcal{F}_{\mathrm{ph}} \ = \ \mathbb{C}\,\Omega \oplus \bigoplus_{n=1}^{\infty} \mathfrak{h}_{\mathrm{ph}}^{\otimes_{sym} n} , \quad \mathfrak{h}_{\mathrm{ph}} \ = \ L^2(\mathbb{R}^3 \times \mathbb{Z}_2) .$$

- On $\mathcal{F}_{\mathrm{ph}}$ we have the usual CCR, i.e.,

$$[a_k, a_{k'}] \ = \ [a_k^*, a_{k'}^*] \ = \ 0,$$
$$[a_k, a_{k'}^*] \ = \delta(k - k') , \quad a_k \Omega \ = \ 0 ,$$

$\forall\, k = (\vec{k}, \tau), k' = (\vec{k}', \tau') \in \mathbb{R}^3 \times \mathbb{Z}_2$, with vacuum $\Omega \in \mathcal{F}_{\mathrm{ph}}$.

- The Hamiltonian $H_{\alpha,\Lambda} := H^*_{\alpha,\Lambda}$ is given by

$$H_{\alpha,\Lambda} := \frac{1}{2m_{\rm el}} \big\{ \tfrac{1}{i} \vec{\nabla}_x + \sqrt{\alpha} \vec{A}_\Lambda(\vec{x}) \big\}^2 + H_{\rm ph}$$

on $\mathcal{D} \subseteq \mathcal{H}$, where

$$H_{\rm ph} = \int |k| \, a_k^* \, a_k \, d^3k,$$

$$\vec{A}_\Lambda(\vec{x}) = \int_{|k| \leq \Lambda} \big\{ e^{-i\vec{k}\cdot\vec{x}} a_k^* + e^{i\vec{k}\cdot\vec{x}} a_k \big\} \, \frac{\vec{\varepsilon}_k}{|k|^{1/2}} \, \frac{dk}{(2\pi)^{3/2}} \, ,$$

- $m_{\rm el} = 1$ is the electron mass, and

$$0 < \alpha \ll 1 \quad \text{fine structure constant,}$$
$$1 \ll \Lambda < \infty \quad \text{UV Cutoff.}$$

- The magnetic vector potential $\vec{A}_\Lambda(\vec{x})$ can be written as

$$\vec{A}_\Lambda(\vec{x}) := a^*(\vec{G}_x) + a(\vec{G}_x)\,, \quad \text{with}$$
$$\vec{G}_x(k) := \frac{\mathbf{1}(|k| \le \Lambda)\, \vec{\varepsilon}_k\, e^{-i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}|k|^{1/2}}\,.$$

- Here, $\{\vec{\varepsilon}_{k,+}\,,\, \vec{\varepsilon}_{k,-}\,,\, \frac{\vec{k}}{|\vec{k}|}\} \subseteq \mathbb{R}^3$ is an ONB, for all $\vec{k} \neq \vec{0}$,
- According to Maxwell theory, the one-photon space consists of divergence-free vector fields,

$$\mathfrak{h}'_{\mathrm{ph}} = \{\vec{f} \in L^2(\mathbb{R}^3; \mathbb{C}^3) \big| \forall\, \vec{k} :\ \vec{k} \cdot \vec{f}(\vec{k}) \equiv 0\}\,,$$

  but the CCR become very complicated to express for $\mathcal{H}'_{\mathrm{ph}}$, and it is customary to use $\mathfrak{h}_{\mathrm{ph}} \simeq \mathfrak{h}'_{\mathrm{ph}}$ instead and write $\vec{f}(k) = f_{k,+}\vec{\varepsilon}_{k,+} + f_{k,-}\vec{\varepsilon}_{k,-}$, for some fixed measurable choice of $\vec{\varepsilon}_{k,\pm} \perp \vec{k}$.

- The ground state energy of the system is

$$E_{\rm gs}(\alpha, \Lambda) \;:=\; \inf \Big\{ \langle \Psi \,|\, H_{\alpha,\Lambda} \Psi \rangle \;\Big|\; \Psi \in \mathcal{H}, \;\; \|\Psi\| = 1 \Big\} \;\geq\; 0\,.$$

- For fixed $\Lambda < \infty$, many results have been derived in the past 30 years, e.g.,
  - self-adjointness and domain of $H_{\alpha,\Lambda}$ [Hiroshima 99, Hasler+Herbst 10] or
  - existence of ground states of $H_{\alpha,\Lambda}$ [Griesemer+Lieb+Loss 00, B+Chen+Fröhlich+Sigal 06].

- Physics require $\Lambda = \infty$, but $H_{\alpha,\Lambda} \geq 0$ is a well-defined operator (with a dense domain) only for $\Lambda < \infty$.
- One is hence interested in the UV limit $\Lambda \to \infty$. This is a difficult problem that has been considered for various approximative models, e.g.,
  - the Nelson model [Gross 62, Nelson 64],
  - the Fröhlich Hamiltonian [Griesemer+Linden 19, Lampart 20], and
  - effective mean-field theories [Hainzl+Lewin+Solovej 07, Gravejat+Lewin+Séré 09, 18].

- Joint work with **Alexander Hach.**
- The Lieb-Loss energy is defined by

$$E_{\mathrm{LL}}(\alpha,\Lambda) := \inf\Big\{\mathcal{E}_{\alpha,\Lambda}(\phi,\psi)\,\Big|\,\phi\in\mathfrak{h}_{\mathrm{el}}\,,\ \psi\in\mathcal{F}_{\mathrm{ph}}\,,\ \|\phi\|=\|\psi\|=1\Big\},$$

where

$$\mathcal{E}_{\alpha,\Lambda}(\phi,\psi) := \langle\phi\otimes\psi\,|H_{\alpha,\Lambda}(\phi\otimes\psi)\rangle = \frac{1}{2}\|\vec{\nabla}\phi\|_2^2 + \Big\langle\psi\Big|\,\mathbb{H}\big(|\phi|^2,\,\mathrm{Im}\{\overline{\phi}\,\vec{\nabla}\phi\}\big)\psi\Big\rangle_{\mathcal{F}},$$

$$\mathbb{H}[\rho,\vec{v}] := H_{\mathrm{ph}} + \frac{\alpha}{2}\int\rho(x)\,\vec{A}_\Lambda^2(x)\,d^3x + \sqrt{\alpha}\int\vec{v}(x)\cdot\vec{A}_\Lambda(x)\,d^3x\,.$$

- Thm 1 [Lieb+Loss 99]: There are $0 < C_1, C_2 < \infty$ such that

$$C_1\, \alpha^{1/2}\, \Lambda^{3/2} \;\leq\; E_{\rm gs}(\alpha, \Lambda) \;\leq\; E_{\rm LL}(\alpha, \Lambda) \;\leq\; C_2\, \alpha^{2/7}\, \Lambda^{12/7}\,.$$

- Second-order perturbation theory about $\phi_0 \otimes \Omega$ yields $E_{\rm gs}(\alpha, \Lambda) \sim C\alpha\Lambda^2$, so Thm 1 implies that perturbation theory is misleading.
- Thm 1 does not take mass renormalization $m_{\rm el} \equiv m_{\rm el}(\Lambda)$ into account, and it cannot be used to compute counterterm explicitly.
- Lieb + Loss have extended Thm 1.
- related to Polaron Model [Griesemer+Møller 10] and recent results in [Breteaux+Faupin+Payet 22].

- Introduce an auxiliary functional

$$\mathcal{F}_1(\phi) \;:=\; \frac{1}{2}\|\vec{\nabla}\phi\|_2^2 + \frac{8\pi\sqrt{2}}{3}\,\|\phi\|_1\,,$$

for $\phi \in Y := H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$. We show that

$$F_1 \;:=\; \inf\left\{\mathcal{F}(\phi) \,\middle|\, \phi \in Y\,,\; \|\phi\|_2 = 1\right\} \;>\; 0\,,$$

- Thm 2 [B+Hach 11]: There is $C < \infty$ and $\delta > 0$ such that

$$\left| \frac{E_{\mathrm{LL}}(\alpha, \Lambda)}{F_1 \alpha^{2/7} \Lambda^{12/7}} \;-\; 1 \right| \;\leq\; C\,\alpha^{\delta}\,\Lambda^{-6\delta}\,.$$

- The Hamiltonian $H_{\alpha,\Lambda}$ commutes with the total momentum operator $\vec{P}_{\rm tot} = -i\vec{\nabla}_x + \vec{P}_{\rm ph}$, where

$$\vec{P}_{\rm ph} \ = \ \int \vec{k} \, a_k^* \, a_k \, dk$$

  is the photon field momentum operator. Hence $\vec{P}_{\rm tot}$ and $H_{\alpha,\Lambda}$ can be diagonalized simultaneously.
- This is implemented by a suitable unitary operator $U : L^2(\mathbb{R}^3_x; \mathcal{F}_{\rm ph}) \to L^2(\mathbb{R}^3_p; \mathcal{F}_{\rm ph})$ which yields

$$U \, H_{\alpha,\Lambda} \, U^* \ = \ \int_{\mathbb{R}^3_p}^{\oplus} H_{\alpha,\Lambda}(\vec{p}) \, d^3p \, ,$$

$$H_{\alpha,\Lambda}(\vec{p}) \ = \frac{1}{2}\big\{ \vec{P}_{\rm ph} - \vec{p} + \sqrt{\alpha}\vec{A}_\Lambda(\vec{0}) \big\}^2 + H_{\rm ph} \, .$$

- Recall that the direct integral representation $M = \int^{\oplus} m(p)\, d^3p$ of an operator M on $L^2(\mathbb{R}^3; \mathfrak{F})$ means that $[M\psi](p) = m(p)\psi(p)$, for all $\psi \in L^2(\mathbb{R}^3; \mathfrak{F})$.
- By unitarity of U, we have that

$$
\begin{aligned}
E_{\rm gs}(\alpha, \Lambda) \;&=\; \inf \big\{ \sigma[H_{\alpha,\Lambda}] \big\} \;=\; \inf \big\{ \sigma[U\, H_{\alpha,\Lambda} U^*] \big\} \\
&=\; \inf_{\vec{p} \in \mathbb{R}^3} \big\{ \inf \sigma[H_{\alpha,\Lambda}(\vec{p})] \big\} \,.
\end{aligned}
$$

- $E_{\rm gs}(\alpha, \Lambda) = \inf \sigma[H_{\alpha,\Lambda}(\vec{0})]$ is plausible, but not proved.
- Note that $H_{\alpha,\Lambda}(\vec{p})$ is not quadratic in the fields,

$$
\begin{aligned}
2\, H_{\alpha,\Lambda}(\vec{p}) \;=\; & \underbrace{\vec{P}_{\rm ph}^{\,2}}_{\rm deg=4} + \underbrace{2\sqrt{\alpha}\vec{A}_\Lambda(\vec{0}) \cdot \vec{P}_{\rm ph}}_{\rm deg=3} + \\
& \underbrace{2\sqrt{\alpha}\vec{p} \cdot \vec{P}_{\rm ph} + \vec{A}_\Lambda(\vec{0})^{\,2} + 2H_{\rm ph}}_{\rm deg=2} + \underbrace{2\sqrt{\alpha}\vec{p} \cdot \vec{A}_\Lambda(\vec{0})}_{\rm deg=1} + \underbrace{\vec{p}^{\,2}}_{\rm deg=0} \,.
\end{aligned}
$$

- Joint work with **Matthias Herdzik.**
- We cannot explicitly compute $\inf \sigma[H_{\alpha,\Lambda}(\vec{p})]$, so we approximate it by the BHF energy

$$E_{\mathrm{BHF}}(\alpha, \Lambda, \vec{p}) := \inf \Big\{ \mathrm{Tr}\big[\rho\, H_{\alpha,\Lambda}(\vec{p})\big] \ \Big|\ \rho \geq 0\,,\ \mathrm{Tr}(\rho) = 1\,,\ \rho \text{ is quasifree} \Big\}$$
$$\geq \inf \Big\{ \mathrm{Tr}\big[\rho\, H_{\alpha,\Lambda}(\vec{p})\big] \ \Big|\ \rho \geq 0\,,\ \mathrm{Tr}(\rho) = 1 \Big\} = \inf \sigma[H_{\alpha,\Lambda}(\vec{p})]\,,$$

- BHF energy was defined in [B+Breteaux+Tzaneteas 13], and it was shown that

$$E_{\mathrm{BHF}}(\alpha, \Lambda, \vec{p}) = \inf_{\eta, B} \Big\{ \big\langle \Omega \big|\, U_B^* \, W_\eta^* \, H_{\alpha,\Lambda}(\vec{p}) \, W_\eta \, U_B \Omega \big\rangle \Big\}$$

where U_B and W_η vary over all (hom.) Bogoliubov transformations and all Weyl operators, resp.

- More explicitly, for a fixed antiunitary involution J on $\mathfrak{h}_{\rm ph}$,

$$U_B^* \, W_\eta^* \, a^*(f) \, W_\eta \, U_B \;=\; a^*(uf) + a(Jvf) + \langle \eta | f \rangle \, ,$$

where $B \equiv B(u, v) = \left(\begin{smallmatrix} u & jvj \\ v & juj \end{smallmatrix} \right)$ fulfills $v \in \mathcal{L}^2(\mathfrak{h}_{\rm ph})$ and

$$B^* \left(\begin{smallmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{smallmatrix} \right) B \;=\; B \left(\begin{smallmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{smallmatrix} \right) B^* \;=\; \left(\begin{smallmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{smallmatrix} \right) .$$

- The BHF energy at $\vec{p} = \vec{0}$ becomes the infimum of the BHF energy functional

$$E_{\rm BHF} \;\equiv\; E_{\rm BHF}(\alpha, \Lambda, \vec{0}) \;=\; \inf_{u,v;\eta} \left\{ \mathcal{E}_{\rm BHF}[u, v; \eta] \right\} ,$$

$$\mathcal{E}_{\rm BHF}[u, v; \eta] \;:=\; \langle \Omega | \, U_B^* W_\eta^* H_{\alpha,\Lambda}(\vec{0}) W_\eta U_B \Omega \rangle \, .$$

- Working out the expectation value, one obtains [B+Breteaux+Tzaneteas 13, Herdzik 22]

$$\begin{aligned}
\mathcal{E}_{\mathrm{BHF}}[u, v; \eta] \;=\; & \langle \Omega | U_B^* W_\eta^* H_{\alpha,\Lambda}(\vec{0}) W_\eta U_B \Omega \rangle \\
= & \frac{1}{2} \sum_{\nu=1}^{3} \Big(\mathrm{Tr}[k_\nu v^* v] + \langle \eta | k_\nu \eta \rangle + 2 \, \mathrm{Re} \langle \eta | G_\nu \rangle \Big)^2 \\
& + \frac{1}{2} \sum_{\nu=1}^{3} \Big\{ \mathrm{Tr}[(v^* J u k_\nu)^2] + \mathrm{Tr}[k_\nu v^* v k_\nu (\mathbf{1} + v^* v)] \\
& \qquad + \langle G_\nu + k_\nu \eta | (1 + 2 v^* v)(G_\nu + k_\nu \eta) \rangle \Big\} \\
& + \mathrm{Tr}\left(|k| v^* v \right) + \big\langle \eta \big| \, |k| \eta \big\rangle \, .
\end{aligned}$$

- Thm 3 [B+Herdzik 23]: Choose the antiunitary $J : \mathfrak{h}_{\mathrm{ph}} \to \mathfrak{h}_{\mathrm{ph}}$ as $[J\psi](\vec{k}, \pm) := \overline{\psi(\vec{k}, \pm)}$. Then

$$E_{\mathrm{BHF}} = \inf \left\{ \mathcal{E}_{\mathrm{BHF}}\left[\sqrt{1+v^2},\ v; \eta\right] \,\middle|\, v \in \mathcal{L}^2(\mathfrak{h}_{\mathrm{ph}}),\ v \geq 0,\ \eta \in \mathfrak{h}_{\mathrm{ph}} \right\},$$

and

$$\begin{aligned} \mathcal{E}_{\mathrm{BHF}}\left[\sqrt{1+v^2},\ v; \eta\right] &= \mathrm{Tr}\left(|k| v^2\right) + \langle \eta|\ |k| \eta\rangle \\ &+ \frac{1}{2}\sum_{\nu=1}^{3} \Big\{ -\mathrm{Tr}\left[\left(k_\nu v \sqrt{1+v^2}\right)^2\right] + \mathrm{Tr}[k_\nu v^2 k_\nu (1+v^2)] \\ &\qquad + \langle G_\nu + k_\nu \eta | (\sqrt{1+v^2} - v)^2 (G_\nu + k_\nu \eta)\rangle \Big\} \\ &+ \frac{1}{2}\sum_{\nu=1}^{3} \Big(\mathrm{Tr}[k_\nu v^2] + \langle \eta | k_\nu \eta\rangle + 2\,\mathrm{Re}\langle \eta | G_\nu\rangle \Big)^2 . \end{aligned}$$

- Using the parametrization $v = \frac{z}{2\sqrt{1+z}}$, one sees that $\sqrt{1+v^2} = \frac{z+2}{2\sqrt{1+z}}$,

$$v \in \mathcal{L}^2(\mathfrak{h}_{\mathrm{ph}}),\ v \geq 0 \quad \Leftrightarrow \quad z \in \mathcal{L}^2(\mathfrak{h}_{\mathrm{ph}}),\ z \geq 0\,,$$

and that the functional simplifies to

$$\widetilde{\mathcal{E}}_{\mathrm{BHF}}[z;\eta] \ := \ \mathcal{E}_{\mathrm{BHF}}\big[\tfrac{z+2}{2\sqrt{1+z}},\ \tfrac{z}{2\sqrt{1+z}}\sqrt{1+v^2};\eta\big]$$

$$= \frac{1}{4}\,\mathrm{Tr}\left(|k|\,z^2\,(1+z)^{-1}\right) + \langle \eta|\ |k|\,\eta\rangle$$

$$+ \frac{1}{4}\sum_{\nu=1}^{3}\Big\{ \mathrm{Tr}\left[(1+z)\,k_\nu\,(1+z)^{-1}k_\nu - k_\nu^2\right]$$

$$+ \langle G_\nu + k_\nu\eta|\,(1+z)^{-1}(G_\nu + k_\nu\eta)\rangle\Big\}$$

$$+ \frac{1}{2}\sum_{\nu=1}^{3}\Big(\tfrac{1}{4}\,\mathrm{Tr}\left[k_\nu\,z^2\,(1+z)^{-1}\right] + \langle\eta|k_\nu\eta\rangle + 2\,\mathrm{Re}\langle\eta|G_\nu\rangle\Big)^2.$$

- So, we have

$$E_{\rm BHF} \;=\; \inf\left\{ \widetilde{\mathcal{E}}_{\rm BHF}[z;\eta] \;\middle|\; z \in \mathcal{L}^2(\mathfrak{h}_{\rm ph}),\; z \geq 0,\; \eta \in \mathfrak{h}_{\rm ph} \right\},$$

- Observe that $\widetilde{\mathcal{E}}_{\rm BHF}[JzJ; J\eta] = \widetilde{\mathcal{E}}_{\rm BHF}[z;\eta]$. We conjecture that

$$E_{\rm BHF} \;=\; \inf\left\{ \widetilde{\mathcal{E}}_{\rm BHF}[z;\eta] \;\middle|\; z \in \mathcal{L}^2(\mathfrak{h}_{\rm ph}),\; z = JzJ \geq 0,\; \eta = J\eta \in \mathfrak{h}_{\rm ph} \right\}.$$

- If $z = JzJ$ and $\eta = J\eta$ then $\widetilde{\mathcal{E}}_{\rm BHF}[z;\eta]$ assumes the simpler form

$$\begin{aligned} \widetilde{\mathcal{E}}_{\rm BHF}[z;\eta] \;=\; & \frac{1}{4}\,{\rm Tr}\left(|k|\, z^2\, (1+z)^{-1}\right) + \langle \eta|\; |k|\, \eta\rangle \\ & + \frac{1}{4}\sum_{\nu=1}^{3} \Big\{ {\rm Tr}\left[(1+z)\, k_\nu\, (1+z)^{-1} k_\nu - k_\nu^2\right] \\ & \qquad + \langle G_\nu + k_\nu \eta|\, (1+z)^{-1} (G_\nu + k_\nu \eta)\rangle \Big\}, \end{aligned}$$

and the optimal $\eta \equiv \eta[z]$ can be computed by completing the square.