Mean-field Quantum Electrodynamics

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Existence of Atoms and Molecules in the Mean-Field Approximation of No-Photon QED

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Ground State and Charge Renormalization in a Nonlinear Model of Relativistic Atoms

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Renormalization and asymptotic expansion of Dirac's polarized vacuum

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Construction of the Pauli-Villars-regulated Dirac vacuum in electromagnetic fields

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Mean-field Quantum Electrodynamics

▶ **Model:**

- quantized Dirac field $\leftrightsquigarrow$ classical electromagnetic field
- interactions solely through the classical field $\Rightarrow$ quadratic in $\Psi(x)^\dagger, \Psi(x) \Rightarrow$ mean-field exact for particles
- quasi-free states for electrons / coherent states for photons

▶ **History:**

- Dirac ('34) wrote first order and suggested self-consistent model
- (Current) Density Functional Theory
- Chaix-Iracane-Lions ('89): purely electrostatic model

▶ **Applicability to real systems?**

- Simple model containing some of the difficulties of full QED
- DFT: chemists plan to include correlation+photons by adding phenomenological terms

Mean-field Quantum Electrodynamics: results

- **Purely electrostatic case:**
  - non-perturbative solutions $\forall \alpha, Z, m, \Lambda > 0$
  - non-perturbative formula for physical charge
  - (perturbative) charge renormalization, Landau pole
  - no mass renormalization needed
  - time-dependent solutions

- **Full electromagnetic case:**
  - perturbative solutions
  - Pauli-Villars regularization
  - Euler-Heisenberg effective action

- **Main open problems:**
  - non-perturbative & time-dependent solutions for $A \neq 0$
  - include correlation & quantized photons perturbatively

QED Lagrangian action

2nd-quantized Dirac field $\Psi(x)$ $\leftrightsquigarrow$ classical EM field $(V(x), A(x))$

Formal time-independent QED Lagrangian action

$$\mathscr{L} = \int_{\mathbb{R}^3} \Psi(x)^\dagger \underbrace{\left(-i \sum_{k=1}^{3} \alpha_k \partial_k + \beta m \right)}_{:= D_{m,0}} \Psi(x)\, dx + e \int_{\mathbb{R}^3} \big(V(x) + V_{\rm ext}(x) \big) \rho(x)\, dx$$

$$- e \int_{\mathbb{R}^3} \big(A(x) + A_{\rm ext}(x) \big) \cdot j(x)\, dx + \frac{1}{8\pi} \int_{\mathbb{R}^3} |\nabla \wedge A|^2 - |\nabla V|^2$$

(units: $\hbar = c = 1$, $\alpha = e^2$)

Density and charge current operators

$$\rho(x) = \sum_{\sigma=1}^{4} \frac{\Psi(x)^\dagger_\sigma \Psi(x)_\sigma - \Psi(x)_\sigma \Psi(x)^\dagger_\sigma}{2}, \quad j(x)_k = \frac{\Psi(x)^\dagger \alpha_k \Psi(x) - \Psi(x) \alpha_k \Psi(x)^\dagger}{2}$$

In one-body space

One particle density matrix

$\left\langle \Psi(x)^\dagger_\sigma \Psi(y)_{\sigma'} \right\rangle = \gamma(x,y)_{\sigma,\sigma'}$ which satisfies $0 \leq \gamma \leq 1$ on $L^2(\mathbb{R}^3, \mathbb{C}^4)$

Action in terms of γ, V, A

$$\langle \mathscr{L} \rangle = \operatorname{tr}\left(D_{m,e(V+V_{\rm ext}),e(A+A_{\rm ext})} \frac{\gamma - \gamma^\perp}{2} \right) + \frac{1}{8\pi} \int_{\mathbb{R}^3} |\nabla \wedge A|^2 - |\nabla V|^2 := \mathcal{L}(\gamma, V, A)$$

where $\gamma^\perp := 1 - \gamma$ and

$$D_{m,\mathcal{V},\mathcal{A}} := \sum_{k=1}^{3} \alpha_k \big(-i\partial_k - \mathcal{A}_k(x) \big) + \beta m + \mathcal{V}(x)$$

Self-consistent time-independent equations

$$\mathcal{L}(\gamma,V,A)=\operatorname{tr}\left(D_{m,e(V+V_{\rm ext}),e(A+A_{\rm ext})}\frac{\gamma-\gamma^\perp}{2}\right)+\frac{1}{8\pi}\int_{\mathbb{R}^3}|\nabla\wedge A|^2-|\nabla V|^2$$

Self-consistent equations

$$\begin{cases} -\Delta V(x) &=& 4\pi e\,\operatorname{tr}_{\mathbb{C}^4}\left(\frac{\gamma-\gamma^\perp}{2}\right)(x,x):=4\pi e\,\rho_{\frac{\gamma-\gamma^\perp}{2}}(x)\\ -\Delta A(x) &=& 4\pi e\,\operatorname{tr}_{\mathbb{C}^4}\left(\alpha\frac{\gamma-\gamma^\perp}{2}\right)(x,x):=4\pi e\,j_{\frac{\gamma-\gamma^\perp}{2}}(x)\\ \nabla\cdot A &=& 0\\ \gamma &=& \mathbb{1}_{(-\infty,\mu)}\left(D_{m,e(V+V_{\rm ext}),e(A+A_{\rm ext})}\right)+\delta\end{cases}$$

Formal variational principle

$$\min_{\substack{\gamma\\0\leq\gamma\leq1}}\ \min_{\substack{A\\\nabla\cdot A=0}}\ \max_{V}\ \mathcal{L}(\gamma,V,A)$$

- If $(V_{\rm ext},A_{\rm ext})=0$, the solution is $(V,A)=0$, $\gamma=\mathbb{1}_{(-\infty,\mu)}(D_{m,0})$ $=$ old Dirac picture of the quantum vacuum

The purely electrostatic case $A = A_{\rm ext} = 0$

$$\max_V \mathcal{L}(\gamma, V, 0) = \operatorname{tr}\left(D_{m,eV_{\rm ext}}\frac{\gamma-\gamma^\perp}{2}\right) + \frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho_{\frac{\gamma-\gamma^\perp}{2}}(x)\rho_{\frac{\gamma-\gamma^\perp}{2}}(y)}{|x-y|}\,dx\,dy$$

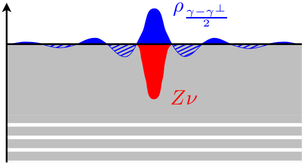
Wick ordering: subtract infinite constant $\operatorname{tr}\left(D_{m,eV_{\rm ext}}\frac{\gamma_0-\gamma_0^\perp}{2}\right) = \operatorname{tr}\left(D_{m,0}\frac{\gamma_0-\gamma_0^\perp}{2}\right)$

Convex minimization problem in electrostatic case

$$\min_\gamma\left\{\operatorname{tr}\left(D_{m,eV_{\rm ext}}Q\right) + \frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho_Q(x)\rho_Q(y)}{|x-y|}\,dx\,dy\right\}$$

where $Q = \gamma - \gamma_0$. Chaix-Iracane-Lions '89

Take $V_{\rm ext}$ such that $\int_{\mathbb{R}^3}|\nabla V_{\rm ext}|^2 < \infty$, for instance $V_{\rm ext} = -eZ\,\nu * |x|^{-1}$



$$\begin{cases} -\Delta V_{\rm tot} &= 4\pi e\left(\rho_{\frac{\gamma-\gamma^\perp}{2}} - Z\nu\right) \\ \gamma &= \mathbb{1}_{(-\infty,0)}\left(D_{m,eV_{\rm tot}}\right) + \delta \end{cases}$$

[HLS05']: no minimizer, no solution to the equation (UV divergences)

Existence with high momentum cut-off

Theorem (∃! non-perturbative solutions [HLS05,HLS05'])

- *Let* $\Lambda, e, m, Z > 0$ *and* ν *as above. Then there exists at least one minimizer living over* $\Pi_\Lambda L^2(\mathbb{R}^3)$ *with* $\Pi_\Lambda := \mathbb{1}(|p| \leq \Lambda)$*. It solves*

$$\begin{cases} \gamma_* = \mathbb{1}_{(-\infty,0)}\big(D_*\big) + \delta \\ D_* = \Pi_\Lambda\big(D_{m,0} + eV_{tot}\big)\Pi_\Lambda \\ -\Delta V_{tot} = 4\pi e\Big(\rho_{\frac{\gamma-\gamma^\perp}{2}} - Z\nu\Big) \end{cases}$$

with $0 \leq \delta \leq \mathbb{1}_{\{0\}}(D_*)$*, and which is such that*

$$\mathrm{tr}\,\gamma_0^\perp\gamma_*\gamma_0^\perp + \mathrm{tr}\,\gamma_0\gamma_*^\perp\gamma_0 + \mathrm{tr}(\gamma_*-\gamma_0)^2 < \infty \text{ and } \rho_{\frac{\gamma-\gamma^\perp}{2}} \in L^2(\mathbb{R}^3)\cap \dot{H}^{-1}(\mathbb{R}^3).$$

All these solutions share the same $\rho_{\frac{\gamma_*-\gamma_*^\perp}{2}} := \rho_{vac}$*, hence* V_{tot} *and* $D_* = D_{m,eV_{tot}}$ *are unique.*

- *If* $e^2\,\|\nabla V_{ext}\|_{L^2} < \pi^{5/6}2^{1/6}$*, then* $\ker(D_*) = \{0\}$ *hence* $\delta \equiv 0$ *and* γ_* *is unique. In addition, the vacuum is neutral*

$$Ind(\gamma_*,\gamma_0) = \text{“}\mathrm{tr}(\gamma_*-\gamma_0)\text{”} := \mathrm{tr}\,\gamma_0^\perp(\gamma_*-\gamma_0)\gamma_0^\perp + \mathrm{tr}\,\gamma_0(\gamma_*-\gamma_0)\gamma_0 = 0.$$

Existence for atoms and molecules

Theorem (Atoms and molecules [HLS07])

Let $\Lambda, e, m, Z > 0$ and $0 \leq \nu \in L^1(\mathbb{R}^3) \cap L^{6/5}(\mathbb{R}^3)$ as above, with $\int_{\mathbb{R}^3} \nu = 1$.

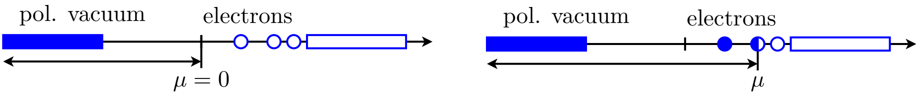
For

$$\alpha Z,\ q > 0,\ \Lambda \text{ fixed and } \alpha \ll 1$$

or for

$$0 < q \leq Z,\ \Lambda \text{ fixed and } \alpha \ll 1$$

there exists a minimizer under the charge constraint "$\mathrm{tr}(\gamma - \gamma_0)$" $= q$. It solves the previous nonlinear equations for some chemical potential $\mu \in (-m, m)$.



Towards charge renormalization

Theorem (The physical charge [GLS09])

For $\nu \in L^1(\mathbb{R}^3)$ *we have* $\rho_{\gamma_*-\gamma_0} \in L^1(\mathbb{R}^3)$ *and*

$$-Z\int_{\mathbb{R}^3}\nu + \int_{\mathbb{R}^3}\rho_{\gamma_*-\gamma_0} = \frac{-Z\int_{\mathbb{R}^3}\nu + \text{“tr”}(\gamma_*-\gamma_0)}{1+\alpha B_\Lambda}$$

where

$$B_\Lambda = \frac{1}{\pi}\int_0^{\frac{\Lambda}{\sqrt{m^2+\Lambda^2}}} \frac{s^2 - s^4/3}{1-s^2}ds = \frac{2}{3\pi}\log\frac{\Lambda}{m} - \frac{5}{9\pi} + \frac{2\log 2}{3\pi} + O(m^2/\Lambda^2).$$

In particular, except when the two terms vanish, $\gamma_* - \gamma_0$ *is never trace-class.*

Physical charge $\equiv$ screening effect of the quantum vacuum

$$e_{\rm ph}^2 = \alpha_{\rm ph} := \frac{e^2}{1+e^2B_\Lambda} = \frac{\alpha}{1+\alpha B_\Lambda}$$

- **Renormalization:** express everything with $\alpha_{\rm ph}$ and study $\Lambda \to \infty$

Problem: cannot keep $\alpha_{\rm ph}$ fixed, since by definition $\alpha_{\rm ph} B_\Lambda < 1$! [Landau pole]

Renormalization order by order

Idea: expand vacuum polarization in powers of $\alpha_{\rm ph}$, keeping $\alpha_{\rm ph}\log\Lambda$ fixed

Theorem (Perturbative renormalization [GLS11])

For $\mu=0$, there exists a sequence $\rho_j\in L^2(\mathbb{R}^3)\cap L^{6/5}(\mathbb{R}^3)$, depending only on $Z\nu$, such that the following holds. For $\epsilon\leq\alpha_{\rm ph}B_\Lambda\leq 1-\epsilon$ and $\alpha_{\rm ph}\ll 1$, we have

$$\left\|\alpha\rho_{tot}-\sum_{j=1}^K(\alpha_{\rm ph})^j\rho_j\right\|_{\dot{H}^{-1}(\mathbb{R}^3)}\leq C_{\epsilon,K,Z\nu}\,(\alpha_{\rm ph})^{K+1}$$

where $\rho_1=-Z\nu$ and

$$\rho_2*|x|^{-1}=-\frac{Z}{3\pi}\int_1^\infty dt\,(t^2-1)^{1/2}\left[\frac{2}{t^2}+\frac{1}{t^4}\right]\int_{\mathbb{R}^3}e^{-2|x-y|t}\frac{\nu(y)}{|x-y|}\,dy$$

is the Uehling potential. (Serber '35, Uehling '35)

- Rough estimates give $C_{\epsilon,K,\rho_{\rm ext}}\leq C(\log K)^{K^2/2}$
- The series is believed to be divergent (Dyson '52)

Back to the electromagnetic case

We integrate fermionic degrees of freedom

Formal Lagrangian action

$$\min_{\gamma} \mathcal{L}(\gamma, V, A) = -\frac{1}{2}\,\mathrm{tr}\,|D_{m,e(V+V_{\rm ext}),e(A+A_{\rm ext})}| + \frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\wedge A|^2 - |\nabla V|^2$$

Pauli & Villars ('49): 2 fictitious fields of masses $m_1, m_2 \gg 1$

$$\mathscr{F}_{\rm PV}(V, V_{\rm ext}, A, A_{\rm ext}) = \frac{1}{2}\,\mathrm{tr}\sum_{j=0}^{2} c_j\Big(|D_{m_j,0}| - |D_{m_j,e(V+V_{\rm ext}),e(A+A_{\rm ext})}|\Big) + \frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\wedge A|^2 - |\nabla V|^2$$

with $m_0 = c_0 = 1$ and $\sum_{j=0}^{2} c_j = \sum_{j=0}^{2} c_j m_j^2 = 0.$

Any other gauge-invariant cut-off probably works the same

Translation invariant case: Euler-Heisenberg '36, Weisskopf '36, Schwinger '51

Existence of perturbative solutions

Theorem (Existence of Pauli-Villars-regulated solutions [GHLS12])

Assume that $c_0 = 1$, $m_2 > m_1 > m_0 > 0$ *and* $\sum_{j=0}^{2} c_j = \sum_{j=0}^{2} c_j m_j^2 = 0$.

- $\mathcal{F}_{PV}$ *is well defined and continuous on the space of potentials* $V, A \in L^6(\mathbb{R}^3)$ *satisfying* $\int_{\mathbb{R}^3} |\nabla V|^2 + |\nabla \wedge A|^2 < \infty$.
- *For any* $\alpha \int_{\mathbb{R}^3} |\nabla V_{ext}|^2 + |\nabla \wedge A_{ext}|^2 < \varepsilon^2\, m_0$, *there exists a unique solution* (V_*, A_*) *to the min-max problem*

$$\min_{\|\nabla V\|_{L^2} < 3\varepsilon\sqrt{\frac{m_0}{\alpha}}} \; \sup_{\|\nabla\wedge A\|_{L^2} < 3\varepsilon\sqrt{\frac{m_0}{\alpha}}} \mathcal{F}_{PV}(V, V_{ext}, A, A_{ext})$$
$$= \max_{\|\nabla\wedge A\|_{L^2} < 3\varepsilon\sqrt{\frac{m_0}{\alpha}}} \; \inf_{\|\nabla V\|_{L^2} < 3\varepsilon\sqrt{\frac{m_0}{\alpha}}} \mathcal{F}_{PV}(V, V_{ext}, A, A_{ext})$$

where ε *only depends on* $\sum_{j=0}^{2} |c_j| m_0/m_j$ *and* α.

- (V_*, A_*) *is a solution to the nonlinear equations.*

Euler-Heisenberg effective action

Theorem (Euler-Heisenberg effective action in magnetic case [GLS17])

Let $B \in C^0(\mathbb{R}^3,\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ with $\nabla B \in L^1(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$ and $\nabla \cdot B = 0$. Let A such that $B = \nabla \wedge A$ and set $A_\varepsilon(x) = \varepsilon^{-1} A(\varepsilon x)$. Then

$$\frac{\varepsilon^3}{2} \operatorname{tr} \sum_{j=0}^{2} c_j \left(|D_{m_j,0,0}| - |D_{m_j,0,A_\varepsilon}| \right) = \int_{\mathbb{R}^3} f_{vac}^{PV}(e|B(x)|)\, dx + O(\varepsilon)$$

where

$$f_{vac}^{PV}(b) := \frac{1}{8\pi^2} \int_0^\infty \left(\sum_{j=0}^{2} c_j\, e^{-sm_j^2} \right) \Big(sb \coth(sb) - 1 \Big) \frac{ds}{s^3}$$

is the Pauli-Villars-regulated Euler-Heisenberg vacuum energy.

- Semi-classical analysis in strong magnetic fields
- Euler-Heisenberg with $E \neq 0$ is not easily well defined

$$\frac{1}{8\pi^2} \int_0^\infty \frac{e^{-sm^2}}{s^3} \left(\frac{e^2 s^2}{3} \left(|E|^2 - |B|^2 \right) - 1 + e^2 s^2 \, (E \cdot B) \, \frac{\Re \cosh \left(es \left(|B|^2 - |E|^2 + iE \cdot B \right)^{\frac{1}{2}} \right)}{\Im \cosh \left(es \left(|B|^2 - |E|^2 + iE \cdot B \right)^{\frac{1}{2}} \right)} \right) ds$$

- Recent confirmation of vacuum birefringence (Mignani et al, 2017)

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