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Ground state properties in non-relativistic QED

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Abstract

We discuss recent results concerning the ground state of non-relativistic quantum electrodynamics as a function of a magnetic coupling constant or the fine structure constant, obtained by the authors in [12, 13, 14].

1 Introduction

We consider a system of finitely many non-relativistic quantum mechanical electrons bound to a static nucleus. The electrons are minimally coupled to the quantized electromagnetic field, and we denote the coupling constant by g. We impose an ultraviolet cutoff on the electromagnetic vector potential appearing in the covariant derivatives.

Models of this type are known as non-relativistic quantum electrodynamics (qed). They provide a reasonable description of microscopic low energy phenomena involving electrons, nuclei, and photons. A systematic mathematical investigation of these models started in the mid 90s with the work of V. Bach, J. Fröhlich, and I.M. Sigal [3, 4, 5]. They showed existence of ground states. Furthermore, they showed that excited bound states of the unperturbed system become unstable and turn into resonances when the electrons are coupled to the radiation field. To prove this result they introduced an operator theoretic renormalization analysis. Later, the existence of ground states was shown in more generality by M. Griesemer, E.H. Lieb, and M. Loss, see [8, 15].

In [13] we showed that the ground state of an atom with spinless electrons is an analytic function of the coupling constant g. That result is explained in Section 2, and it provides an algorithm to determine the ground state to arbitrary precision. To obtain the result we used the operator theoretic renormalization analysis of [3] and that renormalization preserves anlyticity [9].

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In Section 3, we consider expansions in the fine structure constant α. We consider a scaling where the ultraviolet cutoff is of the order of the binding energy of the unperturbed atom. In this scaling lifetimes of excited states of atoms were calculated which agree with experiment [11]. V. Bach, J. Fröhlich, and A. Pizzo [1, 2] showed that there exists an asymptotic expansion of the ground state and the ground state energy with α dependent coefficients. In [13] this result was extended and it was shown that these expansions are convergent. Furthermore, it was shown in [14] that the ground state energy as well as the ground state are k-times continuously differentiable functions of α respectively $\alpha^{1/2}$ on some nonempty k-dependent interval $[0, c_k)$. This result implies that there are no logarithmic terms in this scaling limit. This resolves an open issue raised in [2], since for other scalings of the ultraviolet cutoff logarithmic terms do occur [7, 10, 6].

2 Model and analyticity of the ground state

We introduce the bosonic Fock space over the one photon Hilbert space $\mathfrak{h} := L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ and set

$$\mathcal{F} := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} S_n(\mathfrak{h}^{\otimes^n}),$$

where S_n denotes the orthogonal projection onto the subspace of totally symmetric tensors in $\mathfrak{h}^{\otimes^n}$. By $a^*(k,\lambda)$ and $a(k,\lambda)$, with $(k,\lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$, we denote the so called creation and annihilation operator. They satisfy the following commutation relations, which are to be understood in the sense of distributions,

$$[a(k,\lambda), a^*(k',\lambda')] = \delta_{\lambda\lambda'}\delta(k-k'), \qquad [a^\#(k,\lambda), a^\#(k',\lambda')] = 0 \ ,$$

where $a^\#$ stands for a or a^*. The operator $a(k,\lambda)$ annihilates the vacuum $(1,0,...) \in \mathcal{F}$. We define the operator of the free field energy by

$$H_f := \sum_{\lambda=1,2} \int a^*(k,\lambda)|k|a(k,\lambda)d^3k.$$

For $\lambda = 1,2$ we introduce the so called polarization vectors $\varepsilon(\cdot,\lambda) : S^2 := \{k \in \mathbb{R}^3 | |k| = 1\} \to \mathbb{R}^3$ to be maps such that for each $k \in S^2$ the vectors $\varepsilon(k,1), \varepsilon(k,2), k$ form an orthonormal basis of $\mathbb{R}^3$. For $x \in \mathbb{R}^3$ we define the field operator

$$A_\Lambda(x) := \sum_{\lambda=1,2} \int_{|k|<\Lambda} \frac{d^3k}{\sqrt{2|k|}} \left[e^{-ik\cdot x}\varepsilon(\widehat{k},\lambda)a^*(k,\lambda) + e^{ik\cdot x}\varepsilon(\widehat{k},\lambda)a(k,\lambda) \right] \ , \qquad (1)$$

where $0 < \Lambda$ is a finite ultraviolet cutoff and $\widehat{k} := k/|k|$. The Hilbert space is $\mathcal{H} := \mathcal{H}_{\rm at} \otimes \mathcal{F}$, where

$$\mathcal{H}_{\rm at} := \bigwedge^N L^2(\mathbb{R}^3)$$

is the Hilbert space describing N spin-less electrons. We study the following operator in $\mathcal{H}$

$$H_g := \sum_{j=1}^{N}(p_j + gA_\Lambda(x_j))^2 + V + H_f, \tag{2}$$

where $x_j \in \mathbb{R}^3$ denotes the coordinate of the j-th electron, $p_j = -i\partial_{x_j}$, and V denotes the potential. For the result concerning analyticity in the coupling constant g on a disk $D_r := \{z \in \mathbb{C} | |z| < r\}$, we need the following hypothesis. It contains assumptions about the atomic Hamiltonian $H_{\text{at}} := \sum_{j=1}^{N} p_j^2 + V$ acting in $\mathcal{H}_{\text{at}}$.

Hypothesis (H) The potential V satisfies the following properties:

(i) V is invariant under permutations and rotations.

(ii) V is infinitesimally operator bounded with respect to $\sum_{j=1}^{N} p_j^2$.

(iii) $E_{\text{at}} := \inf \sigma(H_{\text{at}})$ is a non-degenerate isolated eigenvalue of H_{at}.

All assumptions of Hypothesis (H) are satisfied for the hydrogen atom. Part (i) is satisfied for atoms, but not for molecules with static nuclei. We note that (iii) is a restrictive assumption.

Theorem 1. *Suppose (H). Then there exists a positive constant g_0 such that for all $g \in D_{g_0}$ the operator H_g has a non-degenerate eigenvalue $E(g)$ with eigenvector $\psi(g)$ and eigen-projection $P(g)$ satisfying the following properties.*

(i) For $g \in \mathbb{R} \cap D_{g_0}$, $E(g) = \inf \sigma(H_g)$.

(ii) $g \mapsto E(g)$ and $g \mapsto \psi(g)$ are analytic on D_{g_0}.

(iii) $g \mapsto P(g)$ is analytic on D_{g_0} and $P(g)^* = P(\overline{g})$.

Concerning the proof of the theorem, we note that the ground state energy is embedded in continuous spectrum. In such a situation analytic perturbation theory is typically not applicable and other methods have to be employed. In [13] Theorem 1 is proven using a variant of the operator theoretic renormalization analysis. Using the rotation invariance assumption of Hypothesis (H) one can prove that marginal terms in the renormalization analysis are absent. This implies that the renormalization analysis converges. Theorem 1 can then be shown using that renormalization preserves analyticity [12, 9].

Theorem 1 implies that the ground state and the ground state energy admit convergent power series expansions in g. The coefficients of these expansions can be calculated by means of analytic perturbation theory. To this end, one introduces an infrared cutoff which renders all expansion coefficients finite. In [13] it was shown using a continuity argument, that the individual expansion coefficients converge as the infrared cutoff is removed. This is not obvious; the expansion coefficients obtained by regular perturbation theory, [16], can involve cancellations of infrared divergent terms [12].

3 Expansions in the fine structure constant

In this section, we consider the ground state and the ground state energy of a hydrogen atom as a function of the fine structure constant α. We assume that the ultraviolet cutoff is of the order of the binding energy of the unperturbed atom. In suitable units the corresponding Hamiltonian is

$$H_{\alpha,\Lambda} := (p + \alpha^{3/2} A_\Lambda(\alpha x))^2 - \frac{1}{|x|} + H_f.$$

By a scaling transformation we can relate this operator to the operator

$$\widetilde{H}_{\alpha,\Lambda} := (p + \sqrt{\alpha} A_\Lambda(x))^2 - \frac{\alpha}{|x|} + H_f$$

using the following unitary equivalence $\widetilde{H}_{\alpha,\alpha^2\Lambda} \cong \alpha^2 H_{\alpha,\Lambda}$. We are interested in the behavior of the ground state and the ground state energy of $H_{\alpha,\Lambda}$ as $\alpha \downarrow 0$ while Λ remains constant. The ground state and the ground state energy are smooth in the sense of the following theorem [14].

Theorem 2. *Suppose (H) and let $\Lambda > 0$. There exists a positive α_0 such that for $\alpha \in [0, \alpha_0)$ the operator $H_{\alpha,\Lambda}$ has a ground state $\psi(\alpha^{1/2})$ with ground state energy $E(\alpha)$ such that we have the convergent expansions on $[0, \alpha_0)$*

$$E(\alpha) = \sum_{n=0}^{\infty} E_\alpha^{(2n)} \alpha^{3n}, \qquad \psi(\alpha^{1/2}) = \sum_{n=0}^{\infty} \psi_\alpha^{(n)} \alpha^{3n/2}. \tag{3}$$

The coefficients $E_\alpha^{(n)}$ and $\psi_\alpha^{(n)}$ are as functions of α in $C^\infty([0,\infty))$ and $C^\infty([0,\infty); \mathcal{H})$, respectively. For every $k \in \mathbb{N}_0$ there exists a positive $\alpha_0^{(k)}$ such that $\psi(\cdot)$ and $E(\cdot)$ are k-times continuously differentiable on $[0, \alpha_0^{(k)})$.

By the differentiability property of Theorem 2 and Taylor's theorem one can write the ground state and the ground state energy in terms of an asymptotic series with constant coefficients in the sense of [17]. To prove Theorem 2, we consider the Hamiltonian

$$H(g, \beta, \Lambda) := (p + g A_\Lambda(\beta x))^2 - \frac{1}{|x|} + H_f.$$

Using the identity $H(\alpha^{3/2}, \alpha, \Lambda) = H_{\alpha,\Lambda}$, Theorem 2 will follow as an application of Theorem 3, below. A corollary of that theorem is that the ground state of $H(g, \beta, \Lambda)$ is analytic in g with coefficients which are C^∞ functions of β. To state the theorem precisely, let X be a Banach space and let $C_B^k(\mathbb{R}; X)$ denote the space of X-valued functions having bounded, continuous derivatives up to order k normed by $\|f\|_{C_B^k(\mathbb{R};X)} := \max_{0 \le s \le k} \sup_{x \in \mathbb{R}} \|D_x^s f(x)\|_X$.

Theorem 3. *Suppose (H), let $k \in \mathbb{N}_0$, and $\Lambda > 0$. Then there exists a positive g_0 such that for all $(g, \beta) \in D_{g_0} \times \mathbb{R}$ the operator $H(g, \beta, \Lambda)$ has an eigenvalue $E_\beta(g)$ with eigenvector $\psi_\beta(g)$ and eigen-projection $P_\beta(g)$ satisfying the following properties.*

(i) *For $g \in \mathbb{R} \cap D_{g_0}$ we have $E_\beta(g) = \inf \sigma(H_{g,\beta})$, and for all $g \in D_{g_0}$ we have $P_\beta(g)^* = P_\beta(\overline{g})$.*

(ii) *$g \mapsto E_{(\cdot)}(g)$, $g \mapsto \psi_{(\cdot)}(g)$, and $g \mapsto P_{(\cdot)}(g)$ are analytic functions on D_{g_0} with values in $C_B^k(\mathbb{R})$, $C_B^k(\mathbb{R}; \mathcal{H})$, and $C_B^k(\mathbb{R}; \mathcal{B}(\mathcal{H}))$, respectively.*

In [14] Theorem 3 is shown using an operator theoretic renormalization analysis, which involves controlling arbitrary high derivatives with respect to β.

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