Spectral Analysis of Nonrelativistic Quantum Electrodynamics

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Abstract. I review the research results on spectral properties of atoms and molecules coupled to the quantized electromagnetic field or on simplified models of such systems obtained during the past decade. My main focus is on the results I have obtained in collaboration with Jürg Fröhlich and Israel Michael Sigal [8, 9, 10, 11, 12, 13].

1. Introduction

In this lecture I review the progress achieved during the past decade on the mathematical description of quantum mechanical matter interacting with the quantized radiation field. My main focus will be on the results I have obtained in collaboration with Jürg Fröhlich and Israel Michael Sigal [8, 9, 10, 11, 12, 13].

1.1. Basic notions of quantum mechanics

I start by recalling some basic mathematical notions of quantum mechanics. The states of a quantum mechanical system to be described are vectors in a separable Hilbert space, \( \mathcal{H} \). The dynamics on \( \mathcal{H} \) is generated by the self-adjoint Hamiltonian operator, \( H \). That is, given an initial state \( \psi(0) = \psi_0 \in \mathcal{H} \) at time \( t = 0 \), the state at time \( t > 0 \) is given by \( \psi(t) = \exp[-itH]\psi_0 \). The corresponding differential equation fulfilled by \( \psi(t) \) is Schrödinger’s equation,

\[
\frac{d\psi(t)}{dt} = H \psi(t). \tag{1}
\]

Stone’s theorem [43] states that the selfadjointness of \( H \) is equivalent for \( t \mapsto \exp[-itH] \) to be a strongly continuous one-parameter unitary group. Thus selfadjointness of the Hamiltonian is the crucial property for the existence of quantum mechanical dynamics.

As a first example, I describe the above notions for a single, nonrelativistic electron moving in a potential \( V : \mathbb{R}^3 \rightarrow \mathbb{R} \). The Hilbert space of states and the Hamiltonian are, in this case,

\[
\mathcal{H}_{el} := L^2(\mathbb{R}^3 \times \mathbb{Z}_2), \quad H_{el} = -\Delta_x + V(x), \tag{2}
\]

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where $\Delta_x$ is the Laplacian on $\mathbb{R}^3$, and the potential $V(x)$ acts as a multiplication operator, $[V\psi](x,\sigma) := V(x)\psi(x,\sigma)$. Moreover, the $\mathbb{Z}_2$ factor in the definition of $H_{el}$ accounts for the spin of the electron. Under the assumption that $V \in L^2 \cap L^\infty(\mathbb{R}^3;\mathbb{R})$, the Hamiltonian $H_{el}$ is selfadjoint on the standard Sobolev space, $H^2(\mathbb{R}^3 \times \mathbb{Z}_2) \subseteq L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$, the domain $\text{dom}(-\Delta_x)$ of selfadjointness of the Laplacian. If $\lim_{|x|\to \infty} V(x) = 0$, and if $\|(V)\|_{L^{3/2}}$ is not too small, then $H_{el}$ has the following standard spectrum [42], see Fig. 1:

- Below 0, the spectrum is purely discrete, i.e., it consists only of isolated eigenvalues, $E_0 < E_1 < \cdots < 0$, each $E_j$ being of finite multiplicity $n_j < \infty$. Thus there is an orthonormal basis of the corresponding spectral subspace of eigenvectors, $\{\varphi_{j,\alpha}\}_{\alpha=1,\ldots,n_j}$, i.e., $H_{el}\varphi_{j,\alpha} = E_j\varphi_{j,\alpha}$ and $\langle\varphi_{i,\alpha}|\varphi_{j,\beta}\rangle = \delta_{i,j}\delta_{\alpha,\beta}$. If there are infinitely many eigenvalues, they accumulate at 0.
- The positive half-axis supports the purely absolutely continuous spectrum.
- The singular continuous spectrum is empty.

A typical potential to bear in mind is $V(x) := -|x|^{-1}$. Then $H_{el} = -\Delta_x - |x|^{-1}$ is the Hamiltonian of a hydrogen atom. It is actually not more difficult to include more than one electron in the model. The structure (3)-(5) of the spectrum of $\sigma(H_{el})$ would not change, qualitatively. I summarize the assumptions and definitions made in the following hypothesis.

**Hypothesis 1.1.** Let $\mathcal{H}_{el} := L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$, and assume that $V \in L^2 \cap L^\infty(\mathbb{R}^3;\mathbb{R})$ and $\lim_{|x|\to \infty} V(x) = 0$. Let $H_{el} = -\Delta_x + V(x)$ be the corresponding selfadjoint, semibounded on the domain $H^2(\mathbb{R}^3 \times \mathbb{Z}_2)$, and assume that $H_{el}$ as (at least) one negative eigenvalue,

$$E_0 = \inf \sigma(H_{el}) < 0 = \inf \sigma_{\text{ess}}(H_{el}).$$

In my second example, for $N \in \mathbb{N}$, and real numbers $E_0 < E_1 < \cdots < E_N$, the Hilbert space of states is finite dimensional and the Hamiltonian is a diagonal $N \times N$ matrix,

$$\mathcal{H}_{el} := \mathbb{C}^N, \quad H_{el} = \text{diag}[E_0, E_1, \ldots, E_N].$$

![Figure 1. The spectrum of $H_{el}$](image-url)