Spectral Theory of the Operator \((p^2 + m^2)^{1/2} - Ze^2/r\)

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Abstract. Using dilation invariance and dilation analytic techniques, and with the help of a new virial theorem, we give a detailed description of the spectral properties of the operator \((p^2 + m^2)^{1/2} - Ze^2/r\). In the process the norm of the operator \(|x|^{-2}|p|^{-2}\) is calculated explicitly in \(L^p(\mathbb{R}^N)\).

I. Introduction

The classical Hamiltonian describing the interaction of a relativistic particle of charge \(e\) and mass \(m\) with an electromagnetic field [vector potential \(A(x)\) and scalar potential \(\phi(x)\)] is given by [1]

\[
[(p - eA(x))^2 + m^2]^{1/2} + e\phi(x). \tag{1.1}
\]

To make the transition to quantum mechanics, the usual procedure (which is of course fraught with ambiguities) is to change the classical Hamiltonian into an operator on the Hilbert space \(L^2(\mathbb{R}^3)\) by replacing \(p\) by \(-i\nabla\). Because of the troublesome square root in (1.1), the standard procedure just described has received very little attention in treating a relativistic particle in an electromagnetic field. Historically, an alternative procedure was followed resulting in the Klein-Gordon (K.G.) equation [2]. Calling the energy function of (1.1) \(E\), one finds

\[
(E - e\phi(x))^2 - (p - eA(x))^2 - m^2 = 0.
\]

One now makes the Ansatz \(p = -i\nabla\) and tries to solve the implicit eigenvalue problem

\[
\{(E - e\phi(x))^2 - (p - eA(x))^2 - m^2\}\psi(x) = 0 \tag{1.2}
\]

subject to “appropriate” boundary conditions. The K.G. equation has a definite virtue when the interaction is the Coulomb potential \((A \equiv 0, \phi(x) = -Ze/|x|)\): The equation can be solved explicitly. It seems to us that this explicit solvability is the

* Supported in part by NSF Grant MPS 74 22844
main reason for the comparative neglect of the more difficult operator

$$H = (p^2 + m^2)^{1/2} - Ze^2/|x|.$$ (1.3)

This operator describes the same system as the K.G. equation, namely a spin zero particle in the Coulomb field of an infinitely heavy nucleus of charge Z. However, the theory of operator (1.3) does not suffer from the difficulties of interpretation of the K.G. theory [2] which are connected with the fact that the latter is not really a Hamiltonian theory. The operator (1.3) also has the virtue that it is stable over a larger range of Z's than the K.G. theory: The operator $H$ is non-negative if $Ze^2 \leq 2/\pi$ (see Theorem 2.1 below) while the energy of the ground state in the K.G. theory becomes complex when $Ze \geq 1/2$ [2]. (This is to be compared with the Dirac equation for a spin $\frac{1}{2}$ particle in a Coulomb field which is unstable if $Ze^2 > 1$ [2, 3].)

It is thus clear that there is a range of atomic number over which the K.G. energies will differ appreciably from the eigenvalues of the operator in (1.3). It would be very interesting if Nature's preference could be seen experimentally. Unfortunately, this question is clouded by other effects which play an important role in $\pi$ and $K$ mesic atoms [4] and it may be on the borderline of being untestable.

In this paper we examine the spectral properties of the operator of Equation (1.3) from an abstract point of view. Our results are summarized in Theorems 2.1 through 2.5.

II. Spectral Properties

In this section we first state and then prove Theorems 2.1 through 2.5. We use the notation $Q(A) = \mathcal{D}(|A|^{1/2})$ for any self-adjoint operator $A$. We work on $L^2(\mathbb{R}^3)$ unless otherwise stated.

**Theorem 2.1.** Let $H_0 = (p^2 + m^2)^{1/2}, m \geq 0$.

a) If $Ze^2 \leq 2/\pi$, then as a form on $Q(H_0)$

$$H_0 - Ze^2/|x| \geq 0.$$ (2.1)

b) If $Ze^2 > 2/\pi$, then $H_0 - Ze^2/|x|$ is unbounded below as a form on $Q(H_0)$.

c) $||x|^{-1}(H_0 + 1)^{-1}|| = 2$ and thus in particular $\mathcal{D}(|x|^{-1}) \subseteq \mathcal{D}(H_0)$ and $H_0 - Ze^2/|x|$ is essentially self-adjoint on $\mathcal{D}(H_0)$ if $Ze^2 \leq \frac{1}{2}$.

**Remark.** a) Of Theorem 2.1 is stated in Kato [5] (without proof); c) is a well known result [5, 6]. Theorem 2.1 will follow from a more general result proved in Theorem 2.5 below.

**Definition.** We define the operator $H = H_0 - Ze^2/|x|$ for $Ze^2 \leq 2/\pi$ to be the Friedrichs extension of $(H_0 - Ze^2/|x|)^{\lambda(H_0)}$. We remark that because of Theorem 2.1c), if $Ze^2 < 2/\pi$, the Friedrichs extension coincides with the form sum of $H_0$ and $-Ze^2/|x|$.

**Theorem 2.2.** Suppose $Ze^2 < 2/\pi$. Then the spectrum of $H$ in $[0, m)$ is discrete (consisting of eigenvalues of finite multiplicity with no points of accumulation). We have the lower bound

$$H \geq m(1 - (\frac{1}{2}\pi Ze^2)^2)^{1/2}.$$ (2.2)