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Selfadjointness and invariance of the essential spectrum for the Klein-Gordon equation

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Abstract. We consider the selfadjointness and the invariance of the essential spectrum of the Hamiltonian of the Klein-Gordon equation. We prove that the Hamiltonian has a selfadjoint extension such that the essential spectrum coincides with the spectrum of the unperturbed Hamiltonian. We consider a large class of electromagnetic and scalar potentials. In particular we can have potentials of Coulomb type if the coupling constant is not too big. We can even consider magnetic potentials which are divergent at infinity.

1. Introduction

In a previous paper [1] we developed the scattering theory for the Klein-Gordon equation [2]:

$$\left(i\frac{\delta}{\delta t} - b_0\right)^2 \psi(x, t) = \left[\sum_{i=j}^{n} (D_i - b_i)^2 + m^2 + q_s\right]\psi(x, t),$$

$x \in R^n$, $t \in R$, $D_J = -i(\delta/\delta x_J)$, $b_0(x)$ is the electric potential, $b_i(x)$, $1 \leqslant i \leqslant n$, the magnetic potential, and $q_s(x)$ is the scalar potential. We followed the usual procedure of considering an equivalent equation which is first order in time, in the Hilbert space of vector valued functions which have finite energy. We proved existence and completeness of the wave operators, the intertwining relations and the invariance principle as well. In this paper we consider the problem of the selfadjointness and the invariance of the essential spectrum of the Hamiltonian in the case where local singularities of Coulomb type are allowed.

In Section I (Theorem I) we construct a selfadjoint extension, H, of the Hamiltonian such that the essential spectrum coincides with $(-\infty, -m] \cup [m, \infty)$. In particular we can have singularities of Coulomb type if the coupling constant is not too big.

In Section II we give conditions in the magnetic field that allow us to perform a Gauge transformation in the magnetic potential. In particular we consider magnetic potentials which are divergent at infinity.

Concerning the literature: we will only mention the more recent results [8], [9] and [10], where a list of references is given.

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Lundberg [8] considers the case $n = 3$, $b_i(x) \equiv 0$, $1 \leqslant i \leqslant 3$ and

i) $q_s(x)$ and $b_0^2(x)$ square integrable
ii) $b_0(x)$ and $q_s(x)$ behave as $O(|x|^{-3-\varepsilon})$, $\varepsilon > 0$ for $|x| \to \infty$
iii) $\int dx(-b_0^2 + q_s)|f|^2 \geqslant -\alpha \int (|\nabla f|^2 + m^2|f|^2)\, d^3x$ with $0 < \alpha < s$, $f \in C_0^\infty$.

In [9] Eckardt considers the case $n \geqslant 3$, $b_i(x) \equiv 0$, $1 \leqslant i \leqslant n$. He assumes (iii) of [8] and

i) $$M_{\alpha,p}^2 = \sup_{x \in \mathbb{R}^n} \int_{|x-y|<1} |p(y)|^2 |x-y|^{-m+4-\alpha}\, dy < \infty$$
where p is any one of b_0^2 and q_s, and $\alpha \in (0, 1]$.

ii) $$M_{\alpha,p}(x) = \int_{|x-y|<1} |p(y)|^2\, |x-y|^{-m+4-\alpha}\, dy \xrightarrow[|x|\to\infty]{} 0.$$

Kako in [10] considers the case $n = 3$ and $b_i(x)$, $0 \leqslant i \leqslant 3$, and q_s bounded and satisfying

i) $|b_i(x)| \leqslant C|x|^{-2-\varepsilon}$, $0 \leqslant i \leqslant 3$
ii) b_i, $1 \leqslant i \leqslant 3$ are differentiable and $|\partial/\partial x_i\, b_i| \leqslant C|x|^{-2-\varepsilon}$
iii) $|q_s| \leqslant C|x|^{-2-\varepsilon}$.

Our conditions in any one of b_i, $0 \leqslant i \leqslant n$ and $q_s(x)$ are weaker than the conditions of [8], [9] and [10].

In Section II (see also the conclusions) we give a representation of the Klein-Gordon equation as an equation which is first order in time, with a Hamiltonian which is selfadjoint in a Hilbert space, with positive metric, where a position operator and a (positive!) probabitity density is defined (it is often said in the literature that such a representation does not exist). We prove also that if the wave operators exist the scattering matrix is free of Klein paradox. It seems that this representation has not been noticed before in the literature. In fact the Hamiltonian contains a square-root operator which is usually rejected as intractable or expanded in series in the text books on quantum mechanics.

II. Selfadjointness and essential spectrum

We consider the Klein-Gordon equation [2] with electro-magnetic potential $b_i(x)$, $0 \leqslant i \leqslant n$ and scalar potential $q_s(x)$:

$$\left(i\frac{\partial}{\partial t} - b_0(x)\right)^2 \psi(x, t) = \left[\sum_{i=1}^{n} (D_i - b_i)^2 + m^2 + q_s\right]\psi(x, t) \tag{1.1}$$

$$x \in \mathbb{R}^n, \quad t \in \mathbb{R}, \quad D_j = -i\frac{\partial}{\partial x_j}.$$

As in [1] we consider an equivalent equation which is first order in time, we define

$$f_1 = \psi(x, t), f_2 = i\frac{\partial}{\partial t}\psi(x, t) \quad \text{and} \quad f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}.$$

Then (1.1) is equivalent to the following equation $i(\partial/\partial t)f = hf$, where

$$D(h) = \{f \in C_0^{\infty,2} \mid lf_1 \in \mathscr{L}^2 \quad \text{and} \quad Qf_2 \in \mathscr{L}^2\} \tag{1.2}$$

$$h = \begin{bmatrix} 0 & 1 \\ l & Q \end{bmatrix}, \qquad l = \sum_{i=1}^{n} (D_i - b_i)^2 + m^2 + q(x),$$

$$q(x) = q_s - b_0^2, \qquad Q = 2b_0$$

C_0^∞ is the space of infinitely differentiable functions of compact support on $\mathbb{R}^n$, and $C_0^{\infty,2} = C_0^\infty \oplus C_0^\infty$.

Let us first consider the free case, i.e., $q_s(x) \equiv 0$, $b_i(x) \equiv 0$, $0 \leqslant i \leqslant n$. As is well known the energy integral

$$E_0(\psi) = \int d^n x \left\{ \sum_{i=1}^{n} |D_i \psi|^2 + m^2 |\psi|^2 + \left| \frac{\partial}{\partial t} \psi \right|^2 \right\} \tag{1.3}$$

is conserved in time. We associate with (1.3) a scalar product, the 'energy scalar product'

$$(f, g)_0 = \sum_{i=1}^{n} (D_i f_1, D_i g_1) + m^2 (f_1, g_1) + (f_2, g_2) \quad fg \in C_0^{\infty,2}. \tag{1.4}$$

Let $\mathscr{H}_0$ be the completion of $C_0^{\infty,2}$ with this norm.

Let S denote the space of Schwartz, and H_s the Sobolev space of order s, $s \in \mathbb{R}$, i.e., the completion of C_0^∞ with the norm $\|f\|_s = \|(1 + \zeta^2)^{s/2} Ff\|$, $f \in C_0^\infty$ where F denotes the Fourier transform, and $\| \ \|$ the $\mathscr{L}^2$ norm.

The norm (1.3) is equivalent with the norm of $H_1 \otimes \mathscr{L}^2$, and they coincide as sets. In this case the Klein-Gordon equation is equal to

$$i \frac{\partial}{\partial t} f = H_0 f, \qquad H_0 = \begin{bmatrix} 0 & 1 \\ -\Delta + m^2 & 0 \end{bmatrix} \tag{1.5}$$

We denote by $\sigma(A)$, $\sigma_e(A)$, and $\sigma_{ac}(A)$ the spectrum, the essential spectrum and the absolutely continuous spectrum of a selfadjoint operator A, [3]. We have

Theorem 1. *H_0 is selfadjoint in $\mathscr{H}_0$ with domain $D(H_0) = H_2 \otimes H_1$ and is essentially selfadjoint on $C_0^{\infty,2}$. It is absolutely continuous and $\sigma(H_0) = (-\infty, -m] \cup [m, \infty)$.*

Proof: See [1] Q.E.D.

Let us consider again the interacting case. The energy of the field is given by

$$E(\psi) = \int d^n x \left\{ \sum_{i=1}^{n} |(D_i - b_i)\psi|^2 + (m^2 + q)|\psi|^2 + \left| \frac{\partial}{\partial t} \psi \right|^2 \right\} \tag{1.6}$$

where $q(x) = q_s - b_0^2$.

As in the free case we associate with the energy integral a sesquilinear form, 'the energy sesquilinear form'

$$(f, g)_E = \sum_{i=1}^{n} ((D_i - b_i)f_1, (D_i - b_i)g_1) + ((m^2 + q)f_1, g_1) + (f_2, g_2) \tag{1.7}$$

$$f, g \in C_0^{\infty,2}.$$

The operator h is symmetric in the energy sesquilinear form, i.e.,

$$(hf, g)_E = (f, hg)_E, \qquad f, g \in D(h),$$

but the form $(\cdot, \cdot)_E$ will not be positive in general.

We will introduce an assumption assuring that the energy sesquilinear form is positive:

A_0: There is a constant $\varepsilon > 0$ such that

$$\int q^-(x)|f(x)|^2 \, d^n x \leqslant \sum_{i=1}^{n} \|D_i f\|^2 + (m^2 - \varepsilon)\|f\|^2, \quad f \in C_0^\infty$$

by $q^\pm$ we denote the positive and negative parts of $q(x)$.

Lemma 1.2. *If A_0 is satisfied we have*

$$(f, f)_E \geqslant \varepsilon\,((f_1, f_1) + (f_2, f_2)), \quad f \in C_0^{\infty, 2}$$

Proof: See [1] Lemma 2.1. Q.E.D.

Then $(\cdot, \cdot)_E$ is a norm. We denote by $\mathscr{H}_E$ the completion of $C_0^{\infty, 2}$ with that norm.

Before we give a necessary and sufficient condition for A_0 to be satisfied let us see what it means for an electric potential of Coulomb type, i.e., $q_s(x) \equiv 0$ and $b_0(x) = e/|x|$.

A_0 is satisfied if

$$e^2 \int \frac{1}{|x|^2} |f(x)|^2 \, dx \leqslant \int (k^2 + \lambda)|Ff(k)|^2 \, d^n k, \quad f \in C_0^\infty$$

but by Hardy's inequality for $n \geqslant 3$

$$\int \frac{1}{|x|^2} |f(x)|^2 \, d^n x \leqslant \left(\frac{2}{n-2}\right)^2 \int k^2 |Ff(k)|^2 \, d^n k,$$

Then A_0 is satisfied if $|e| \leqslant (n-2)/2$.

It is known that the constant in Hardy's inequality is the best possible. In the usual system of unities this means, for $n = 3$, $Z \leqslant 68.5$, where Z is the atomic number.

Let us define [5]

$$B_\lambda(q) = \inf_{\psi > 0} \sup_x \frac{1}{\psi} \int |q(y)| \sigma_{2,\lambda}(x - y)\psi(y) \, dy,$$

where $\sigma_{2,\lambda}(x)$ is the inverse Fourier transform of $(2\pi)^{-n/2}(\lambda + |\zeta|^2)^{-1}$, $\lambda > 0$. Then

Lemma 1.3. *A_0 is satisfied if and only if $B_\lambda(q^-) \leqslant 1$ for some $\lambda < m^2$.*

Proof: See [1], Lemma 1.1. Q.E.D.

Let us introduce

$$S_\lambda(q) = \sup_x \int |q(y)| \sigma_{2,\lambda}(x - y) \, dy.$$

We have $B_\lambda(q) \leqslant S_\lambda(q)$. Then A_0 is satisfied if $S_\lambda(q^-) \leqslant 1$ for some $\lambda < m^2$. In the case of a scalar potential of Coulomb type, i.e. $b_0 \equiv 0$, $q_s = e/|x|$, this gives, for $n = 3$, $e < 2m$.

Let us introduce some notations [4]. For $\alpha > 0$ let

$$\begin{aligned} \omega_\alpha(|y|) &= |y|^{\alpha-n}, \quad 0 < \alpha < n, \\ &= 1 - \lg|y|, \quad \alpha = n, \\ &= 1, \quad \alpha > n. \end{aligned}$$

$$N_{\alpha,\delta,x}(q) = \int_{|y|<\delta} |q(x-y)|^2 \omega_\alpha(y)\, dy.$$

$$N_{\alpha,\delta}(q) = \sup_x N_{\alpha,\delta,x}(q), \qquad N_{\alpha,x}(q) = N_{\alpha,1,x}(q)$$

$$N_\alpha(q) = N_{\alpha,1}(q).$$

We denote by N_α the set of functions q such that $N_\alpha(q) < \infty$.

We introduce a new assumption

A_1:

1) $b_i(x) \in N_2$, $1 \leqslant i \leqslant n$ and if $n \geqslant 2$, $N_{2,\delta}(b_i) \xrightarrow[\delta\to 0]{} 0$

2) $q(x) = q_1(x) + q_c(x)$, $|q_1|^{1/2} \in N_2$, and if $n \geqslant 2$, $N_{2,\delta}(|q_1|^{1/2}) \xrightarrow[\delta\to 0]{} 0 \cdot q_c(x) \equiv 0$ if $n \leqslant 2$, and $q_c(x) = -e^2/|x|^2$, $|e| \leqslant (n-2)/2$ if $n > 2$.

Lemma 1.4. *If A_0 and A_1 are satisfied there exist two constants C_1, $C_2 > 0$ such that*

$$C_2(\|f_1\|_1^2 + \|f_2\|^2) \leqslant (f,f)_E \leqslant C_1(\|f_1\|_1^2 + \|f_2\|^2).$$

Proof:

$$\begin{aligned} (f,f)_E &= \sum_{i=1}^n \|(D_i - b_i)f_1\|^2 + ((m+q)f_1, f_1) + (f_2, f_2) \\ &\leqslant C_1(\|f_1\|_1^2 + \|f_2\|). \end{aligned}$$

where we applied Hardy's inequality and Lemma 2.2 of [1]. Finally

$$\begin{aligned} (f,f)_E \geqslant{} & \sum_{i=1}^n \|D_i f_1\|^2 - 2\sum_{i=1}^n \|D_i f_1\|\,\|b_i f_1\| - \varepsilon\|f_1\|_1^2 - K\|f_1\|^2 - \\ & - \left(\frac{2e}{n-2}\right)^2 \|f_1\|_1^2 + \|f_2\|^2, \end{aligned}$$

then

$$\left(1 - \varepsilon - \left(\frac{2e}{n-2}\right)^2\right)\|f_1\|_1^2 + \|f_2\|^2 \leqslant (f,f)_E + \|f_2\|^2,$$

hence $(f,f)_E \geqslant C_2(\|f_1\|_1^2 + \|f_2\|^2)$, for some $C_2 > 0$. Q.E.D.

This implies that the norm of $\mathscr{H}_E$ is equivalent to the norm of $H_1 \otimes \mathscr{L}^2$ and they coincide as sets.

We need the following assumption:

A_2:

$$N_{4,x}(b_i) + N_{4,x}(|q_1|^{1/2}) \xrightarrow[|x|\to\infty]{} 0, \ 1 \leqslant i \leqslant n$$

Lemma 1.5. *Let A_1 be satisfied. Then l (see 1.2) has a self-adjoint bounded below extension, denoted by L, (a 'quadratic form extension'). If A_2 is also satisfied the essential spectrum of L coincides with $[m^2, \infty)$.*

Proof: We define the sesquilinear form

$$\tilde{l}(f, g) = \sum_{i=1}^{n} (D_i - b_i)f, (D_i - b_i)g) + ((m^2 + q)fg), \quad f, g \in C_0^\infty.$$

As in Lemma 1.4 we have

$$|\tilde{l}(f, f)| \leqslant C\|f\|_1^2, \quad f \in C_0^\infty, \quad C > 0$$

and

$$(1 - \varepsilon)\|f\|_1^2 \leqslant \tilde{l}(f, f) + K(f, f), \quad f \in C_0^\infty, \varepsilon < 1.$$

Then $\tilde{l}$ extends to a closed, symmetric, bounded below form with domain H_1. The associated selfadjoint operator is the extension of L that we need.

If A_2 is also satisfied we prove as in Theorem 1 of [6] that the essential spectrum of L coincides with $[m^2, \infty)$. Q.E.D.

Note that if A_0 is also satisfied $L \geqslant \varepsilon > 0$. Then $\sqrt{L}$ is selfadjoint, positive, with domain $D(\sqrt{L}) = H_1$. Moreover it is essentially selfadjoint on C_0^∞, and $\sigma_e(\sqrt{L}) = [m, \infty)$. The energy norm is given by

$$(f, f)_E = (\sqrt{L} f_1, \sqrt{L}, g_1) + (f_2, g_2), \quad f, g \in \mathscr{H}_E.$$

We define

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} \sqrt{L} & 1 \\ \sqrt{L} & -1 \end{bmatrix}$$

U is a unitary operator from $\mathscr{H}_E$ onto $\mathscr{H} = \mathscr{L}^2 \oplus \mathscr{L}^2$. Let H_L be

$$H_L = \begin{bmatrix} 0 & 1 \\ L & 0 \end{bmatrix},$$

then

$$\hat{H}_L = UH_LU^{-1} = \begin{bmatrix} \sqrt{L} & 0 \\ 0 & -\sqrt{L} \end{bmatrix}$$

$D(\hat{H}_L) = H_1 \otimes H_1$. Also let

$$V = \begin{bmatrix} 0 & 0 \\ 0 & Q \end{bmatrix}$$

then

$$\hat{V} = Q\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad Q = 2b_0(x).$$

We will prove that $\hat{H} = \hat{H}_L + \hat{V}$ is selfadjoint in $\mathscr{H}$ with domain $D(\hat{H}) = H_1 \otimes H_1$. Then h (see 1.2):

$$h = \begin{bmatrix} 0 & 1 \\ l & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & Q \end{bmatrix}$$

will have a selfadjoint extension, H,

$$H = U^{-1}\hat{H}U = H_L + V, \qquad D(H) = D(L) \otimes H_1.$$

To do that we introduce the following assumptions:

A_3: $b_0 = b_0^1 + b_0^c$, $b_0^1 \in N_2$ and if $n \geqslant 2$

$N_{2,j}(b_0^1) \xrightarrow[\delta \to 0]{} 0$. $b_0^c(x) \equiv 0$ if $n \leqslant 2$

$n \geqslant 3$ $b_0^c(x) = \dfrac{e}{|x|}$, where $|e| < \dfrac{n-2}{2\sqrt{17}}$.

A_4: $N_{2,x}(b_0^1) \xrightarrow[|x| \to \infty]{} 0$.

Theorem 2. *Let A_0 A_1 and A_3 be satisfied. Then h (see 1.2) has a selfadjoint extension, H, with domain $D(H) = D(L) \otimes H_1$. If A_2 and A_4 are also satisfied the essential spectrum of H coincides with $(-\infty, -m] \cup [m, \infty)$.*

Proof: Let us define
$\hat{V} = \hat{V}_1 + \hat{V}_2$,

where

$$\hat{V}_1 = 2b_0^1(x)\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \text{and} \quad \hat{V}_2 = 2b_0^c(x)\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$

Then

$$\|\hat{V}_1 f\|^2 = 8\int |b_0^1|^2 |f_1 - f_2|^2\, dx \leqslant$$
$$\leqslant 16\int |b_0^1|^2(|f_1|^2 + |f_2|^2)\, dx \leqslant$$
$$\leqslant 16(\|b_0 f_1\|^2 + \|b_0 f_2\|^2).$$

But for any $\varepsilon > 0$

$$\|b_0 f_i\| \leqslant \varepsilon \|f_i\|_1 + K\|f_i\|, \quad i = 1, 2$$

by Lemma 2.2 of [1].

Then for any $\varepsilon > 0$ there is a K such that

$$\|\hat{V}_1 f\| \leqslant \varepsilon(\|\sqrt{L} f_1\| + \|\sqrt{L} f_2\|) + K(\|f_1\| + \|f_2\|)$$

Thus $\hat{V}_1$ is $\hat{H}_L$ bounded with relative bound zero.

We must prove that

$$\| \hat{V}_2 f \|^2 \leqslant \varepsilon \| \hat{H}_L f \|^2 + K \| f \|^2$$

for some $\varepsilon < 1$ and any $f \in C_{0}^{\infty}{}_{,}{}^{2}$. It follows from an easy calculation that this is true if

$$17\, e^2 \left\| \frac{1}{|x|} f \right\|^2 + \| \, |q_1|^{1/2} f \, \|^2 \leqslant \varepsilon \sum_{i=1}^{n} (\|(D_i - b_i) f\|^2 + K \| f \|^2),$$

for any $f \in C_0^\infty$. But by A_3, Hardy's inequality, Lemma 2.2 of [1] and Lemma 1.2, page 168 of [4], this is true.

Then $\hat{V}$ is $\hat{H}_L$-bounded with relative bound less than one. Hence $\hat{H}$ is selfadjoint with domain

$$D(\hat{H}) = H_1 \otimes H_1.$$

Moreover $\hat{V}_1$ is $\hat{H}_L$ compact (see Lemma 2.3 of [1]) Then

$$\sigma_e(\hat{H}_L + \hat{V}_1) = \sigma_e(\hat{H}_L) = (-\infty, -m] \cup [m, \infty).$$

Moreover since $\hat{V}_2$ is $\hat{H}_L + \hat{V}_1$ bounded we have:

$$\begin{aligned}(\hat{H} - Z)^{-1} - (\hat{H}_L + \hat{V}_1 - Z)^{-1} &= \\ &= (\hat{H} - Z)^{-1} \frac{1}{|x|^{1/2}} \frac{l}{|x|^{1/2}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} (\hat{H}_L + V - Z)^{-1} \\ &= \left[\frac{1}{|x|^{1/2}} (\hat{H} - Z)^{-1} \right]^* \frac{l}{|x|^{1/2}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} (\hat{H}_L + \hat{V}_1 - Z)^{-1}\end{aligned}$$

which is a compact operator. Then

$$\sigma_e(\hat{H}) = (-\infty, -m] U [m, \infty) \qquad \text{Q.E.D.}$$

The condition $|e| < (n - 2)/2\sqrt{17}$ is not optimal.

III. Gauge invariance

As in [1] we give conditions in the magnetic field that allow us to perform a Gauge transformation in the magnetic potential $b_i(x)$, $1 \leqslant i \leqslant n$. We assume, for simplicity, that $n > 2$ and that $b_i(x) \in \mathscr{L}^2{}_{\text{loc}}$, $1 \leqslant i \leqslant n$.

We denote

$$M_{\alpha,1}(q) = \sup_x \int_{|y|<1} |q(x - y)| |y|^{\alpha - n} \, dy$$

$M_{\alpha,1}$ is the set of functions q such that $M_{\alpha,1}(q) < \infty$. We also say that q is locally in $M_{\alpha.1}$ if $\mathscr{G} q \in M_{\alpha,1}$ for every $\mathscr{G} \in C_0^\infty$.

We introduce the following assumption A_T: Let $b_i(x)$ $1 \leqslant i \leqslant n$ be locally $M_{2,1}$ and suppose that $(\operatorname{Rot} b)_{ij}$ is a locally Hölder continuous tensor such that

$$C_{iJ}^T(x) = \int |D_i b_J - D_J b_i| r^{1-n} \, dy < \infty$$

for every x, where $1 \leqslant i, j \leqslant n$, $r = |x - y|$. Then (see Lemma 2.1 of [6])

$$b_i = b_i^T + \frac{\partial}{\partial x_i}\phi(x), \quad 1 \leqslant i \leqslant n$$

where

$$b_i^T(x) = K\int (\text{Rot } b)_{Ji}\left(\frac{\partial}{\partial x_J} r^{2-n}\right) dy,$$

$$\phi(x) = \int_C (b_i - b_i^T)\, dS^i, \qquad K = -\Gamma(\tfrac{1}{2}n)/2(n-2)\pi^{n/2}$$

C is any curve from a fixed point to x (the integral is independent of the curve) and the summation convention is used.

We introduce the following assumption:

A_1^T:

1) $C_{ij}^T \in N_2$ and $N_{2,\delta}(C_{ij}^T) \xrightarrow[\delta\to 0]{} 0$.

2) $q(x) = q_1(x) + q_c(x)$, $|q_1|^{1/2} \in N_2$ and $N_{2,\delta}(|q_1|^{1/2}) \xrightarrow[\delta\to 0]{} 0$.

$$q_c(x) = -\frac{e^2}{|x|^2}, \qquad |e| \leqslant \left(\frac{n-2}{2}\right).$$

We define $\mathscr{H}_T$ to be the completion of $C_0^{\infty,2}$ with the norm (1.7) but with b_i^T instead of b_i. The Klein-Gordon equation with b_i^T is equal to

$$i\frac{\partial}{\partial t}f = h_T f; \qquad h_T = \begin{bmatrix} 0 & 1 \\ l_T & Q \end{bmatrix}$$

$$l_T = \sum_{i=1}^{n} (D_i - b_i^T)^2 + m^2 + q(x), \qquad Q = 2b_0(x) \tag{2.1}$$

$$D(h_T) = \{f \in C_0^{\infty,2} \mid l_T f_1 \in \mathscr{L}^2 \quad \text{and} \quad Qf_2 \in \mathscr{L}^2\}$$

Then as in Lemma 1.5 we prove that l_T has a selfadjoint extension L_T. As in Theorem 2 we prove that L_T has a selfadjoint extension with domain $D(H_T) = D(L_T) \otimes H_1$.

We define [1]

$$\mathscr{H}_E = \{f \in \mathscr{L}^2 \quad \text{such that} \quad f = U^{-1}f^T \quad \text{for some} \quad f^T \in \mathscr{H}_T\}$$

with the scalar product

$$(f, g)_E = (f^T, g^T)_T \quad \text{where} \quad U^{-1}f^T(x) = e^{-i\phi(x)}f^T(x)$$

U is a unitary operator from $\mathscr{H}_E$ onto $\mathscr{H}_T$ by construction. Since

$$(D_i + b_i^T)Uf = (D_i + b_i^T)\, e^{i\phi(x)}f(x) = U(D_i + b_i)f,$$

$\mathscr{H}_E$ is the completion of $U^{-1}C_0^{\infty,2}$ with the scalar product (1.7). Then

Theorem 3. *If A_0, A^T, A_1^T and A_3 are satisfied h (see 1.2) has a selfadjoint extension, H in $\mathscr{H}_E$. If A_2 and A_4 are also satisfied then*

$$\sigma_e(H) = (-\infty, -m]U[m, \infty).$$

Proof: We define

$$H = U^{-1} H_T U.$$

We only need to prove that H is an extension of L. But

$$H = U^{-1} \begin{bmatrix} 0 & 0 \\ L_T & Q \end{bmatrix} U = \begin{bmatrix} 0 & 0 \\ U^{-1} L_T U & Q \end{bmatrix}$$

so we must prove that $L = U^{-1} L_T U$ is an extension of l. But if $f \in D(l)$, then

$$(Ulf, Ug) = \sum_{i=1}^{n} ((D_i - b_i^T)Uf, (D_i - b_i^T)Ug) + \\ + ((m^2 + q)f, g) = l_T(Uf, Ug), \quad Ug \in C_0^\infty.$$

then $f \in D(L_T)$ and $L_T U f = Ulf$, i.e.

$$lf = U^{-1} L_T U f = Lf. \qquad \text{Q.E.D.}$$

Conclusions

We derived two representations of (1.1) as an equation which is first order in time. Namely

$$i \frac{\partial}{\partial t} f = Hf, \qquad H = \begin{bmatrix} 0 & 1 \\ L & Q \end{bmatrix}, \qquad f \in \mathscr{H}_E$$

and

$$i \frac{\partial}{\partial t} \hat{f} = \hat{H} \hat{f}, \qquad \hat{H} = \begin{bmatrix} \sqrt{L} & 0 \\ 0 & -\sqrt{L} \end{bmatrix} + Q \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$\hat{f} = \begin{pmatrix} \hat{f}_+ \\ \hat{f}_- \end{pmatrix} \in \mathscr{H} = \mathscr{L}^2 \otimes \mathscr{L}^2.$$

They are unitary equivalent. The second one has the advantage that the scalar product in the Hilbert space where the representation is given does not depend on the interaction, and is more suitable for the physical interpretation. In the free case we have

$$i \frac{\partial}{\partial t} \hat{f} = \begin{bmatrix} \sqrt{-\Delta + m^2} & 0 \\ 0 & -\sqrt{-\Delta + m^2} \end{bmatrix} \hat{f},$$

We see then that the $\hat{f}_+$, $\hat{f}_-$ are the usual positive and negative energy components (this is sometimes called the free particle representation, see [7]). We can define a position operator as multiplication by x; and $|\hat{f}_+(x)|^2$ and $|\hat{f}_-(x)|^2$ can be interpreted as the (positive!!) probability density for particles with positive and negative energy respectively. The negative energy solutions are interpreted in terms of antiparticles in the usual way.

If $b_0(x) \equiv 0$, i.e., if we only have scalar and magnetic field the Hamiltonian $\hat{H}$ is still diagonal, and the positive and negative energy solutions evolve in an independent way.

However, if the electric field is different from zero, the Hamiltonian is not diagonal anymore. But if the wave operators exist (see [1]) and the intertwining relations are satisfied, i.e., $\psi(\hat{H})\omega_{\pm} = \omega_{\pm}\psi(\hat{H}_0)$, we have

$$S\psi(\hat{H}_0) = \omega_{+}^{*}\omega_{-}\psi(\hat{H}_0) = \psi(\hat{H}_0)S.$$

Then the scattering matrix commutes with any Borel function of the free Hamiltonian, in particular with the projectors onto the positive and negative energy subspaces, and asymptotically there is no Klein paradox.

Of course this representation is possible only if A_0 is satisfied, i.e., if the external fields are not too strong. But in fact a description of a relativistic spin zero particle by a one particle quantum mechanical equation is only expected to hold for weak, slowly varying external fields (see [2] page 199).

We have seen then that the Klein-Gordon equation gives, for weak fields, a relativistic quantum mechanical description of a spin zero particle with a selfadjoint Hamiltonian, in a Hilbert space, with positive metric, where a position operator and a (positive!) density of probability is defined (it is often said in the literature that such a representation does not exist).

It seems that this representation has not been noticed before in the literature. In fact the Hamiltonian $\hat{H}$ contains the operator $\sqrt{L}$ which is usually rejected as intractable or is expanded in series in the text-books in quantum mechanics.

It should be noted that $\sqrt{L}$ is not a local operator, but the equation $i(\partial/\partial t)\hat{f} = \hat{H}f$ is local because it is equivalent to the Klein-Gordon equation (1.1.) which is local.

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