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Qualitative properties of the Dirac equation in a central potential

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Abstract. The Dirac equation for a massive spin-$\frac{1}{2}$ field in a central potential V in three dimensions is studied without fixing *a priori* the functional form of V. The second-order equations for the radial parts of the spinor wavefunction are shown to involve a squared Dirac operator for the free case, whose essential self-adjointness is proved by using the Weyl limit point-limit circle criterion, and a 'perturbation' resulting from the potential. One then finds that a potential of Coulomb type in the Dirac equation leads to a potential term in the above second-order equations which is not even infinitesimally form-bounded with respect to the free operator. Moreover, the conditions ensuring essential self-adjointness of the second-order operators in the interacting case are changed with respect to the free case, i.e. they are expressed by a majorization involving the parameter in the Coulomb potential and the angular momentum quantum number. The same methods are applied to the analysis of coupled eigenvalue equations when the anomalous magnetic moment of the electron is not neglected.

1. Introduction

In the same year when Dirac derived the relativistic wave equation for the electron [1], the work of Darwin and Gordon had already exactly solved such an equation in a Coulomb potential in three spatial dimensions [2, 3]. Since those early days, several efforts have been produced in the literature to solve the Dirac equation with other forms of central potentials, until the recent theoretical attempts to describe quark confinement [4–8]. In the present paper we study the mathematical foundations of the eigenvalue problem for a massive spin-$\frac{1}{2}$ field in a central potential $V(r)$ on $\mathbb{R}^3$, without specifying *a priori* which function we choose for $V(r)$. In other words, we prefer to draw conclusions on $V(r)$ from a careful mathematical investigation.

By doing so, we hope to elucidate the general framework of relativistic eigenvalue problems on the one hand, and to develop powerful tools to understand some key features of central potentials on the other. For this purpose, in section 2 we focus on the radial parts of the spinor wavefunction, casting the corresponding second-order differential operators in a convenient form for the subsequent analysis. In section 3, the Weyl limit point-limit circle criterion [9] is used to prove that the squared Dirac operator for the free problem is essentially self-adjoint on the set $C_0^\infty(0,\infty)$ of smooth functions on $(0,\infty)$ with compact support away from the origin. In section 4 some boundedness criteria for perturbations [9, 10] are first described and then applied when the potential in the original Dirac equation consists of terms of Coulomb and/or linear type. The effects of the anomalous magnetic moment of the electron are studied in section 5. Concluding remarks and open problems are presented in section 6.

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2. Second-order equations for stationary states

For a charged particle with spin in a central field, the angular momentum operator and the parity operator with respect to the origin of the coordinate system commute with the Hamiltonian. Thus, states with definite energy, angular momentum and parity occur. The corresponding spinor wavefunction for stationary states reads [11, 12]

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} g(r)\Omega_{j,l,m} \\ (-1)^{\frac{1+l-l'}{2}} f(r)\Omega_{j,l',m} \end{pmatrix}$$

where $\Omega_{j,l,m}$ and $\Omega_{j,l',m}$ are the spinor harmonics defined, for example, in [11, 12], and $l = j \pm \frac{1}{2}, l' = 2j - l$.

The stationary Dirac equation in a central potential $V(r)$ takes the form (m_0 being the rest mass of the particle of linear momentum $\vec{p}$)

$$\begin{pmatrix} m_0c^2 + V(r) & \vec{\sigma}\cdot\vec{p} \\ \vec{\sigma}\cdot\vec{p} & -m_0c^2 + V(r) \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = E \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

and leads eventually to the following coupled system of first-order differential equations (having defined $F(r) \equiv rf(r)$ and $G(r) \equiv rg(r)$):

$$\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r}\right) G(r) = (\lambda_1 - W(r))F(r) \tag{2.1}$$

$$\left(-\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r}\right) F(r) = (-\lambda_2 - W(r))G(r) \tag{2.2}$$

where $k = -l - 1$ (if $j = l + \frac{1}{2}$) or l (if $j = l - \frac{1}{2}$), and we have defined

$$W(r) \equiv \frac{V(r)}{\hbar c} \tag{2.3}$$

$$\lambda_1 \equiv \frac{E + m_0c^2}{\hbar c} \tag{2.4}$$

$$\lambda_2 \equiv \frac{-E + m_0c^2}{\hbar c}. \tag{2.5}$$

Equation (2.1) yields a formula for $F(r)$ which, upon insertion into equation (2.2), leads to the second-order equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + p(r)\frac{\mathrm{d}}{\mathrm{d}r} + q(r)\right] G(r) = 0 \tag{2.6}$$

where

$$p(r) \equiv \frac{W'(r)}{(\lambda_1 - W(r))} \tag{2.7}$$

$$q(r) \equiv -\frac{k(k+1)}{r^2} + \frac{k}{r}p(r) + W^2(r) + (\lambda_2 - \lambda_1)W(r) - \lambda_1\lambda_2. \tag{2.8}$$

Equation (2.6) should be supplemented by the boundary condition $G(0) = 0$. It then describes a Sturm–Liouville equation nonlinear in the spectral parameter. In [13], the equivalence has been proved of the radial Dirac equations (2.1) and (2.2) to the parameter-dependent Sturm–Liouville equation (2.6) (the parameter λ used in [13] corresponds to our E, and $m_0c^2 = 1$ units are used therein). By equivalence we mean that, under suitable assumptions on the potential, the function G solving equation (2.6) is found to belong to the prescribed space $H_0^1(\mathbb{R}_+)$, i.e. the space of absolutely continuous functions on $[0, \infty)$ which are square integrable on $\mathbb{R}_+$ jointly with their first derivative and vanish at the origin. Now we can use a well known technique

to transform equation (2.6) into a second-order equation where the coefficient of $\frac{\mathrm{d}}{\mathrm{d}r}$ vanishes. This is achieved by defining the new function Ω such that [14]

$$\Omega(r) \equiv G(r) \exp \tfrac{1}{2} \int p(r)\, \mathrm{d}r. \tag{2.9}$$

In the few cases where exact analytic formulae are available in the literature one studies equation (2.6) and its counterpart for F (see equation (2.13)). However, equation (2.9) has the advantage of leading to a second-order equation for Ω in a form as close as possible to 'perturbations' of Schrödinger operators, and is hence preferred in our paper devoted to qualitative and structural properties. In non-relativistic quantum mechanics, such a method leads to a unitary map [9] transforming the radial Schrödinger equation in a central potential into an equation involving a radial Schrödinger operator $-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + U(r)$ acting on square-integrable functions on $\mathbb{R}_+$ which vanish at the origin. In our relativistic eigenvalue problem the transformation of the Hilbert space of square-integrable functions is no longer unitary, but remains of practical value. All nonlinear properties of the resulting Sturm–Liouville boundary-value problem are in fact encoded into a single function playing the role of a parameter-dependent potential term (see below), rather than two functions p and q as in (2.6)–(2.8). The function Ω is then found to obey the differential equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} + P_{W,E}(r) \right] \Omega(r) = \frac{(E^2 - m_0^2 c^4)}{\hbar^2 c^2} \Omega(r) \tag{2.10}$$

having defined

$$P_{W,E}(r) \equiv -W^2(r) + \frac{1}{2} \frac{W''}{(\lambda_1 - W)} + \frac{3}{4} \left(\frac{W'}{\lambda_1 - W} \right)^2 - \frac{k}{r} \frac{W'}{(\lambda_1 - W)} + \frac{2E}{\hbar c} W(r). \tag{2.11}$$

Such an equation may be viewed as follows: since the potential W 'perturbs' the 'free' problem for which W vanishes in equations (2.1) and (2.2), in the corresponding second-order equation (2.10) one deals with a 'free operator'

$$A_r^l \equiv -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} \qquad \text{for all} \quad l = 0, 1, \ldots \tag{2.12}$$

perturbed by the multiplication operator $P_{W,E}(r)$ defined in (2.11). An interesting programme is therefore emerging at this stage:

(i) First, prove (essential) self-adjointness of the 'free' operator A_r^l on a certain domain.
(ii) Second, try to understand whether the operator $A_r^l + P_{W,E}(r)$ in equation (2.10) remains self-adjoint on the same domain. If this condition is too restrictive, try to derive all properties of this 'perturbed' second-order operator.

If one first uses equation (2.2) to relate $G(r)$ to $\frac{\mathrm{d}F}{\mathrm{d}r}$ and F, one finds instead the Sturm–Liouville equation (cf [13])

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \tilde{p}(r) \frac{\mathrm{d}}{\mathrm{d}r} + \tilde{q}(r) \right] F(r) = 0 \tag{2.13}$$

supplemented by the boundary condition $F(0) = 0$, where (cf (2.7) and (2.8))

$$\tilde{p}(r) \equiv -\frac{W'(r)}{(\lambda_2 + W(r))} \tag{2.14}$$

$$\tilde{q}(r) \equiv -\frac{k(k-1)}{r^2} - \frac{k}{r} \tilde{p}(r) + W^2(r) + (\lambda_2 - \lambda_1) W(r) - \lambda_1 \lambda_2. \tag{2.15}$$

Thus, after defining (cf (2.9))

$$\tilde{\Omega}(r) \equiv F(r) \exp \tfrac{1}{2} \int \tilde{p}(r)\, \mathrm{d}r \tag{2.16}$$

one finds for $\tilde{\Omega}(r)$ the second-order differential equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{k(k-1)}{r^2}+\tilde{P}_{W,E}(r)\right]\tilde{\Omega}(r)=\frac{(E^2-m_0^2c^4)}{\hbar^2c^2}\tilde{\Omega}(r) \tag{2.17}$$

having now defined (cf (2.11))

$$\tilde{P}_{W,E}(r)\equiv -W^2(r)-\frac{1}{2}\frac{W''}{(\lambda_2+W)}+\frac{3}{4}\left(\frac{W'}{\lambda_2+W}\right)^2-\frac{k}{r}\frac{W'}{(\lambda_2+W)}+\frac{2E}{\hbar c}W(r). \tag{2.18}$$

Since $k=-l-1$ if $j=l+\frac{1}{2}$, and $k=l$ if $j=l-\frac{1}{2}$, the 'free' operator in equation (2.17) reads now

$$\tilde{A}_r^l\equiv -\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{(l+1)(l+2)}{r^2}\qquad \text{for all}\quad l=0,1,\ldots \tag{2.19a}$$

$$\tilde{A}_r^l\equiv -\frac{d^2}{dr^2}+\frac{l(l-1)}{r^2}\qquad \text{for all}\quad l=1,2,\ldots. \tag{2.19b}$$

Note that $P_{W,E}(r)$ has a second-order pole at $\lambda_1=W$ (see (2.11)) and $\tilde{P}_{W,E}(r)$ has a second-order pole at $\lambda_2=-W$. Thus, the analysis of the interacting case (i.e. with $W(r)\neq 0$) is performed in section 4 at fixed values of E and away from such singular points.

3. Weyl criterion for the squared Dirac operator in the free case

The self-adjointness properties of the free operator (2.12) should be studied by considering separately the case $l>0$ and the case $l=0$. For positive values of the quantum number l, A_r^l turns out to be essentially self-adjoint. This means, by definition, that its closure (i.e. the smallest closed extension) is self-adjoint, which implies that a unique self-adjoint extension of A_r^l exists [15]. In general, if several self-adjoint extensions exist, one has to understand which one should be chosen, since they are distinguished by the physics of the system being described [9, 15]. This is why it is so desirable to make sure that the operator under investigation is essentially self-adjoint. We here rely on a criterion due to Weyl, and the key steps are as follows [9].

The function V is in the *limit circle* case at zero if for some, and therefore all λ, *all* solutions of the equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\varphi(x)=\lambda\varphi(x) \tag{3.1}$$

are square integrable at zero, i.e. for them

$$\int_0^a|\varphi(x)|^2\,\mathrm{d}x<\infty \tag{3.2}$$

with finite values of a, e.g. $a\in]0,1]$. If $V(x)$ is not in the limit circle case at zero, it is said to be in the *limit point* case at zero. The Weyl limit point-limit circle criterion states that, if V is a continuous real-valued function on $(0,\infty)$, then the operator

$$\mathcal{O}\equiv -\frac{d^2}{dx^2}+V(x) \tag{3.3}$$

is essentially self-adjoint on $C_0^\infty(0,\infty)$ if and only if $V(x)$ is in the limit point case at both zero and infinity. The property of being in the limit point at zero relies on the following theorem [9].

Theorem 3.1. *Let V be continuous and positive near zero. If*

$$V(x) \geqslant \tfrac{3}{4}x^{-2} \tag{3.4}$$

near zero, then $\mathcal{O}$ is in the limit point case at zero.

The limit point property at ∞ means that the limit circle condition at ∞ is not fulfilled, i.e. the condition

$$\int_a^\infty |\varphi(x)|^2 \,\mathrm{d}x < \infty \tag{3.5}$$

does not hold. To understand when this happens, one can use the following [9].

Theorem 3.2. *If V is differentiable on $(0, \infty)$ and bounded above by a parameter K on $[1, \infty)$, and if*

$$\int_1^\infty \frac{\mathrm{d}x}{\sqrt{K - V(x)}} = \infty \tag{3.6}$$

$$V'(x)|V(x)|^{-\frac{3}{2}} \qquad \textit{is bounded near } \infty \tag{3.7}$$

then $V(x)$ is in the limit point case at ∞.

Thus, a necessary and sufficient condition for the existence of a unique self-adjoint extension of $\mathcal{O}$ is that its eigenfunctions should fail to be square integrable at zero and at ∞. Powerful operational criteria are provided by the check of (3.4), (3.6) and (3.7), which only involve the potential.

In our problem, for all $l \geqslant 1$, the 'potential' $\tilde{V}_l(r) \equiv \frac{l(l+1)}{r^2}$ is of course in the limit point at zero, since the inequality (3.4) is then satisfied. Moreover, $\tilde{V}_l(r)$ is differentiable on $(0, \infty)$, bounded above by $\chi_l \equiv l(l+1)$ on $[1, \infty)$, and such that

$$\int_1^\infty \frac{\mathrm{d}x}{\sqrt{\chi_l - \tilde{V}_l(x)}} = \frac{1}{\sqrt{l(l+1)}} \int_1^\infty \frac{x}{\sqrt{x^2 - 1}} \,\mathrm{d}x = \infty \tag{3.8}$$

$$\tilde{V}_l'(r)|\tilde{V}_l(r)|^{-\frac{3}{2}} = -\frac{2}{\sqrt{l(l+1)}} \qquad \text{for all} \quad r. \tag{3.9}$$

Hence all conditions of theorem 3.2 are satisfied, which implies that $\tilde{V}_l(r)$ is in the limit point at ∞ as well. By virtue of the Weyl limit point-limit circle criterion, the free operator A_r^l defined in (2.12) is then essentially self-adjoint on $C_0^\infty(0, \infty)$ for all $l > 0$.

When $l = 0$, however (for which $k = -1$), A_r^l reduces to the operator $-\frac{\mathrm{d}^2}{\mathrm{d}r^2}$, which has deficiency indices $(1, 1)$. Recall that for an (unbounded) operator B with adjoint $B^\dagger$, deficiency indices are the dimensions of the spaces of solutions of the equations $B^\dagger u = \pm \mathrm{i}u$. More precisely, one first defines the deficiency sub-spaces ($D(B^\dagger)$ being the domain of $B^\dagger$)

$$\mathcal{H}_+(B) \equiv \{u \in D(B^\dagger) : B^\dagger u = \mathrm{i}u\} \tag{3.10}$$

$$\mathcal{H}_-(B) \equiv \{u \in D(B^\dagger) : B^\dagger u = -\mathrm{i}u\} \tag{3.11}$$

with the corresponding deficiency indices

$$n_+(B) \equiv \dim \mathcal{H}_+(B) \tag{3.12}$$

$$n_-(B) \equiv \dim \mathcal{H}_-(B). \tag{3.13}$$

The operator B is self-adjoint if and only if $n_+(B) = n_-(B) = 0$, but has self-adjoint extensions provided that $n_+(B) = n_-(B)$ [9, 15]. In our case, half of the solutions of the equations $(A_r^0)^\dagger u = \pm \mathrm{i}u$ are square-integrable on $\mathbb{R}_+$, which implies that $n_+(A_r^0) = n_-(A_r^0) = 1$. This

is easily proved because such equations with complex eigenvalues reduce to the ordinary differential equation [9]

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\mathrm{e}^{\alpha r} = \mathrm{i}\mathrm{e}^{\alpha r} \tag{3.14}$$

and

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\mathrm{e}^{\omega r} = -\mathrm{i}\mathrm{e}^{\omega r}. \tag{3.15}$$

In the former case, on setting $\alpha = \rho\mathrm{e}^{\mathrm{i}\theta}$, with ρ and $\theta \in \mathbb{R}$, one finds $\rho = \pm 1, \theta = -\frac{\pi}{4}$, which leads to the two roots of the equation $-\alpha^2 = \mathrm{i}$:

$$\alpha_1 = \frac{1}{\sqrt{2}} - \frac{\mathrm{i}}{\sqrt{2}} \tag{3.16}$$

$$\alpha_2 = -\frac{1}{\sqrt{2}} + \frac{\mathrm{i}}{\sqrt{2}}. \tag{3.17}$$

In the latter case, ω solves the algebraic equation $\omega^2 = \mathrm{i}$, and hence one finds the roots

$$\omega_1 = \frac{1}{\sqrt{2}} + \frac{\mathrm{i}}{\sqrt{2}} \tag{3.18}$$

$$\omega_2 = -\frac{1}{\sqrt{2}} - \frac{\mathrm{i}}{\sqrt{2}}. \tag{3.19}$$

Only the roots α_2 and ω_2 are compatible with the request of square-integrable solutions of (3.14) and (3.15) on $\mathbb{R}_+$, and hence one finds $n_+(A_r^0) = n_-(A_r^0) = 1$ as we anticipated. This property implies that a one-parameter family of self-adjoint extensions of A_r^0 exists, with domain $D(A_r^0)$ given by

$$D(A_r^0) = \{u \in L^2(\mathbb{R}_+) : u, u' \in AC_{\mathrm{loc}}(\mathbb{R}_+); u'' \in L^2(\mathbb{R}_+); u(0) = \beta u'(0)\}. \tag{3.20}$$

Here $AC_{\mathrm{loc}}(\mathbb{R}_+)$ denotes the set of locally absolutely continuous functions on the positive half-line, the prime denotes differentiation with respect to r, and β is a real-valued parameter. Bearing in mind the limiting form of equation (2.10) when $l = 0$ and $W = 0$, this means that one is studying the case characterized by

$$\lambda \equiv \frac{(E^2 - m_0^2c^4)}{\hbar^2c^2} < 0 \tag{3.21}$$

for which the square-integrable eigenfunction of $-\frac{\mathrm{d}^2}{\mathrm{d}r^2}$ reads (σ being a real constant to ensure reality of E)

$$u(r) = \sigma\mathrm{e}^{-r\sqrt{|\lambda|}}. \tag{3.22}$$

On defining

$$(u, v) \equiv \int_0^\infty u^*(r)v(r)\,\mathrm{d}r$$

the boundary condition in (3.20) is obtained after integrating twice by parts in the integral defining the scalar product (A_r^0u, v) to re-express it in the form $(u, (A_r^0)^\dagger v)$, with u in the domain of A_r^0 and v in the domain of the adjoint $(A_r^0)^\dagger$. One then finds that both u and v should obey the boundary condition (3.20). In the light of (3.20)–(3.22) one obtains the very useful formula

$$1 = -\beta\sqrt{|\lambda|} \tag{3.23}$$

which implies

$$E^2 = m_0^2 c^4 - \frac{\hbar^2 c^2}{\beta^2}. \tag{3.24}$$

This means that in a relativistic problem a lower limit for β^2 (and hence for $|\beta|$) exists, to avoid having $E^2 < 0$.

To complete the analysis of squared Dirac operators in the free case, one has also to consider the operators $\tilde{A}_r^l$ defined in (2.19*a*) and (2.19*b*). The former has a 'potential' term $\frac{(l+1)(l+2)}{r^2}$ which is in the limit point case at both zero and infinity for all $l \geqslant 0$. The latter has a 'potential' term $\frac{l(l-1)}{r^2}$ which is in the limit point at zero with the exception of the value 1 of the quantum number l, for which $\tilde{A}_r^l$ reduces to the operator $-\frac{\mathrm{d}^2}{\mathrm{d}r^2}$, and hence we repeat the logical steps proving that such an operator has a one-parameter family of self-adjoint extensions. Once more, their domain is given by equation (3.20).

4. Second-order operators in the interacting case

Now we would like to understand whether the general results on perturbations of self-adjoint operators make it possible to obtain a better understanding of effects produced by the central potential $W(r)$ in equations (2.10) and (2.17) (the essential self-adjointness of the Dirac Hamiltonian with non-vanishing W is studied in [16], and several comments can be found in the following sections). For this purpose, the key steps are as follows [9].

(i) Let A and B be densely defined linear operators on a Hilbert space H with domains $D(A)$ and $D(B)$, respectively. If $D(A) \subset D(B)$ and if, for some a and b in $\mathbb{R}$,

$$\|B\varphi\| \leqslant a\|A\varphi\| + b\|\varphi\| \qquad \text{for all} \quad \varphi \in D(A) \tag{4.1}$$

then B is said to be *A-bounded*. The infimum of such a is called the *relative bound* of B with respect to A. If the relative bound vanishes, the operator B is said to be *infinitesimally small* with respect to A.

(ii) The Kato–Rellich theorem states that if A is self-adjoint, B is symmetric, and B is A-bounded with relative bound $a < 1$, then $A + B$ is self-adjoint on $D(A)$.

(iii) If the potential V can be written as

$$V = V_1 + V_2 \tag{4.2}$$

with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$, and if V is real-valued, then the operator $-\triangle + V(x)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ and self-adjoint on $D(-\triangle)$. As a corollary, the operator $-\triangle - \frac{e^2}{r}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

(iv) An analogue of the Kato–Rellich theorem exists which can be used to study the case when B is not A-bounded. The result can be stated after recalling the following definitions.
Let A be a self-adjoint operator on H. On passing to a spectral representation of A with associated measures $\{\mu_n\}_{n=1}^N$ on the spectrum of A, so that A is multiplication by x on the direct sum $\oplus_{n=1}^N L^2(\mathbb{R},\ \mathrm{d}\mu_n)$, one can consider

$$\mathcal{I} \equiv \left\{ \{\psi_n(x)\}_{n=1}^N : \sum_{n=1}^N \int_{-\infty}^{\infty} |x||\psi_n(x)|^2 \,\mathrm{d}\mu_n < \infty \right\} \tag{4.3}$$

and hence define, for ψ and $\varphi \in \mathcal{I}$,

$$q(\varphi, \psi) \equiv \sum_{n=1}^N \int_{-\infty}^{\infty} x\varphi_n^*(x)\psi_n(x)\,\mathrm{d}\mu_n. \tag{4.4}$$

Such a q is called the *quadratic form* associated with A, and one writes

$$Q(A) \equiv \mathcal{I}. \tag{4.5}$$

The *form domain* of the operator A is then, by definition, $Q(A)$, and can be viewed as the largest domain on which q can be defined.

(v) The KLMN theorem states that, if A is a positive self-adjoint operator and if $\beta(\varphi, \psi)$ is a symmetric quadratic form on $Q(A)$ such that

$$|\beta(\varphi, \varphi)| \leqslant a(\varphi, A\varphi) + b(\varphi, \varphi) \qquad \text{for all} \quad \varphi \in D(A) \tag{4.6}$$

for some $a < 1$ and $b \in \mathbb{R}$, then there exists a unique self-adjoint operator C with

$$Q(C) = Q(A) \tag{4.7}$$

and

$$(\varphi, C\psi) = (\varphi, A\psi) + \beta(\varphi, \psi) \qquad \text{for all} \quad \varphi, \psi \in Q(C). \tag{4.8}$$

Such a C is bounded below by $-b$.

(vi) If A is a positive self-adjoint operator, and B is a self-adjoint operator such that

$$Q(A) \subset Q(B) \tag{4.9}$$

and

$$|(\varphi, B\varphi)| \leqslant a(\varphi, A\varphi) + b(\varphi, \varphi) \qquad \text{for all} \quad \varphi \in D(A) \tag{4.10}$$

for some $a > 0$ and $b \in \mathbb{R}$, then B is said to be *relatively form-bounded* with respect to A. Furthermore, if a can be chosen arbitrarily small, B is said to be *infinitesimally form-bounded* with respect to A.

(vii) If the operator B is self-adjoint and relatively form-bounded, the parameter a being < 1, with respect to a positive self-adjoint operator A, then the KLMN theorem makes it possible to define the 'sum' $A + B$, although this mathematical construction may differ from the operator sum. In particular, B can be form-bounded with respect to A even though the intersection of their domains may be the empty set.

(viii) The KLMN theorem is physically relevant because it leads to the definition of Hamiltonians even when the Kato–Rellich criterion is not fulfilled. In other words, the request of dealing with $L^2 + L^\infty$ potentials is too restrictive. For example, the potential $V_\alpha(r) = -r^{-\alpha}$ belongs to $L^2 + L^\infty$ only if $\alpha < \frac{3}{2}$. However, if $\alpha \in [\frac{3}{2}, 2)$, one can use the KLMN theorem because, for all $\alpha < 2$, one can prove that $-r^{-\alpha}$ is infinitesimally form-bounded with respect to $-\triangle$ [9].

In our problem, the 'potential' terms in equations (2.10) and (2.17) are given by (2.11) and (2.18), respectively. If the potential $W(r)$ is of Coulomb type, i.e. (γ being a dimensionful constant)

$$W(r) = \frac{\gamma}{r} \tag{4.11}$$

the singular behaviour of $P_{W,E}(r)$ as $r \to 0$ is dominated by (for a *fixed value* of E)

$$-\frac{(\gamma^2 + \frac{1}{4} + k)}{r^2}$$

and the singular behaviour of $\tilde{P}_{W,E}(r)$ as $r \to 0$ is given instead by (again for a fixed value of E)

$$-\frac{(\gamma^2 + \frac{1}{4} - k)}{r^2}.$$

Thus, as $r \to 0$, the operators on the left-hand sides of both (2.10) and (2.17) reduce to

$$L_r \equiv \left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{(k^2 - \gamma^2 - \frac{1}{4})}{r^2} \right]. \tag{4.12}$$

In the operator L_r, the coefficient of r^{-2} is no longer greater than or equal to $\frac{3}{4}$ (see (3.4)) for the same values of l ensuring essential self-adjointness of the free problem. The inequality

$$k^2 - \gamma^2 - \tfrac{1}{4} \geqslant \tfrac{3}{4} \tag{4.13}$$

is instead fulfilled by

$$(l+1)^2 \geqslant \gamma^2 + 1 \qquad \text{for all} \quad l = 0, 1, \ldots \tag{4.14}$$

if $k = -l - 1$, and by

$$l^2 \geqslant \gamma^2 + 1 \qquad \text{for all} \quad l = 1, 2, \ldots \tag{4.15}$$

if $k = l$. Our result implies that, for all $|k| \geqslant 2$, essential self-adjointness on $C_0^\infty(0, \infty)$ of the second-order operators on the left-hand sides of (2.10) and (2.17) is obtained provided that $|\gamma| \leqslant \sqrt{3}$. This reflects the fact that a Coulomb potential in the first-order system (2.1) and (2.2) leads to 'potential' terms in the second-order equations (2.10) and (2.17) which are not even infinitesimally form-bounded with respect to the squared Dirac operators in the free case, because both the potential terms and the free operators contain terms proportional to r^{-2}. To study the limit point condition at infinity, we try to majorize the 'potential' $P_{W,E}$ obtained from the Coulomb potential (4.11), and we find that

$$|P_{W,E}(r)| \leqslant 2\frac{|E\gamma|}{\hbar c} + \frac{[|\gamma(1+k)|(\lambda_1 + |\gamma|) + \frac{3}{4}\gamma^2]}{\lambda_1^2}$$

if $r \in [1, \infty)$. Moreover, the integral (3.6) diverges when V is replaced by $P_{W,E}$, and the condition (3.7) is fulfilled as well, because

$$P'_{W,E}(r)|P_{W,E}(r)|^{-\frac{3}{2}} \propto r^{-\frac{1}{2}} \qquad \text{as} \quad r \to \infty.$$

The check of (3.6) and (3.7) for $\tilde{P}_{W,E}$ leads to the same results, and hence we use the Weyl criterion of section 3 to conclude that, *for fixed values* of E, essential self-adjointness on $C_0^\infty(0, \infty)$ of the second-order operators in equations (2.10) and (2.17) holds provided that the inequality $k^2 - \gamma^2 \geqslant 1$ is satisfied. This rules out $l = 0$ in (4.14) and $l = 1$ in (4.15). One then finds that $|\gamma| \leqslant \sqrt{3}$ as we said before.

The limiting form (4.12) is not affected by the addition of parts linear in r [6, 17, 18] to the right-hand side of (4.11), because the singular behaviour of $P_{W,E}(r)$ at fixed values of E as $r \to 0$ is still dominated by the Coulomb potential. In contrast, a purely linear potential

$$W(r) = \Gamma r \tag{4.16}$$

satisfies the request of infinitesimal form-boundedness of $P_{W,E}(r)$ with respect to the squared Dirac operators in the free case, because then the singular behaviour of $P_{W,E}(r)$ as $r \to 0$ is expressed by $-\frac{k\Gamma}{\lambda_1}\frac{1}{r}$ and the singular part of $\tilde{P}_{W,E}(r)$ as $r \to 0$ reads $-\frac{k\Gamma}{\lambda_2}\frac{1}{r}$. However, one might consider linear terms with compact support, i.e. vanishing for all r greater than some finite r_0, or weighted with exponential functions which ensure a fall-off condition at infinity, e.g. the potential (cf [17])

$$W(r) = \frac{\gamma}{r} + \Gamma r \mathrm{e}^{-\mu r} \tag{4.17}$$

where μ is positive. In such a case, the limiting behaviours of $P_{W,E}$ as $r \to 0$ and as $r \to \infty$ are still dominated by the Coulomb part in the potential W, and hence we again find essential self-adjointness on $C_0^\infty(0, \infty)$ provided that $k^2 - \gamma^2 \geqslant 1$.

In the physical literature, however, the potential has not been written in the form (4.17). To achieve quark confinement, a purely linear term has instead been added to the Coulomb part, also considering a split of the additional part into Lorentz scalar-type and Lorentz vector-like potentials. Furthermore, such a vector contribution is sometimes omitted in a phenomenological analysis, bearing in mind its non-perturbative nature (since the perturbative part has vector nature instead) [19]. Needless to say, such arguments are not compelling.

5. Inclusion of the anomalous magnetic moment

The second-order operators that we have analysed in the interacting case (see again equations (2.10) and (2.17)) are not 'squared Dirac operators' because the eigenvalues of the Dirac operator occur in their 'potential term'. It is therefore important to compare more carefully the predictions of the second-order equation for Ω (and $\tilde{\Omega}$) with the results obtained from squared Dirac operators studied in [16]. The latter are used in [16] because a theorem ensures that, given the (abstract) Dirac Hamiltonian

$$T = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix} + \begin{pmatrix} W_+ & 0 \\ 0 & W_- \end{pmatrix} \tag{5.1}$$

if one of the operators D_-D_+ or D_+D_- is essentially self-adjoint, then the operator T is essentially self-adjoint as well, where W_+ and W_- take into account the rest mass and the potential (see theorem 5.9 in [16]).

Let us now consider the effect of the anomalous magnetic moment μ of the electron in a central potential $V(r)$. With the notation of our section 2, the resulting set of coupled eigenvalue equations is found to be [16]

$$\left[\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r} - \mu W'(r)\right] G(r) = (\lambda_1 - W(r))F(r) \tag{5.2}$$

$$\left[-\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r} - \mu W'(r)\right] F(r) = (-\lambda_2 - W(r))G(r) \tag{5.3}$$

which implies, on using again the definition (2.9), that $\Omega(r)$ obeys the second-order equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} + P^{(\mu)}_{W,E}(r)\right]\Omega(r) = \frac{(E^2 - m_0^2c^4)}{\hbar^2c^2}\Omega(r) \tag{5.4}$$

where we have defined (cf equation (5.48) in [16])

$$P^{(\mu)}_{W,E}(r) \equiv P_{W,E}(r) + \mu\left[W'' + W'^2(\mu + (\lambda_1 - W)^{-1}) - 2\frac{k}{r}W'\right]. \tag{5.5}$$

For example, if a potential W of Coulomb type is considered, one finds from (4.11) and (5.5) that the limiting form of the eigenvalue equation (5.4) as $r \to 0$ is entirely dominated by the term proportional to μ. More precisely, in such a limit equation (5.4) reduces to

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\mu^2\gamma^2}{r^4}\right]\Omega(r) = 0 \tag{5.6}$$

which is solved by

$$\Omega(r) = r\mathrm{e}^{-\frac{\mu\gamma}{r}}. \tag{5.7}$$

An analogous method can be used for $\tilde{\Omega}(r)$ defined in (2.16), finding a parameter-dependent potential

$$\tilde{P}^{(\mu)}_{W,E}(r) \equiv \tilde{P}_{W,E}(r) + \mu\left[-W'' + W'^2\left(\mu + \frac{1}{(\lambda_2 + W)}\right) - 2\frac{k}{r}W'\right] \tag{5.8}$$

which leads again to the limiting behaviour (5.7) when $W(r) = \frac{\gamma}{r}$, but now for $\tilde{\Omega}(r)$, as $r \to 0$. We can therefore see, in a physically relevant example, that our approach, leading to second-order equations for Ω and $\tilde{\Omega}$, recovers qualitative agreement with the analysis in [16], where it is shown that, no matter how singular the central potential at $r = 0$ is, the Dirac operator is always well defined as long as $\mu \neq 0$. In other words, our formula (5.5) clearly accounts for the dominating effect of the anomalous magnetic moment with all potentials diverging at the origin. However, a rigorous result on the relation between our approach and the squared Dirac operators studied in [16] remains an interesting technical problem whenever $W(r) \neq 0$ (cf [13]).

6. Concluding remarks

The contributions of our paper, of a technical nature, consist in the application of analytic techniques that can help us to understand some key qualitative features of central potentials for the Dirac equation, with emphasis on the mathematical formulation of relativistic eigenvalue problems. Although the methods used in our investigation are well known in the literature, the overall picture remains, to our knowledge, original (see comments below). In particular, we would like to mention the following points (at the risk of slight repetitions).

(i) The forms (2.10) and (2.17) of the second-order equations for the radial parts of the spinor wavefunction, with $P_{W,E}(r)$ and $\tilde{P}_{W,E}(r)$ defined in (2.11) and (2.18), respectively, is very convenient if one wants to understand whether the potential can affect the self-adjointness domain of the free problem.

(ii) The identification of the domains of (essential) self-adjointness of the operators defined in (2.12), (2.19*a*) and (2.19*b*) is helpful as a first step towards the problem with non-vanishing potential $W(r)$, and clarifies the general framework.

(iii) A potential of Coulomb type, although quite desirable from a physical point of view, leads to some non-trivial features with respect to the non-relativistic case. We have in fact seen that $P_{W,E}(r)$ and $\tilde{P}_{W,E}(r)$ fail to be infinitesimally form-bounded with respect to the squared Dirac operators in the free case, if $W(r)$ contains a Coulomb term. Moreover, the limit-point condition at zero for the potential in the second-order operators in the interacting case is only fulfilled if the inequalities (4.14) or (4.15) hold. In other words, the essential self-adjointness on $C_0^\infty(0, \infty)$ of the second-order operators with non-vanishing potential is still obtained, but under more restrictive conditions expressed by (4.14) and (4.15). This may have non-trivial physical implications: if essential self-adjointness fails to hold, we know from section 3 that different self-adjoint extensions of the second-order operators exist, characterized by the choice of a regular boundary condition at $r = 0$ (cf (3.20)). The lowest values of l (for which (4.13) does not hold), corresponding to the bound states of greater phenomenological interest, might therefore find an appropriate mathematical description within the framework of self-adjoint extensions of symmetric operators. It remains to be seen how much freedom is left, on physical grounds, to specify the boundary conditions for the self-adjoint extension.

(iv) On considering the effect of the anomalous magnetic moment, equation (2.10) is replaced by equation (5.4), with the potential term defined in (5.5). For all potentials diverging at the origin, the effect of the anomalous magnetic moment is then dominating as $r \to 0$.

Indeed, as far as the Dirac operator is concerned, one can prove its essential self-adjointness on $C_0^\infty(\mathbb{R}^3 - \{0\})$ in the presence of a Coulomb potential provided that $|\gamma|$ (see (4.11)) is majorized by $\frac{1}{2}\sqrt{3}$, as is shown in [16], following work by Weidmann (see p 130 in [16]

and references therein). In our paper, however, we have focused on second-order differential operators, and the consideration of a central potential, with the associated Hilbert space

$$L^2(\mathbb{R}_+, r^2\,\mathrm{d}r) \otimes L^2(S^2,\ \mathrm{d}\Omega)$$

has eventually led to the second-order operators occurring in (2.10) and (2.17) and acting on square-integrable functions on the positive half-line. Our calculations, summarized in the points (i)–(iv) above, remain therefore original. We should notice that the condition $|\gamma| < \frac{1}{2}\sqrt{3}$ found in [16] is compatible with our inequalities (4.14) and (4.15) for all $l \geqslant 2$. In other words, the condition on γ ensuring essential self-adjointness of the Dirac operator leads also to essential self-adjointness of the second-order operators studied in our paper, whereas the converse does not hold (one may find a $|\gamma|$ smaller than $\sqrt{3}$ but greater than $\frac{1}{2}\sqrt{3}$). Our analysis has possibly the merit of having shown that some extra care is necessary when $l = 0, 1$, but this should not be unexpected, if one bears in mind from section 3 that already in the free case the values $l = 0, 1$ make it necessary to perform a separate analysis (cf [20]).

We should also acknowledge that in [21] the essential self-adjointness of powers of the Dirac operator had been proved, but in cases when the potential V is smooth. In particular, when the potential is a C^∞ function on $\mathbb{R}^3$, no growth conditions on it are necessary to ensure essential self-adjointness of any power of the Dirac operator [9, 21]. In our problem, however, we have considered a Coulomb term in the potential, which is singular at the origin. Although a regular solution of the eigenvalue problem exists [8, 18], since the origin remains a Fuchsian singular point, the domain of essential self-adjointness of the second-order operators in the interacting case is changed. This is reflected by the inequality (4.13) for the fulfillment of the limit-point condition at zero, which now involves γ, and hence the atomic number [11, 12]. Note also that, to find a real-valued solution which is regular at the origin in a Coulomb field, one only needs the weaker condition $k^2 \geqslant \gamma^2$ [11, 12]. Thus, a careful investigation of the essential self-adjointness issue picks out a subset of the general set of real-valued regular solutions.

For simplicity, we have considered at the end of section 4 only one 'linear' term. More precisely, however, two linear terms are often studied, of a scalar and vector nature, respectively [8]. Moreover, a naturally occurring question is whether one can extend our qualitative analysis to study the (essential) self-adjointness issue for operators involving the square root of the Laplacian [22], i.e. $\sqrt{-c^2\hbar^2\,\triangle + m_0^2c^4} - \frac{Ze^2}{r}$. Such problems have been the object of intensive investigations, but more work could be done from the point of view of rigorous mathematical foundations. In the light of the above remarks, there is some encouraging evidence that new insight into the choice of phenomenological central potentials can be gained by applying some powerful analytic techniques along the lines described in our paper. In the near future, one might therefore hope to re-interpret from a deeper perspective the previous work in the literature, including the class of potentials responsible for quark confinement.

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References

[1] Dirac P A M 1928 *Proc. R. Soc.* A **117** 610
[2] Darwin C G 1928 *Proc. R. Soc.* A **118** 654
Darwin C G 1928 *Proc. R. Soc.* A **120** 621

[3] Gordon W 1928 *Z. Phys.* **48** 11
[4] Kaburagi M, Kawaguchi M, Morii T, Kitazoe T and Morishita J 1980 *Phys. Lett.* B **97** 143
[5] Eichten E and Feinberg F 1981 *Phys. Rev.* D **23** 2724
[6] Kaburagi M, Kawaguchi M and Morii T 1981 *Z. Phys.* C **9** 213
[7] Baker M, Ball J S and Zachariasen F 1995 *Phys. Rev.* D **51** 1968
[8] Franklin J 1998 A simple Dirac wavefunction for a Coulomb potential with linear confinement *Preprint* HEP-PH 9812464
[9] Reed M and Simon B 1975 *Methods of Modern Mathematical Physics. II. Fourier Analysis and Self-Adjointness* (New York: Academic)
[10] Kato T 1995 *Perturbation Theory for Linear Operators* (Berlin: Springer)
[11] Landau L D and Lifshitz E M 1971 *Relativistic Quantum Theory* (Oxford: Pergamon)
[12] Greiner W 1990 *Relativistic Quantum Mechanics: Wave Equations* (Berlin: Springer)
[13] Griesemer M and Lutgen J 1999 *J. Funct. Anal.* **162** 120
[14] Whittaker E T and Watson G N 1927 *Modern Analysis* (Cambridge: Cambridge University Press)
[15] Reed M and Simon B 1980 *Methods of Modern Mathematical Physics. I. Functional Analysis* 2nd edn (New York: Academic)
[16] Thaller B 1992 *The Dirac Equation* (Berlin: Springer)
[17] Eichten E and Gottfried K 1977 *Phys. Lett.* B **66** 286
[18] Mur V D, Popov V S, Simonov A Yu and Yurov V P 1994 *JETP* **78** 1
[19] Becirevic D and Le Yaouanc A 1999 *J. High Energy Phys.* 03(1999)021
(Becirevic D and Le Yaouanc A 1999 Affine g coupling ($g_{B^*B\pi}$, $g_{D^*D\pi}$): a quark model with Dirac equation *Preprint* HEP-PH 9901431)
[20] Fewster C J 1993 On the energy levels of the hydrogen atom *Preprint* HEP-TH 9305102
[21] Chernoff P R 1973 *J. Func. Anal.* **12** 401
[22] Herbst I 1977 *Commun. Math. Phys.* **53** 285