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DIRAC OPERATORS WITH A SPHERICALLY SYMMETRIC δ-SHELL INTERACTION

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1. Introduction

Dirac Hamiltonians with external potentials have attracted a lot of attention recently [1,2]. Of course, they require a fixed inertial frame and represent an approximative description of the true relativistic two-particle dynamics only, but nevertheless they can provide us with various useful and physically interesting models. Unfortunately, the number of situation when a Dirac-operator model is exactly solvable is very low comparing to the non-relativistic quantum mechanics [3].

In the non-relativistic case many new solvable models have appeared recently as a result of extensive investigation of point and contact interaction phenomena - cf.the monograph [4] for summary and further references. One of these models concerns the three-dimensional Schroedinger operator with the interaction formally given by the δ-shell potential

$$g\,\delta(r-R), \qquad R = \mathrm{const} \tag{1.1}$$

cf.[5-12] and [13-15] for some generalizations. The aim of the present paper is to investigate Dirac operator with this sort of interaction, and to add thereby a new item to the short list of exactly solvable problems of relativistic quantum mechanics. We are going to construct all rotationally invariant contact interactions supported by the sphere, and to specify those among them which correspond to a mixture of electrostatic and Lorentz scalar δ-shell potentials with coupling constants g_v and g_s

respectively:

$$g_v\ \delta(r-R)\ +\ g_s\ \beta\delta(r-R)\ . \tag{1.2}$$

In distinction to the Schroedinger case, such a shell can confine a particle within it at finite values of the coupling constants provided its scalar component is strong enough: we will show that it happens if

$$g_v^2 - g_s^2 + 4 = 0\ . \tag{1.3}$$

Other properties of the corresponding Dirac operators, in particular, their spectra will be also discussed. In a sequel to this paper, we are going to discuss Dirac operators with a δ-shell plus Coulomb potential, the non-relativistic limit and the approximation of the δ-shell interaction by short-range potentials.

2. Partial wave decomposition

Our construction starts from the Dirac Hamiltonian on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ defined by

$$H_D\ :\ \ H_D\,\psi = -i\vec{\alpha}\,\vec{\partial}\,\psi + \beta\, m\,\psi \tag{2.1}$$

with the domain

$$D(H_D) = H^{1,2}(\mathbb{R}^3)\otimes\mathbb{C}^4\ .$$

The Dirac matrices are taken as

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} , \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} .$$

For the definition of other quantities related to the Dirac equation (spherical spinors, etc.) we follow the convention of [16]. The operator H_D is self-adjoint and $C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$ is its core. Moreover, $C_0^\infty(\mathbb{R}^3\backslash\{0\}) \otimes \mathbb{C}^4$ is also a core of H_D as can be seen from its density in $D(H_D)$ in the $H^{1,2}$ norm. It illustrates the known fact that there is no non-trivial point interaction for a three-dimensional Dirac operator [17].

Our construction of the δ-shell interaction proceeds in a usual way: one restricts the starting operator to a set of functions with supports disjoint with the support of the interaction, and constructs self-adjoint extensions of the obtained operator. Since in our case the support is the sphere $S_R = \{ \vec{x} \in \mathbb{R}^3;\ |\vec{x}| = R \}$, where R is a given positive number, we are interested in the operator

$$H_1 := H_D \mid C_0^\infty(\mathbb{R}^3\backslash S_R) \otimes \mathbb{C}^4 \qquad (2.2)$$

From the technical reasons it is useful to consider also its restriction

$$H_0 := H_D \mid C_0^\infty(\mathbb{R}^3\backslash(S_R \cup \{0\})) \otimes \mathbb{C}^4 . \qquad (2.3)$$

Since $\overline{H}_0 = \overline{H}_1$ as one can check in the above mentioned way, the two operators have identical families of self-adjoint extensions.

The operators (2.2) and (2.3) have infinite deficiency indices and hence a vast family of extensions. In this paper we restrict our attention to those of them which are <u>rotationally invariant</u>; it will give us a possibility of reducing the problem to analysis of ordinary differential operators. It does not mean, however, that other self-adjoint extensions are not physically attractive. On the contrary, one should expect existence of interesting extensions which are rotationally non-invariant and at the same time specified by local boundary conditions. These problems will be discussed elsewhere. In addition to the rotational symmetry requirement we shall consider only <u>reflection-symmetric</u> extensions, i.e., our group of symmetry will be the universal covering group SU(2) of O(3).

These requirements mean that there is a single-valued unitary representation U of SU(2) such that an arbitrary self-adjoint extension H of H_0 from the considered class fulfills

$$U(R)\ H\ U(R)^{-1} = H \tag{2.4}$$

for any $R \in SU(2)$. One can decompose the state Hilbert space into orthogonal sum of subspaces referring to the total angular momentum j, its third component m and the parity $(-1)^l$ as

$$\mathcal{H} = \bigoplus_{j=1/2}^{\infty} \bigoplus_{l=j-1/2}^{j+1/2} \bigoplus_{\mu=-j}^{j} \mathcal{H}_{jl\mu} \tag{2.5a}$$

with

$$\mathcal{H}_{jl\mu} = \left\{ \psi \in \mathcal{H} : \psi(r,\vec{n}) = \begin{pmatrix} f(r)\Omega_{jl\mu}(\vec{n}) \\ g(r)\Omega_{jl'\mu}(\vec{n}) \end{pmatrix} ;\ f,g \in L^2(\mathbb{R}_+, r^2dr) \right\}, \tag{2.5b}$$

where $\Omega_{jl\mu}$ are the spherical spinors [16] and $l'=j\mp 1/2$ for $l=j\pm 1/2$. It follows from (2.4) that H commutes with all functions of the operator U(R), in particular, with the projection corresponding to the representation of U(2) with a given j,μ and parity. Hence we have the decomposition

$$H = \bigoplus_{j=1/2}^{\infty} \bigoplus_{l=j-1/2}^{j+1/2} \bigoplus_{\mu=-j}^{j} H_{jl\mu} \tag{2.6}$$

where the "component operators" $H_{jl\mu}$ are self-adjoint with the domains $D(H_{jl\mu}) = D(H) \cap \mathcal{H}_{jl\mu}$.

In each subspace $\mathcal{H}_{jl\mu}$, one can separate the radial part of the operator $\mathcal{H}_{jl\mu}$. To this aim we introduce the isomorphisms

$$U_{jl\mu}: \mathcal{H}_{jl\mu} \rightarrow \hat{\mathcal{H}} = L^2(\mathbb{R}_+) \otimes \mathbb{C}^2$$

by

$$(U_{jl\mu}\psi)(r) = \begin{pmatrix} rf(r) \\ (-1)^{j-l-1/2}\, rg(r) \end{pmatrix}, \tag{2.7}$$

where f,g are related to ψ as in (2.5b). We want to check first the inclusion

$$H_0 \subset \bigoplus_{j=1/2}^{\infty} \bigoplus_{l=j-1/2}^{j+1/2} \bigoplus_{\mu=-j}^{j} H^{(0)}_{jl\mu}, \tag{2.8}$$

where the operators $H^{(0)}_{jl\mu}$ are equal to $U^{-1}_{jl\mu}\, H^{(0)}_{jl}\, U_{jl\mu}$ the last named operator being defined by

$$\hat{H}^{(0)}_{jl} := \begin{pmatrix} m \; ; -\frac{d}{dr} + \frac{\varkappa_{jl}}{r} \\ \frac{d}{dr} + \frac{\varkappa_{jl}}{r} \; ; \; -m \end{pmatrix} \tag{2.9a}$$

on $D(\hat{H}^{(0)}_{jl}) = C_0^{\infty}((0,R)\cup(R,\infty))\otimes\mathbb{C}^2$ with

$$\varkappa_{jl} = (-1)^{j-l+1/2}\,(j+1/2) \tag{2.9b}$$

(we note that here the capped quantities refer to the two-component space $\hat{\mathcal{H}}$). Now we want to prove that a decomposition analogous to (2.8) holds for any rotation-invariant self-adjoint operators on $\mathcal{H}$.

2.1 Proposition : For a self-adjoint operator H in $\mathcal{H}$, the equality (2.4) holds for all $R \in SU(2)$ iff

$$H = \bigoplus_{j=1/2}^{\infty} \bigoplus_{l=j-1/2}^{j+1/2} \bigoplus_{\mu=-j}^{j} U^{-1}_{jl\mu}\hat{H}_{jl}U_{jl\mu}\,, \tag{2.10}$$

where $\hat{H}_{jl}$ is a self-adjoint operator in $\hat{\mathcal{H}}$ independent on μ.

Proof: The sufficient condition is trivial. The requirement (2.4) implies the decomposition (2.6) and one defines naturally $\hat{H}_{jl\mu}=U_{jl\mu}H_{jl\mu}U^{-1}_{jl\mu}$, so it is only necessary to check its independence of μ.

Let us show first that $D(\hat{H}_{jl\mu}) = D(\hat{H}_{jl\mu'})$. The operator $U^{-1}_{jl\mu}$ maps $D(\hat{H}_{jl\mu})$ onto $D(H_{jl\mu})$ and the vector

$$U(R)\begin{pmatrix} r^{-1}f\,\Omega_{jl\mu} \\ (-1)^{j-l-1/2}r^{-1}g\,\Omega_{jl'\mu} \end{pmatrix} = \sum_{\mu'=-j}^{j} \mathcal{D}^{(j)}_{\mu'\mu}(R)\begin{pmatrix} r^{-1}f\,\Omega_{jl\mu'} \\ (-1)^{j-l-1/2}r^{-1}g\,\Omega_{jl'\mu'} \end{pmatrix}$$

belongs to D(H) for any $\begin{pmatrix} f \\ g \end{pmatrix} \in D(\hat{H}_{jl\mu})$ and $R \in SU(2)$ according to (2.4). Since $\mathscr{H}_{jl\mu} \perp \mathscr{H}_{jl\mu'}$ for $\mu \neq \mu'$ each term on the rhs. must belong to $D(H_{jl\mu'})$. One always find R such that $\mathscr{D}^{(j)}_{\mu'\mu}(R) \neq 0$ due to the Burnside theorem [18]; then applying $U_{jl\mu'}$ we find that

$$\begin{pmatrix} f \\ g \end{pmatrix} \in D(H_{jl\mu'})$$

for all $\mu' = -j, \dots ,j$. The index $\mu = -j,\dots,j$ can be chosen arbitrarily so the equality of the domains is obtained

Consider now a vector $\psi \in D(H)$ referring to fixed j,l, i.e.,

$$\psi(r,\vec{n}) = \sum_{\mu=-j}^{j} \begin{bmatrix} r^{-1} f_{jl\mu}(r)\ \Omega_{jl\mu}(\vec{n}) \\ (-1)^{j-l-1/2} r^{-1} g_{jl'\mu}(r)\ \Omega_{jl'\mu}(\vec{n}) \end{bmatrix}$$

with

$$\hat{\psi}_{jl\mu} \equiv \begin{pmatrix} f_{jl\mu} \\ g_{jl'\mu} \end{pmatrix} \in \hat{D}_{jl} \equiv D(\hat{H}_{jl\mu}$$

for $\mu = -j,\dots,j$. Denoting

$$\hat{H}_{jl\mu} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{bmatrix} \hat{H}^{(1)}_{jl\mu}\ (f,g) \\ \hat{H}^{(2)}_{jl\mu}\ (f,g) \end{bmatrix}$$

we can calculate easily

$U(R)HU(R)^{-1}\psi =$

$$= \sum_{\mu=-j}^{j} \sum_{\nu,\sigma} \mathscr{D}^{(j)}_{\mu\nu}(R)\ \mathscr{D}^{(j)}_{\nu\sigma}(R^{-1}) \begin{bmatrix} r^{-1}\hat{H}^{(1)}_{jl\nu}\ (f_{jl\sigma}; g_{jl'\sigma})\ \Omega_{jl\mu} \\ (-1)^{j-l-1/2}\hat{H}^{(2)}_{jl\nu}\ (f_{jl\sigma}; g_{jl'\sigma})\ \Omega_{jl'\mu} \end{bmatrix}.$$

Since this should equal to $H\psi$, we get the relation

$$\sum_{\nu,\sigma} \mathcal{D}^{(j)}_{\mu\nu}(R)\ \mathcal{D}^{(j)}_{\nu\sigma}(R^{-1})\ \hat{H}_{jl\nu}\hat{\psi}_{jl\sigma} = \hat{H}_{jl\mu}\hat{\psi}_{jl\mu}$$

valid for any $\hat{\psi}_{jl\rho} \in \hat{D}_{jl}$, $\rho = -j,\dots,j$. Multiplying it by $\mathcal{D}^{(j)}_{\rho\mu}(R^{-1})$ from the left and summing over μ, we obtain

$$\sum_{\sigma} \mathcal{D}^{(j)}_{\rho\sigma}(R^{-1}) \left[\hat{H}_{jl\rho}\hat{\psi}_{jl\sigma} - \hat{H}_{jl\sigma}\hat{\psi}_{jl\sigma} \right] = 0$$

for each $R \in SU(2)$. Using the Burnside theorem again we get

$$\hat{H}_{jl\rho}\hat{\psi}_{jl\sigma} = \hat{H}_{jl\sigma}\hat{\psi}_{jl\sigma}$$

for all $\rho,\sigma = -j,\dots,j$. ∎

It follows now easily from the proved assertion and the decomposition (2.8) that in order to construct all rotationally invariant δ-shell interactions for the operator (2.1), one has to construct all self-adjoint extensions $\hat{H}_{jl}$ of $\hat{H}^{(0)}_{jl}$ in each partial wave subspace and to insert them into the formula (2.10)

3. Self-adjoint extensions of the radial operators

We have reduced the problem to analysis of ordinary differential operators corresponding to the formal expression

$$\tau = \begin{pmatrix} 0, & -1 \\ 1, & 0 \end{pmatrix} \frac{d}{dr} + \begin{pmatrix} m & , \frac{\varkappa_{jl}}{r} \\ \frac{\varkappa_{jl}}{r} & , -m \end{pmatrix} \tag{3.1}$$

which can be handled by standard methods (e.g., that of [19], chap.XIII), because the coefficient of the derivative is a constant and non-singular matrix. The adjoint operator $\hat{H}^{(0)*}_{jl}$ to (2.9) acts as (3.1) on the domain $D(\hat{H}^{(0)*}_{jl})$ consisting of the functions $\hat{\psi} \in \hat{\mathscr{H}}$ which are absolutely continuous in $(0,R)$ and (R,∞) with $\tau\hat{\psi} \in \hat{\mathscr{H}}$. Since τ is formally self-adjoint its deficiency indices are equal and self-adjoint extensions of the operator (2.9) exist.

The deficiency indices fulfill $d \le 4$, because they correspond to solutions of a two-component first-order differential equation in the intervals $(0,R)$ and (R,∞). In order to find them explicitly consider the equation

$$(\tau - i)\,\varphi = 0 \tag{3.2}$$

whose solutions are obtained easily by analytic continuation of the well-known stationary solutions of the free radial Dirac equation to imaginary values of energy.

$$\varphi_z(r) = \begin{bmatrix} r^{1/2} Z_\nu(i(1+m^2)^{1/2} r) \\ (-1)^{j-l+1/2} \left(\frac{1+im}{1-im} \right)^{1/2} r^{1/2} Z_{\nu'}(i(1+m^2)^{1/2} r) \end{bmatrix}, \tag{3.3}$$

where $\nu=l+1/2$, $\nu'=l'+1/2$ and the cylindrical function Z_ν stands for J_ν or $H_\nu^{(1)}$. The first choice yields a solution which is square integrable in $(0,R)$ but not in (R,∞), while the reverse is true for the second case. Extending the square integrable solutions by zero in the other interval, we get $d = 2$.

One could use this explicit form of deficiency vectors for construction of the self-adjoint extensions via the von Neumann formulae, but this is not very practical. Instead, we are going to characterize the extensions by suitable boundary conditions. Since $H_D \mid C_0^\infty(\mathbb{R}^3\setminus\{0\})\otimes\mathbb{C}^4$ is e.s.a., there are no non-trivial boundary values at 0 and ∞.

<u>3.1 Proposition</u>: There is a complete set of four independent boundary values on $D(\hat{H}_{jl}^{(0)*})$, namely

$$\psi \longmapsto \psi(R_\pm) \equiv \lim_{r\to R_\pm} \psi(r)$$

(recall that ψ is a two component vector)

<u>Proof</u>: consider $\psi = \begin{pmatrix} f \\ g \end{pmatrix} \in D(\hat{H}_{jl}^{(0)*})$. The functions f,g are absolutely continuous inside $(0,R)$ and (R,∞) and square integrable on $\mathbb{R}_+$ with $\tau\psi \in L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$. Then, for instance, f is square integrable in a left neighbourhood of R and

$$| \; f(r) - f(s) \; | \le |r-s|^{1/2} \left| \int_r^s |f'(t)|^2 dt \; \right|^{1/2}$$

so $\lim_{r\to R_-} f(r)$ exist and in the same way one checks the existence of the other three limits. Since we have $4=2d$ linearly independent boundary values , they form a complete set for $\hat{H}^{(0)}_{jl}$ [19] ∎

Self adjoint extensions of $\hat{H}^{(0)}_{jl}$ are restrictions of $\hat{H}^{(0)*}_{jl}$ to a subspace of $D(\hat{H}^{(0)*}_{jl})$ specified by a symmetric set of two linearly independent boundary conditions. We define the boundary form

$$F(\psi,\varphi;r) := \psi^{+}(r)\ \tau_0\ \varphi(r),$$

where $\tau_0 = \begin{pmatrix}0,-1\\1,0\end{pmatrix}$. Integration by parts yield for any $\varphi,\ \psi \in D(\hat{H}^{(0)*}_{jl})$ the equality

$$\int_r^s \psi^{+}\tau\varphi\ dt - \int_r^s (\tau\psi)^{+}\varphi\ dt = F(\psi,\varphi;s) - F(\psi,\varphi;r)$$

provided R is not contained in the interval (r,s). Since the integrals on the *lhs* converge in any subinterval of $\mathbb{R}_+$, one can establish existence of the limits of $F(\psi,\varphi;.)$ at the points 0, R_-, R_+, ∞ similarly as in Proposition 3.1. Furthermore,

$$\lim_{r\to 0_+} F(\psi,\varphi;r) = \lim_{r\to\infty} F(\psi,\varphi;r) = 0$$

for any $\varphi,\psi \in D(\hat{H}^{(0)*}_{jl})$ since otherwise one could define an additional independent boundary value in contradiction to Proposition 3.1. Hence we get

$$(\psi,\hat{H}^{(0)*}_{jl}\ \varphi) - (\hat{H}^{(0)*}_{jl}\psi,\varphi) = F(\psi,\varphi;R_-) - F(\psi,\varphi;R_+) \qquad (3.4)$$

for any $\varphi,\psi \in D(\hat{H}^{(0)*}_{jl})$ and we have to choose those boundary conditions for which the *rhs* of (3.4) vanishes.

3.2 Theorem: Any self-adjoint extension $\hat{H}_{jl}$ of $\hat{H}^{(0)}_{jl}$ in $\hat{\mathcal{H}}$ acts as $\hat{H}_{jl}\psi = \tau\psi$ for $\psi \in D(\hat{H}_{jl})$ where τ is given by (3.1) and $D(\hat{H}_{jl})$ consists of the functions $\psi \in L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$ which are absolutely continuous inside $(0,R)$ and (R,∞), $\tau\psi \in L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$, and satisfy the following boundary conditions:

$$\psi(R_-) = e^{i\alpha} A\, \psi(R_+), \qquad (3.5a)$$

where $\alpha \in [0,2\pi)$ and A is a real 2x2 matrix with det A = 1, or

$$\begin{pmatrix} c_1 , & c_2 \\ 0 , & 0 \end{pmatrix} \psi(R_-) + \begin{pmatrix} 0 , & 0 \\ d_1 , & d_2 \end{pmatrix} \psi(R_+) = 0 , \qquad (3.5b)$$

where c_1, c_2, d_1, d_2 are real and both matrices are non-zero. Conversely, any operator of this form is a self-adjoint extension of $\hat{H}^{(0)}_{jl}$ in $\hat{\mathcal{H}}$.

Proof: It remains to check that (3.5) are all symmetric sets of pairs of linearly independent boundary conditions. According to the Proposition 3.1, the general form of such boundary conditions is

$$C\psi(R_-) + D\psi(R_+) = 0 , \qquad (3.6)$$

where C,D are 2x2 matrices such that the 2x4 matrix (C,D) has rank two. The symmetry conditions according to (3.4) reads

$$\psi(R_-)^+\tau_0\varphi(R_-) - \psi(R_+)^+\tau_0\varphi(R_+) = 0 \qquad (3.7)$$

for any $\varphi,\psi \in D(\hat{H}^{(0)*}_{jl})$ satisfying (3.6). We distinguish the following three cases:

(i) C is non-singular, then (3.6) can be written as $\psi(R_-) = B\psi(R_+)$ and substitution into (3.6) gives

$$\psi(R_+)^+(B^+\tau_0 B - \tau_0)\varphi(R_+) = 0 .$$

Since this equation should hold for any $\psi(R_+)$, $\varphi(R_+)$, we get

$$B^+\tau_0 B = \tau_0 . \qquad (3.8)$$

So $|\det B| = 1$ and B is non-singular. A simple algebra shows that (3.8) is equivalent to (3.5a) with $B = \exp(i\alpha)A$.

(ii) D is non-singular, then (3.6) can be written as $\psi(R_+)=\tilde{B}\psi(R_-)$, where $\tilde{B}$ is non-singular due to (3.7), so this case reduces to the previous one.

(iii) Both C,D are of rank one but (C,D) has rank two. Multiplying (3.6) by a suitable non-singular matrix, we can write it as

$$\begin{pmatrix} c_1 , & c_2 \\ 0 , & 0 \end{pmatrix} \psi(R_-) + D_1 \, \psi(R_+) = 0 , \qquad (3.9)$$

where at least one of the numbers c_1, c_2 is non-zero. Since D_1 is again a rank-one matrix, one can write it as

$$D_1 = \begin{pmatrix} \lambda d_1 , & \lambda d_2 \\ d_1 , & d_2 \end{pmatrix}$$

with at least one of the numbers d_1, d_2 non-zero (the other possibility when only the first row is non-zero is excluded because the combined 2x4 matrix should be of rank two). It is easy to see that (3.9) is in that case equivalent to (3.5b) or to

$$\begin{bmatrix} c_1 , & c_2 \\ 0 , & 0 \end{bmatrix} \psi(R_-) = \begin{bmatrix} 0 , & 0 \\ d_1 ; & d_2 \end{bmatrix} \psi(R_+) = 0 , \qquad (3.5b')$$

i.e., that the boundary conditions decouple in this case. The coefficients c_1,c_2,d_1,d_2 might be still complex. The condition (3.5b′) , however, means that the two-dimensional complex vector $\psi(R_-)$ is for any $\psi \in D(\hat{H}_{jl}^{(0)*})$ orthogonal to $\begin{pmatrix}\bar{c}_1\\ \bar{c}_2\end{pmatrix}$, i.e.,

$$\psi(R_-) = \alpha_\pm(\psi) \begin{bmatrix} \bar{c}_2 \\ -\bar{c}_1 \end{bmatrix}$$

and the corresponding expression for $\psi(R_+)$ in terms of d_1,d_2. Substituting it to the expression (3.7) where now both terms on the lhs must be zero , we get $\mathrm{Im}\ \bar{c}_1 c_2 = \mathrm{Im}\ \bar{d}_1 d_2 = 0$. Thus c_1,c_2 and d_1,d_2 must have the same phases. ∎

<u>3.3 Remark</u>: In addition to the stated symmetry requirements, one may want the constructed Hamiltonians to be time-reversal invariant. The corresponding antiunitary operator T can be defined as in the free-particle case [16]

$$T\psi = \begin{bmatrix} \sigma_2 , & 0 \\ 0 , & \sigma_2 \end{bmatrix} K \ \psi ,$$

where K means the complex conjugation. After the partial-wave decomposition, we see that H is time-reversal invariant iff $D(\hat{H}_{jl})$ is invariant with respect to the complex conjugation for all j,l. The just proved theorem shows that this is the case when $\hat{H}_{jl}$ are specified by the boundary conditions (3.5b) or by (3.5a) with $\alpha=0$.

4. δ-shells

As we have mentioned in the introduction, we are interested primarily in the potentials (1.2), i.e., a combination of the scalar external field $g_s\beta\delta(r-R)$ and the vector field described in the given reference frame by ($g_v\delta(r-R),\vec{0}$) with real coupling constants. In the radial Hamiltonians $\hat{H}_{jl}$, this interaction corresponds to the formal potential

$$\begin{pmatrix} g_v+g_s & , 0 \\ 0 & , g_v-g_s \end{pmatrix} \delta(r-R) \qquad (4.1)$$

with g_v, g_s independent of j,l. More generally one can consider the potential

$$G\delta(r-R) \qquad (4.2)$$

where G is a 2x2 matrix. Our aim is now to specify the self-adjoint extensions $\hat{H}_{jl}$ that can be associated with the formal Dirac operator with the potential (4.2). Suppose that ψ satisfies the equation

$$[\tau + G\delta(r-R)]\psi = E\psi$$

and the limits $\psi(R_\pm)$ exist. Integrating over $(R-\varepsilon,R+\varepsilon)$ and taking the limit $\varepsilon \to 0_+$, we get

$$\left[1 - \frac{1}{2}\tau_0 G \right] \psi(R_+) - \left[1 + \frac{1}{2}\tau_0 G \right]\psi(R_-) = 0 \qquad (4.3)$$

provided we have chosen the relation

$$\int_{R-\varepsilon}^{R+\varepsilon} \delta(r-R)\psi(r)dr = \frac{1}{2}\left(\psi(R_+) + \psi(R_-)\right) \tag{4.4}$$

as a definition of the *lhs*. Of course, only those matrices G are acceptable for which the boundary condition (4.3) is compatible with (3.5). As one expects, the following assertion is true.

<u>4.1 Proposition</u>: Boundary conditions (4.3) define a self-adjoint extension of $\hat{H}^{(0)}_{jl}$ iff $G^+ = G$.

<u>Proof</u>: The matrix $(1-\tau_0 G/2, 1+\tau_0 G/2)$ has rank two since the sum of the submatrices is nonsingular. It remains to check that (4.3) implies (3.7) iff $G^+ = G$. We start with the necessary condition and distinguish four cases denoting $B = \frac{1}{2}\tau_0 G$:

(i) 1-B is nonsingular, then (4.3) is equivalent to $\psi(R_+)=(1-B)^{-1}(1+B)\psi(R_-)$; substituting it into (3.7) we get after a simple algebra $G^+ = G$.

(ii) 1+B is nonsingular, then the same procedure with the interchange $G \longrightarrow -G$ can be used.

(iii) 1-B =0 or 1+B =0; in that case $G=\pm 2\tau_0 \neq G^+$, but the condition (4.3) reads $\psi(R_\pm) = 0$, while $\psi(R_\mp)$ is arbitrary. Hence the rhs of (3.7) equals $\mp\psi(R_\pm)^+\tau_0\varphi(R_\pm)$ so these boundary conditions cannot define a self-adjoint extension.

(iv) both 1+B and 1-B have rank one. As in the proof of the

Theorem 3.2, one can find a nonsingular matrix V which converts them into non-zero matrices of the following form

$$V(1+B) = \begin{pmatrix} c_1 , & c_2 \\ 0 , & 0 \end{pmatrix} , \quad V(1-B) = \begin{pmatrix} 0 , & 0 \\ d_1 , & d_2 \end{pmatrix}$$

one can express V and VB form there. Furthermore, V is nonsingular so one can calculate B and

$$G = -2\tau_0 B = \frac{2}{c_2 d_1 - c_1 d_2} \begin{pmatrix} 2c_1 d_1 , & c_1 d_2 + c_2 d_1 \\ c_1 d_2 + c_2 d_1 , & 2c_2 d_2 \end{pmatrix} . \quad (4.5)$$

Since we can choose V so that the numbers c_1, c_2, d_1, d_2 are real, G is real symmetric, and therefore Hermitean.

On the contrary, assume $G^+=G$ and let us prove that (4.3) defines a self-adjoint extension. For the cases (i) and (ii) we have done it already, the case (iii) does not occur. It remains to complete the proof for the case (iv). Any Hermitian G is of the form

$$G = \begin{pmatrix} a , & b \\ \bar{b} , & c \end{pmatrix}$$

with a,c real. It gives

$$1+B = \begin{pmatrix} 1-\bar{b}/2 , & -c/2 \\ a/2 , & 1+b/2 \end{pmatrix} , \qquad 1-B = \begin{pmatrix} 1+\bar{b}/2 , & c/2 \\ -a/2 , & 1-b/2 \end{pmatrix} .$$

Since det(1+B) = det(1-B) =0, b must be real and $b^2=4+ac$. For any a,b,c satisfying this restriction, one can choose c_1, c_2, d_1, d_2 so that G is expressed in the form (4.5) ,e.g., by taking $c_1 = d_1 = 1$ for $a \neq 0$ and $c_1=0$ or $d_1=0$ for $a=0$. ∎

Let us return now to the physically interesting case (4.1). The corresponding matrix G is Hermitean and the boundary conditions (4.3) read

$$\begin{pmatrix} 1 & , \frac{g_v - g_s}{2} \\ -\frac{g_v + g_s}{2} & , 1 \end{pmatrix} \psi(R_+) - \begin{pmatrix} 1 & , \frac{g_s - g_v}{2} \\ \frac{g_v + g_s}{2} & , 1 \end{pmatrix} \psi(R_-) = 0 \cdot \qquad (4.6)$$

It is clear that they can be cast into the form (3.5a) iff $g_v^2 - g_s^2 + 4 \neq 0$; otherwise they belong to the type (3.5b). Remark 3.3 shows the corresponding operators, as well as the more general Hamiltonians referring to the δ-shell interaction (4.2) with **real** G, are time-reversal invariant. They do not cover, of course, the class of all self-adjoint extensions $\hat{H}_{jl}$ described by Theorem 3.2; a possible interpretation of the remaining ones is discussed in the Appendix.

5. Confinement

In some cases, the contact interaction of the sphere may separate the two spatial regions fully, i.e., the particle under consideration is either confined in the ball $B_R = \{ x \in \mathbb{R}^3 : |\vec{x}| \le R \}$ or lives outside B_R and cannot enter it. In other words, the sphere S_R is impenetrable for the particles.

Let us denote $\mathcal{H}_R = \{ \psi \in \mathcal{H} : \text{supp}\, \psi \subset B_R \}$; we are interested in the situation when $\mathcal{H}_R$ is invariant under $\exp(-iHt)$ for all $t \in \mathbb{R}$ or equivalently $E_R H \subset H E_R$, where E_R is the projection onto $\mathcal{H}_R$ in $\mathcal{H}$

$$(E_R\psi)(\vec{x}) = \Theta(R-|\vec{x}|)\psi(\vec{x}).$$

In the spherically symmetric case it is further equivalent to

$$\hat{E}_R D(\hat{H}_{jl}) \subset D(\hat{H}_{jl})$$

for all j,l, where $\hat{E}_R$ is the projection into $L^2(0,R)\otimes\mathbb{C}^2$ in $\hat{\mathcal{H}}$. Combining the last requirements with Theorem 3.2, we arrive at the following conclusion.

5.1 Proposition: Let H be a rotationally and space-reflection symmetric Dirac operator with contact interaction on the sphere S_R, then S_R is impenetrable for the particles iff the corresponding partial-wave operators $\hat{H}_{jl}$ are defined by the boundary conditions (3.5b) for all j,l.

As an example, consider again the physically interesting case of the interaction (4.1) corresponding to the boundary conditions (4.6). The observation made at the end of the previous section shows that the sphere S_R is impenetrable in this case iff

$$g_v^2 - g_s^2 + 4 = 0 . \qquad (5.1)$$

Notice that presence of the scalar component is essential here,

$$|g_s| = \left[g_v^2 + 4 \right]^{1/2} \geq 2 .$$

In particular a purely scalar δ-shell confines the particles iff $g_s = \pm 2$. We remark also that the relation (5.1) has been found recently (on a heuristic level) as the impenetrability condition for a δ-shaped separable potential in one-dimensional Dirac operator [20]

6. Spectral properties

6.1 Point spectrum

In order to solve the eigenvalue problem $\hat{H}_{jl}\psi = \lambda\psi$, one has to find $\psi = (f,g) \in D(\hat{H}_{jl})$ so that the equations

$$-g' + \frac{\varkappa}{r} g + m f = \lambda f \qquad (6.1a)$$

$$f' + \frac{\varkappa}{r} f - m g = \lambda g \qquad (6.1b)$$

are fulfilled in $(0,R)$ and (R,∞) together with the appropriate boundary conditions coupling the solutions at the point R ; for simplicity we write $\varkappa \equiv \varkappa_{jl}$.

6.1 Proposition: For any of the boundary conditions (3.5), the operator $\hat{H}_{jl}$ has at most two eigenvalues (with account of multiplicity) in $[-m,m]$.

Proof: One has only to modify slightly the argument leading to Corollary 1 to Proposition 8.19 in [21]. Denote by A_1, A_2 two extensions $\hat{H}_{jl}$, where the first corresponds to the free Dirac Hamiltonian, and suppose there are more then two eigenvalues in $[-m,m]$. Since both the the operators A_1, A_2 are self-adjoint extensions of an operator with deficiency indices (2,2), there has to exist a nonzero vector $\psi \in \mathrm{Ran}\, E_{A_2}([-m,m]) \cap D(\hat{H}_{jl}^{(0)})$. We have

$$\| A_2\psi \|^2 = \int_{\mathbb{R}} \lambda^2 d(\psi, E_\lambda^{(2)}\psi) \le m^2 \|\psi\|^2$$

where we have denoted by $\{E_\lambda^{(j)}\}$ the spectral decomposition of A_j. At the same time, the spectrum of A_1 is contained in $(-\infty,-m]\cup[m,\infty)$ and the endpoints $\pm m$ are not its eigenvalues so

$$\| A_1\psi \|^2 = \int_{(-\infty,-m]\cup[m,\infty)} \lambda^2 d(\psi, E_\lambda^{(1)}\psi) > m^2 \|\psi\|^2$$

but $A_1\psi = A_2\psi$ since $\psi \in D(\hat{H}_{jl}^{(0)})$ so we arrive at a contradiction.∎

The points $\lambda = \pm m$ can be eigenvalues of $\hat{H}_{jl}$ for particular boundary conditions. For instance, consider $\lambda = -m$ and $l=j-1/2$, i.e., $\varkappa = -(l+1)$. The equations (6.1) have then the following square integrable solutions

$$f(r) = ar^{-\varkappa},\ g(r) = \frac{2ma}{1-2\varkappa} r^{1-\varkappa} \text{ for } r\in(0,R)$$

$$f(r) = 0,\ g(r) = br^{\varkappa} \quad \text{for } r \in (R,\infty).$$

Substituting them into the boundary conditions (3.5) one can find the cases when $\lambda=-m$ is an eigenvalue. In particular, for the boundary conditions (4.6) this is true if

$$g_v^2 - g_s^2 - 4 + \frac{8mR}{1-2\varkappa}(g_v-g_s) = 0.$$

Similarly one can handle the remaining cases.

Let us turn now to eigenvalues $\lambda \in (-m,m)$ for fixed boundary conditions (3.5) which we shall write for simplicity in the form (3.6),

$$C\psi(R_-) + D\psi(R_+) = 0 .$$

It is clear from (6.1) that the functions f,g are continuously differentiable to any order in (0,R) and (R,∞). Expressing g from (6.1b) and substituting into (6.1a), we get the Bessel equation whose solutions in (0,R) and (R,∞) are of the form (3.3) with $i\mp m$ replaced by $\lambda\mp m$. Substituting them into the boundary conditions, we get the following eigenvalue equation

$$\det\left[C\varphi^{(-)}(\lambda), D\varphi^{(+)}(\lambda)\right] = 0 , \qquad (6.2a)$$

where

$$\varphi^{(-)}(\lambda) = \begin{pmatrix} J_\nu(i(m^2-\lambda^2)^{1/2}R) \\ (-1)^{j-l+1/2} i \left(\frac{m-\lambda}{m+\lambda}\right)^{1/2} J_{\nu'}(i(m^2-\lambda^2)^{1/2}R) \end{pmatrix} \qquad (6.2b)$$

$$\varphi^{(+)}(\lambda) = \begin{pmatrix} H_\nu^{(1)}(i(m^2-\lambda^2)^{1/2}R) \\ (-1)^{j-l+1/2} i \left(\frac{m-\lambda}{m+\lambda}\right)^{1/2} H_{\nu'}^{(1)}(i(m^2-\lambda^2)^{1/2}R) \end{pmatrix} \qquad (6.2c)$$

with $\nu=l+1/2$, $\nu'=l'+1/2$ and $l'=j\mp 1/2$ for $l=j\pm 1/2$, according to Proposition 6.1, it has at most two solutions, or even less if some of the points $\lambda=\pm m$ is an eigenvalue.

Similarly one can proceed for $|\lambda|>m$. There are non-zero square integrable solutions in (R,∞) in this case and therefore $\hat{H}_{jl}$ referring to the boundary conditions (3.5a) has no eigenvalues of that type. On the other hand, the boundary conditions (3.5b) yield the eigenvalue equation

$$c_1 J_\nu((\lambda^2-m^2)R) + c_2(-1)^{j-l+1/2} \frac{(\lambda^2-m^2)^{1/2}}{\lambda+m} J_{\nu'}((\lambda^2-m^2)^{1/2}R) = 0 . \quad (6.3)$$

It is clear that it has for any real c_1, c_2 two infinite sequences of solutions accumulating at $\lambda = \pm\infty$.

6.2 Continuous spectrum

The spectrum of the free Dirac operator is known [22] to be purely (and absolutely) continuous and equals to $(-\infty,-m] \cup [m,\infty)$. We are going to show that the same is true for the operators with the δ-shell interaction.

The resolvents of the self-adjoint extensions $\hat{H}_{jl}$ with fixed j,l differ mutually by a rank-two operator (this fact follows immediately from the Krein resolvent formula [4]) and have therefore the same continuous spectrum

$$\sigma_c(\hat{H}_{jl}) = \sigma_{ess}(\hat{H}_{jl}) = \sigma_{ess}(\hat{H}^{(D)}_{jl}) = (-\infty,-m] \cup [m,\infty)$$

for all j,l , where $\hat{H}^{(D)}_{jl}$ denotes the partial-wave "component" of H_D. The essential spectrum of $\hat{H}^{(D)}_{jl}$ can be easily computed just solving the equations (6.1) in $\mathbb{R}_+$ for each $\lambda \in (-\infty,-m] \cup [m,\infty)$ and taking a suitable sequence of cut-off functions. Moreover, the spectrum of $\hat{H}^{(D)}_{jl}$ is absolutely continuous for all j,l. ; this follows immediately from the decomposition

$$\bigcup_{j,l} \sigma_c(\hat{H}_{jl}^{(D)}) = \sigma_c(H_D) = \sigma_{a.c}(H_D) = (-\infty,-m] \cup [m,\infty) .$$

It remains in such a way to check that

$$\sigma_{ess}(\hat{H}_{jl}) = \sigma_{a.c}(\hat{H}_{jl})$$

for all j,l and all self-adjoint extensions $\hat{H}_{jl}$. To this purpose we use once more the Krein resolvent formula which yields the following relation for the resolvent of $\hat{H}_{jl}$

$$(\hat{H}_{jl}-z)^{-1} = (\hat{H}_{jl}^{(D)}-z)^{-1} + \sum_{m,n=1}^{2} \mu_{m,n}^{(jl)}(z) \; |g_m(z)\rangle\langle g_n(\bar{z})| ,$$

where the matrix $\mu^{(jl)}(z)$ is meromorphic and represents a solution to the equation

$$[\mu^{(jl)}(z)]_{mn}^{-1} = [\mu^{(jl)}(z_0)]_{mn}^{-1} - (z-z_0) \; (g_m(\bar{z}),g_n(z_0))$$

and the vectors $g_m(z)$ solve

$$g_m(z) = g_m(z_0) + (z - z_0) \; (\hat{H}_{jl}^{(D)} - z)^{-1} \; g_m(z_0)$$

being therefore analytic in $\rho(\hat{H}_{jl}^{(D)})$. Let us now take $z \in (a,b) \subset (-\infty,-m] \cup [m,\infty)$ where a,b are chosen in such a way that

$$(\varphi,(\hat{H}_{jl}-z)^{-1}\varphi) \qquad (6.4)$$

is analytic in (a,b) for all $\varphi \in C_0^\infty(\mathbb{R}_+)\otimes\mathbb{C}^2$; the above argument shows that it is always possible. Then the known criterion [23] shows that $(a,b) \cap \sigma_{sc}(\hat{H}_{jl}) = \emptyset$. Since the poles of (6.4) are isolated it follows that $\sigma_{sc}(\hat{H}_{jl}) = \emptyset$. Summarizing the above results we get

<u>6.2 Theorem</u>: For any of the boundary conditions (3.5), the operator $\hat{H}_{jl}$ has at most two eigenvalues (with the account of multiplicities) in $[-m,m]$. For (3.5a), there are no eigenvalues in $(-\infty,-m] \cup [m,\infty)$ while for (3.5b) there are two infinite sequences of eigenvalues accummulating at $\lambda = \pm\infty$. Furthermore, one has

$$\sigma_c(\hat{H}_{jl}) = \sigma_{ess}(\hat{H}_{jl}) = \sigma_{ac}(\hat{H}_{jl}) = (-\infty,-m] \cup [m,\infty)$$

and $\sigma_{sc}(\hat{H}_{jl}) = \emptyset$.

<u>Appendix: Asymmetric δ-shells</u>

The δ-shells do not exhaust the class of extensions covered by Theorem 3.2. Though it might be physically not interesting, we are going to demonstrate that the remaining extensions correspond to "asymmetric" δ-shells with (4.2) replaced by $G\delta_a(r-R)$, where G is again a 2x2 matrix and δ_a is defined by

$$\int_{R-\varepsilon}^{R+\varepsilon} \delta_a(r-R)\psi(r)dr = a\psi(R_+) + (1-a)\psi(R_-) \qquad (A.1)$$

for $\psi \in D(\hat{H}_{jl}^{(0)*})$, where a is a complex number. Condition (4.3) is now replaced by

$$(1-aB)\psi(R_+) - (1+bB)\psi(R_-) = 0 , \qquad (A.2)$$

where we have denoted $B = \tau_0 G$ and $b = 1-a$. Let us denote further $\hat{H}_{jl}^{(G,a)}$ the restriction of $\hat{H}_{jl}^{(0)*}$ to the subset of its domain specified by the boundary conditions (A.2)

<u>A.1 Proposition</u>: $\hat{H}_{jl}^{(G,a)}$ is a self-adjoint extension of $\hat{H}_{jl}^{(0)}$ iff

$$G - G^+ = (1-2\mathrm{Re}a)G^+\tau_0 G . \qquad (A.3)$$

<u>Proof</u>: The relation (A.2) represents two linearly independent boundary conditions since rank(1-aB,1+aB) = rank(1-aB,B) = rank(1,B) = 2. It remains to check that it is symmetric iff (A.3) is valid. We distinguish again several cases:

(i) 1-aB is nonsingular. Then $\psi(R_+)=(1-aB)^{-1}(1+aB)\psi(R_-)$ so the requirement gives

$$\tau_0 - (1+\bar{b}B^+)(1-\bar{a}B^+)^{-1}\tau_0(1-aB^+)^{-1}\,(1+bB^+) = 0 \qquad (A.4)$$

multiplying this relation by $(1-\bar{a}B^+)$ and (1-aB) from the left and right, respectively, we arrive after a short calculation at the relation (4.9)

(ii) An analogous argument can be used if 1+bB is nonsingular

(iii) Suppose that rank(1-aB)=1 and $\hat{H}_{jl}^{(G,a)}$ is self-adjoint. Then (A.2) must be equivalent to (3.5b), i.e., there is a nonsingular V such that

$$V(1+bB) = \begin{pmatrix} c_1, & c_2 \\ 0, & 0 \end{pmatrix}, \quad V(1-aB) = \begin{pmatrix} 0, & 0 \\ -d_1, & -d_2 \end{pmatrix} \qquad \text{(A.5)}$$

by a suitable choice of V one can have one of the following possibilities:

(a) $c_1=d_1=1$

(b) $c_1=d_2=1,\ d_1=0$

(c) $c_2=d_1=1,\ c_1=0$.

One can calculate the matrices VB and V from here obtaining, in particular, $\det V = a(1-a)(c_2d_1 - c_1d_2)$. Since it is nonzero, one has $a \neq 0,1$ and $c_2 \neq d_2$ in the case (a). Furthermore one can calculate

$$G = -\tau_0\mathcal{B} = \frac{1}{\det V}\begin{pmatrix} c_1d_1, & (1-a)c_2d_1+c_1d_2 \\ (1-a)c_1d_2+ac_2d_1, & c_2d_2 \end{pmatrix}.$$

Thus one has to check that this matrix fulfills the condition (A.3) iff all the coefficients c_1, c_2, d_1, d_2 are real. For each of the possibilities this can be done by a straightforward algebra.

(iv) The case $1-aB=0$ is excluded similarly as in the proof of proposition 4.1. ∎

The operators $\hat{H}_{jl}^{(G,a)}$ with $a \in (0,1)$ cover almost all extensions covered by Theorem 3.2:

<u>A.2 Proposition:</u> The set of the self-adjoint operators $\hat{H}_{jl}^{(G,a)}$ as well as its subset corresponding to $a \in (0,1)$ coincides with the set of self-adjoint extensions $\hat{H}_{jl}$ from Theorem 3.2 with the exception of those given by the boundary conditions (3.5b) with $c_1=d_1,\ c_2=d_2$.

Proof: First we check that the condition (A.2) with $\det(1+bB) \neq 0$ is equivalent to (3.5a). Using (A.4) one can check that $1-aB$ is also nonsingular, and therefore (A.2) is equivalent to $\psi(R_-)=A_1\psi(R_+)$ for a nonsingular A_1. Since the (A.2) defines self-adjoint operator by definition, it must hold $A_1 = e^{i\alpha}A$ for some α, A. Conversely, consider (3.5a) with some $A_1=e^{i\alpha}A$. Since A_1 is nonsingular and det is a continuous function, $\det(a1+bA_1)\neq 0$ for all $|a|$ small enough. We choose such an a and set $B=(1-A_1)(a1+bA_1)^{-1}$. Then $1+bB=(a1+bA_1)^{-1}$ and $A_1=(1+bB)^{-1}(1-aB)$ so we arrive back at (A.2). It is clear that there are many pairs of a,B corresponding to a given A_1.

Next one has to check that (A.2) with $\det(1+bB)=0$ is equivalent to (3.5b) with $c_1\neq d_1$ or $c_2\neq d_2$. As in the previous proof, there is a nonsingular V such that the relation (A.5) holds. From here, one can calculate VB and V, and also $\det V = a(a-1)(c_1d_2 - c_2d_1)$. The last relation shows that it cannot hold for $c_1=d_1$ and $c_2=d_2$. Conversely, consider (3.5b) with $c_1\neq d_1$ or $c_2\neq d_2$. Choosing $a\neq 0,1$ and

$$V = \begin{pmatrix} ac_1 & ac_2 \\ (1-a)d_1 & (a-1)d_2 \end{pmatrix}$$

we can define

$$B = V^{-1} \begin{pmatrix} c_1 & c_2 \\ d_1 & d_2 \end{pmatrix}$$

and $G=-\tau_0 B$ so we arrive back at (A.5) and (3.5b) implies (A.2) ∎

Finally, let us remark that the remaining extensions of Theorem 3.2 can be described as "asymmetric" δ-shells with the parameter a being a 2x2 matrix.

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