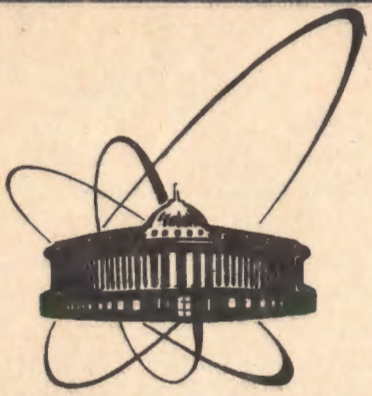

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DIRAC HAMILTONIAN WITH COULOMB POTENTIAL AND SPHERICALLY SYMMETRIC SHELL CONTACT INTERACTION

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1990

Dedicated to the memory of recently deceased Professor Václav Votruba, the founder of modern Czech theoretical physics

1. Introduction

Dirac equation with external Coulomb potential is used successfully in atomic physics, and at the same time, it is one of the rather few exactly solvable models in "relativistic quantum mechanics". Another solvable model (up to numerical solution of a transcendental equation for eigenvalues) is the Dirac equation with spherically symmetric shell interactions like the potential $\delta(r-R)$, R=const (Dittrich *et al* 1989, Domínguez-Adame 1990). The combination of both Coulomb and contact shell interactions still gives a solvable model as we are going to show in this paper.

In addition to extension of the list of solvable models, the results might be of some phenomenological interest if the contact shell interaction is used as a simulation of strong interaction in hadronic atoms (Mur and Popov 1985). For the Schrödinger Hamiltonian , the problem of Coulomb plus shell contact interactions have been studied in a number of papers (e.g., Mur and Popov 1985, Antoine *et al* 1987).

In the present paper, we consider Dirac Hamiltonian with Coulomb potential and contact interaction on the sphere of radius R with Coulomb source in its centre. We consider only Hamiltonians which are symmetric with respect to the space rotations and reflections. This allows us to separate different partial waves with given angular momentum j, parity $(-1)^l$, and the third component of angular momentum (Dittrich *et al* 1989). Then we may consider ordinary differential radial operators for each partial wave only.

The shell contact interaction is constructed by the known method based on self-adjoint extensions (Albeverio *et al* 1988) : the sought Hamiltonians H are self-adjoint extensions of the operator H_0 in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$, where

$$H_0\psi := \left[-i\vec{\alpha}\cdot\vec{\nabla} + \beta m - \frac{2\alpha}{r}\right]\psi \qquad (1.1)$$

for .

$$\psi \in D(H_0) := C_0^\infty(\mathbb{R}^3 \setminus ((0) \cup S_R)) \otimes \mathbb{C}^4 \; ; \qquad (1.2)$$

in other words, H_0 is the restriction of the Dirac-Coulomb Hamiltonian to the functions which vanish in the vicinity of the shell-interaction support. In (1.1), $\vec{\alpha}$, β are Dirac matrices, m is the particle mass, Z is the charge number, α is the fine structure constant, and

$$S_R := \{ \vec{x} \in \mathbb{R}^3 \mid |\vec{x}| = R \} \qquad (1.3)$$

2. The radial operators

From now on we shall consider one partial wave with given j, $(-1)^l$ and j_3. After separation of the angular variables and the unitary transfomation removing the weight factor r^2 from the measure, we shall use the Hilbert space

$$\hat{\mathcal{H}} := L^2(\mathbb{R}_+) \otimes \mathbb{C}^2 \; ; \qquad (2.1)$$

the construction starts from the operator $\hat{H}_0$ of the form

$$\hat{H}_0 := \begin{pmatrix} m - \frac{Z\alpha}{r} & -\frac{d}{dr} + \frac{\varkappa}{r} \\ \frac{d}{dr} + \frac{\varkappa}{r} & -m - \frac{Z\alpha}{r} \end{pmatrix} \qquad (2.2)$$

with

$$D(\hat{H}_0) := C_0^\infty((0,R) \cup (R,\infty)) \otimes \mathbb{C}^2 \qquad (2.3)$$

and $\varkappa = (-1)^{j-l+1/2}(j + 1/2)$. We are interested in self-adjoint extensions of the operator $\hat{H}_0$ in $\hat{\mathcal{H}}$ which correspond to

spherically symmetric self-adjoint extensions of the operator H_0 in $\mathcal{H}$.

First of all, we have to calculate the deficiency indices $d_\pm := \dim \mathrm{Ker}(\hat{H}_0^* \mp i)$; it requires to solve the equations

$$(\hat{H}_0^* \mp i)\varphi = 0 \; . \qquad (2.4)$$

To this end, it is necessary to find square integrable solutions of the equation with $\hat{H}_0^*$ replaced by the differential operator of the form (2.2) in (0,R) and (R,∞) (Dunford and Schwartz 1963). The differential equations corresponding to (2.4) can be solved in a similar way as the equations for the stationary states of the hydrogen atom (Beresteckii *et al* 1980). The functions from the deficiency spaces are written in the form $\varphi = \begin{pmatrix} f \\ g \end{pmatrix} \in \hat{\mathcal{H}}$ corresponding to the matrix form of the operator (2.2). Since the latter is real, $d_+ = d_-$ and we may consider the upper signs in (2.4) only. We denote

$$\gamma := (\varkappa^2 - Z^2\alpha^2)^{1/2} \; , \quad \lambda := (m^2 + 1)^{1/2} \; , \quad \varrho := 2\lambda r \qquad (2.5)$$

and we assume $0 < |Z|\alpha < 1$ for simplicity (the case Z=0 have been studied in Dittrich *et al* (1989) ; on the other hand, the case $|Z|\alpha > 1$ is not very interesting from the physical point of view, but probably can be treated in a similar manner with a complex γ if necessary). We use the following substitution (Beresteckii *et al* 1980)

$$\begin{aligned} f(r) &= (m+i)^{1/2}\, e^{-\varrho/2}\, \varrho^\gamma\, [Q_1(\varrho) + Q_2(\varrho)] \; , \\ g(r) &= -(m-i)^{1/2}\, e^{-\varrho/2}\, \varrho^\gamma\, [Q_1(\varrho) - Q_2(\varrho)] \; . \end{aligned} \qquad (2.6)$$

The function Q_1 here must satisfy the degenerate hypergeometric equation with the parameters

$$a = \gamma - \frac{Z\alpha}{\lambda} i \; , \quad c = 2\gamma + 1 \; , \qquad (2.7)$$

and Q_2 should satisfy that equation with the parameters a+1, c. The general solution is of the form

$$Q_1(\varrho) = A\Phi(a,c;\varrho) + B\Psi(a,c;\varrho)$$

$$Q_2(\varrho) = \frac{i\frac{Z\alpha}{\lambda} - \gamma}{\varkappa - \frac{Z\alpha m}{\lambda}} A\Phi(a+1,c;\varrho) + \left(\varkappa + \frac{Z\alpha m}{\lambda}\right) B\Psi(a+1,c;\varrho). \qquad (2.8)$$

Here Φ is the degenerate hypergeometric function and Ψ is the other solution of the degenerate hypergeometric equation in the notation of Bateman and Erdélyi (1953). Under our assumptions, $|\frac{Z\alpha m}{\lambda}| < |Z\alpha| < 1 < |\varkappa|$ and (2.8) is defined for all values of the parameters ; A and B are constants in the intervals (0,R) and (R,∞).

The square integrability of the functions (2.6) in (0,R) is governed by the asymptotics of the solutions (2.8) at $\varrho \to 0+$:

$$\Phi(a,c;\varrho) \approx 1 \ , \quad \Phi(a+1,c;\varrho) \approx 1$$

$$\Psi(a,c;\varrho) \approx \frac{\Gamma(2\gamma)}{\Gamma(a)} \varrho^{-2\gamma} \ , \quad \Psi(a+1,c;\varrho) \approx \frac{\Gamma(2\gamma)}{\Gamma(a+1)} \varrho^{-2\gamma} .$$

The leading terms $\varrho^{-2\gamma}$ of Q_1, Q_2 cannot cancel in both the functions (2.6) for $B \neq 0$, i.e., at least one of f and g then has the asymptotics of the order of $\varrho^{-\gamma}$ which is square integrable iff

$$Z^2\alpha^2 > \varkappa^2 - \frac{1}{4} . \qquad (2.9)$$

Since $\varkappa^2 \geq 1$, the last inequality can be solved for some values of $\varkappa$ if

$$|Z| > \frac{\sqrt{3}}{2\alpha} \approx 118.68 . \qquad (2.10)$$

In the following, we assume $|Z| \leq \frac{\sqrt{3}}{2\alpha}$. There are two reasons for this assumption. The first is that $Z \leq 118$ is

sufficient for all physical atoms, heavy ion collisions being at the best only roughly approximated by our static one-centre problem. On the other hand, it is well known that for $Z > 118$ the Dirac Hamiltonian with Coulomb field (without a shell interaction) is not self-adjoint and additional requirements are used to specify the "correct" self-adjoint extension (Rellich 1943-44, Nenciu 1976 and 1977, Klaus and Wüst 1979, Klaus 1980, Karnarski 1985). It follows for our problem that the case $Z > 118$ can be treated in the same way as that of $Z \leq 118$, the only difference being an additional boundary condition which must be imposed at the origin.

For $|Z| \leq \frac{\sqrt{3}}{2\alpha}$, the square integrability requires B = 0 while A may be arbitrary in (0,R). The integrability of (2.6) in (R,∞) is governed by the asymptotics of (2.8) at $\varrho \to \infty$:

$$\Phi(a,c;\varrho) \approx \frac{\Gamma(c)}{\Gamma(a)} e^{\varrho} \varrho^{a-c} \ , \quad \Phi(a+1,c;\varrho) \approx \frac{\Gamma(c)}{\Gamma(a+1)} e^{\varrho} \varrho^{a+1-c} ,$$

$$\Psi(a,c;\varrho) \approx \varrho^{-a} \ , \quad \Psi(a+1,c;\varrho) \approx \varrho^{-a-1} .$$

The square integrability of (2.6) now requires A = 0 while B may be arbitrary in (R,∞). Consequently, there are two linearly independent solutions of the equation (2.4) (within $D(\hat{H}_0^*)$) and $d_+ = d_- = 2$.

The self-adjoint extension $\hat{H}$ of the operator $\hat{H}_0$ in $\hat{\mathcal{H}}$ is then defined by imposing two linearly independent boundary conditions on the functions from $D(\hat{H})$. The presence of the Coulomb potential, which is regular in the vicinity of R , does not affect the construction of boundary conditions and other considerations from Sections III-V and Appendix of (Dittrich *et al*, 1989). We may therefore adopt the main results of this paper without any modifications ; we shall formulate here only the main theorem on the form of boundary conditions. For $\psi \in D(\hat{H}_0^*)$, the finite limits

$$\psi(R\pm) = \lim_{r \to R\pm} \psi(r)$$

exist and form a complete set of boundary values.

Theorem. Any self-adjoint extension $\hat{H}$ of $\hat{H}_0$ in $\hat{\mathcal{H}}$ acts as formal differential operator of the form (2.2) in $D(\hat{H})$. The domain $D(\hat{H})$ consists of all functions $\psi \in \hat{\mathcal{H}}$ such that

(i) ψ is absolutely continuous inside the intervals $(0,R)$ and (R,∞),

(ii) formal differential operator (2.2) maps ψ to a function from $\hat{\mathcal{H}}$,

(iii) ψ satisfies one of the following boundary conditions

$$\psi(R-) = e^{i\theta} A\, \psi(R+) \tag{2.11}$$

where θ is real (θ can be taken in $[0,\pi)$) and A is a real 2x2 matrix with $\det(A) = 1$, or

$$\begin{bmatrix} c_1 & c_2 \\ 0 & 0 \end{bmatrix} \psi(R-) + \begin{bmatrix} 0 & 0 \\ d_1 & d_2 \end{bmatrix} \psi(R+) = 0 \tag{2.12}$$

where c_1, c_2, d_1, d_2 are real and both matrices in (2.12) are nonzero. Conversely, any operator of the described form is a self-adjoint extension of $\hat{H}_0$ in $\hat{\mathcal{H}}$.

Both the boundary conditions (2.11), (2.12) can be written in the form

$$C\psi(R-) + D\psi(R+) = 0 \tag{2.13}$$

with suitable matrices C and D . We can always take $c_1 = 1$, c_2 real or $c_1 = 0$, $c_2 = 1$ and similarly for d_1, d_2.

3. The point spectrum

This section is devoted to discussion of spectral properties of the radial operator $\hat{H}$. Before we pass to the point spectrum which is our main topic, let us comment on the essential spectrum

Proposition. $\sigma_{ess}(\hat{H}) = (-\infty,-m] \cup [m,\infty)$.

Proof. Since the essential spectra for all self-adjoint extensions are the same provided the deficiency indices are finite (Weidmann 1980) which is our case, it is sufficient to prove the statement for the Dirac-Coulomb operator without the shell interaction, i.e., for $\theta = 0$ and $A = I$ and arbitrary j, l which we shall assume in the rest of the proof.

Notice first that $\sigma_{ess}(H) = (-\infty,-m] \cup [m,\infty)$. Weidmann (1980) proves this for $|Z\alpha| < 1/2$, however, the restriction is used only to check the self-adjointness. We know that H is self-adjoint for all $|Z\alpha| \le \sqrt{3}/2$ so the remaining part of the proof in Weidmann (1980) can be used for the respective values of Z. Naturally, $\sigma_{ess}(\hat{H}) \subset \sigma_{ess}(H)$ holds for all j,l. It remains to prove that $\sigma_{ess}(\hat{H}) \supset (-\infty,-m] \cup [m,\infty)$.

For any $E \in (-\infty,-m) \cup (m,\infty)$, we shall construct a sequence $(\psi_n)_{n=1}^{\infty} \subset \hat{\mathcal{H}}$ such that $\|\psi_n\| = 1$, $\|(\hat{H} - E)\psi_n\| \to 0$ which proves that $E \in \sigma(\hat{H})$, and also $E \in \sigma_{ess}(\hat{H})$ since E is not an isolated point of $\sigma(\hat{H})$. To construct the sequence $(\psi_n)_{n=1}^{\infty}$, denote by η the formal differential operator in (2.2). One has to solve the equation

$$(\eta - E)\varphi = 0 .$$

We use a substitution similar to (2.5-7) with i is replaced by E , i.e.,

$$\lambda := (m^2 - E^2)^{1/2} = i(E^2 - m^2)^{1/2} ,$$

$$\varrho := 2\lambda r = 2i(E^2 - m^2)^{1/2} r ,$$

$$a := \gamma - \frac{Z\alpha}{\lambda} E = \gamma + iZ\alpha E(E^2 - m^2)^{-1/2} .$$

and take the solution with the degenerate hypergeometric function Φ (i.e., A=1 , B=0 in (2.8)). The solution is regular at 0 and its absolute value approaches a non-zero constant as $r \to \infty$. Next we choose a function $h \in C_0^\infty(\mathbb{R})$ such that $|h(x)| \le 1$ for $x \in \mathbb{R}$, $h(x) = 1$ for $x < 0$, and $h(x) = 0$ for $x > 1$; we define $h_n(x) := h(x-n)$ and

$$\varphi_n(r) := h_n(r)\varphi(r) .$$

Now $\|\varphi_n\| \to \infty$ for $n \to \infty$, $\varphi_n \in D(\hat{H})$,

$$(\hat{H}-E)\varphi_n = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} h_n' \varphi$$

and $\|(\hat{H}-E)\varphi_n\| \le C$ for all n and a suitable C. The functions $\psi_n := \varphi_n / \|\varphi_n\|$ then form the sought sequence. ∎

According to the proved Proposition, the spectra $\sigma(\hat{H})$ of various self-adjoint extensions $\hat{H}$ may differ only in eigenvalues lying in $(-m,m)$. To be exact, we have in mind here differences in spectra in the set-theoretical sense ; possible eigenvalues embedded in the continuum (which are expected to exist in the case of impenetrable sphere) may be different too.

We are looking for the eigenvalues $E \in (-m,m)$ and eigenfunctions ψ satisfying

$$(\hat{H} - E)\psi = 0 . \qquad (3.1)$$

For $r \neq R$, ψ must satisfy the corresponding differential equation whose solutions are well known (Beresteckii *et al*, 1980). We use again the substitutions

$$\psi = \begin{pmatrix} f \\ g \end{pmatrix} ,$$

$$\gamma := (\varkappa^2 - Z^2\alpha^2)^{1/2} , \quad \lambda := (m^2 - E^2)^{1/2} , \quad \varrho := 2\lambda r \qquad (3.2)$$

$$f(r) = (m+E)^{1/2} e^{-\varrho/2} \varrho^\gamma [Q_1(\varrho) + Q_2(\varrho)] ,$$

$$g(r) = -(m-E)^{1/2} e^{-\varrho/2} \varrho^\gamma [Q_1(\varrho) - Q_2(\varrho)] , \qquad (3.3)$$

$$a := \gamma - \frac{Z\alpha}{\lambda} E , \quad c := 2\gamma + 1 . \qquad (3.4)$$

First we have to find Q_1, Q_2 which yield f, g square integrable in $(0,R)$ and (R,∞). To find two linearly independent solutions and to look for their asymptotics at 0 and ∞ is rather straightforward but a little tedious ; we sketch this procedure only briefly.

It is known that Q_1 satisfies the degenerate hypergeometric equation with the parameters a, c while Q_2 obeys the same equation with the parameters a+1, c. Let us denote

$$a_1 := \varkappa - \frac{Z\alpha}{\lambda} m , \quad a_2 := \varkappa + \frac{Z\alpha}{\lambda} m ,$$

$$Q_1^{(1)}(\varrho) := a_1 \Phi(a,c;\varrho) , \quad Q_2^{(1)}(\varrho) := -a\Phi(a+1,c;\varrho)$$

$$Q_1^{(2)}(\varrho) := \Psi(a,c;\varrho) , \quad Q_2^{(2)}(\varrho) := a_2 \Psi(a+1,c;\varrho)$$

$$Q_1^{(3)}(\varrho) := a_1 e^\varrho \Psi(c-a,c;-\varrho) , \quad Q_2^{(3)}(\varrho) := e^\varrho \Psi(c-a-1,c;-\varrho).$$

$$Q_1^{(4)}(\varrho) := (1+a-c)\Phi(a,c;\varrho) , \quad Q_2^{(4)}(\varrho) := a_2 \Phi(a+1,c;\varrho)$$

$(Q_1^{(1)},Q_2^{(1)})$ and $(Q_1^{(2)},Q_2^{(2)})$ are two linearly independent solutions of the equations for (Q_1,Q_2) if $a \neq 0,-1,-2,\ldots$ since $c > 0$ holds always under our assumptions ; $(Q_1^{(2)},Q_2^{(2)})$ and $(Q_1^{(3)},Q_2^{(3)})$ are linearly independent solutions in all cases. Furthermore, $(Q_1^{(1)},Q_2^{(1)})$ and $(Q_1^{(4)},Q_2^{(4)})$ are always linearly dependent but one of them can be zero for some value of the energy.

For $a \neq 0,-1,-2,\ldots$, $(Q_1^{(2)},Q_2^{(2)})$ does not yield (f,g) square integrable in $(0,R)$ if $|Z| \leq \sqrt{3}/(2\alpha)$; then $(Q_1^{(1)},Q_2^{(1)})$ gives the only square integrable solution. Consider the case $a = 0,-1,-2,\ldots$ when $(Q_1^{(1)},Q_2^{(1)})$ and $(Q_1^{(2)},Q_2^{(2)})$ are linearly dependent. For $a \leq 0$ and $|Z| \leq \sqrt{3}/(2\alpha)$, $(Q_1^{(3)},Q_2^{(3)})$ does not give square integrable (f,g) in $(0,R)$. If $|a|^2 + |a_1|^2 \neq 0$, $(Q_1^{(1)},Q_2^{(1)})$ leads again to a nontrivial square integrable solution. If $a = a_1 = 0$, we have $(Q_1^{(1)},Q_2^{(1)}) = (0,0)$ but $(Q_1^{(4)},Q_2^{(4)})$ leads to a square integrable solution while the same is not true for $(Q_1^{(2)},Q_2^{(2)})$. As a result, the only square integrable (f,g) in $(0,R)$ is given by $(Q_1^{(1)},Q_2^{(1)})$ or $(Q_1^{(4)},Q_2^{(4)})$ in all cases.

In the interval (R,∞), $(Q_1^{(3)},Q_2^{(3)})$ does not yield a square integrable solution (f,g) while $(Q_1^{(2)},Q_2^{(2)})$ does. Let us denote by $\psi^{(1)}$ the function given by $(Q_1^{(1)},Q_2^{(1)})$ according to (3.3) ; if $a = a_1 = 0$, we replace $(Q_1^{(1)},Q_2^{(1)})$ by $(Q_1^{(4)},Q_2^{(4)})$. Similarly, $\psi^{(2)}$ is given by $(Q_1^{(2)},Q_2^{(2)})$. The eigenfunction must be then of the form

$$\psi(r) = \begin{cases} u\psi^{(1)}(r) & \text{for } r < R \\ v\psi^{(2)}(r) & \text{for } r > R \end{cases}$$

where the complex numbers u,v are chosen in such a way that the boundary condition (2.13) is satisfied, i.e.,

$$uC\psi^{(1)}(R) + vD\psi^{(2)}(R) = 0.$$

Nontrivial (u,v) exist iff

$$\det\left[C\psi^{(1)}(R), D\psi^{(2)}(R)\right] = 0 \qquad (3.5)$$

which is the sought equation for eigenvalues E (in the used notation, $C\psi^{(1)}(R)$ and $D\psi^{(2)}(R)$ are two columns of the matrix in the square bracket).

4. Numerical results

Equation (3.5) can be solved numerically and we are going to present here several examples illustrating how the eigenvalues of the radial operator $\hat{H}$ with Coulomb potential and scalar δ-shell (simulating strong interaction) situated in the gap $(-mc^2,mc^2)$ behave with respect to the coupling constant. In the following, the units where $mc^2 = 1$ are used for simplicity, i.e., the energies are normalized to mc^2.

The scalar δ-shell interaction with a coupling constant g, which means symbolically the potential

$$g\,\beta\,\delta(r-R) \qquad (4.1)$$

in the Hamiltonian of a Dirac particle, corresponds to the boundary condition (2.13) with matrices

$$C = \begin{bmatrix} 1 & g/2 \\ g/2 & 1 \end{bmatrix} , \quad D = \begin{bmatrix} -1 & g/2 \\ g/2 & -1 \end{bmatrix} \qquad (4.2)$$

like in the case without the Coulomb potential (Dittrich *et al*, 1989 ; the relation to alternative definition of Dominguez-Adame (1990) is discussed in the Appendix).

Because our purpose is only illustrative, we have not tried to make the computer program for solving equation (3.5) very sophisticated. It has two major shortcomings. First of all, it cannot handle the cases with $R \gtrsim 8$ which means most hadronic

atoms in the model mentioned below. In addition, the procedure becomes numerically unstable at the points close to the edges of the gap. For this reason, we restrict our attention mostly to the energy interval $[-0.99,0.99]$. Of course, these limitations of numerical accuracy are not a matter of principle and could be undoubtedly overcome if necessary.

The system we consider is a natural model for a relativistic atom with one orbiting particle and the strong interaction supported by the nucleus surface. In particular, one can try to model in this way the Zeldovich (1959) effect, i.e., level shifting and rearrangement due to the strong interaction for atoms with a heavy orbiting particle.

In order to illustrate the main features of the relativistic Coulomb plus strong sphere interaction, we calculate the spectra for two values of the sphere radius, namely $R = 6$ and $R = 2.71$. Recall that the seemingly dimensionless quantities refer in fact to the Compton wavelength of the orbiting particle. Adopting therefore $R \approx 1.2\, Z^{1/3}$ fm as the nucleus radius, we see that two cases correspond roughly to the antiproton hydrogen atom and to a muonic heavy atom, respectively.

On Fig.1a-d, several "lowest" eigenvalues for $R = 6$ and a few values of nuclear charge Z are plotted versus the coupling constant. As we remarked, only the first of them corresponds in some sense to a real physical system, however keeping R fixed makes it possible to show how the spectrum changes when the Coulomb interaction becomes stronger. We see that the shell is most "attractive" at the value $g = -2$ at which the inner and outer part of the sphere are separated. We also see that there is a critical value $g_Z < 0$ such that for $g > g_Z$ there are positive eigenvalues in the gap only. For larger values of Z, the effect of almost level crossing (or cascading - see Gesztesy *et al*, 1988) for $\varkappa = -1$ begins to appear; comparing to Fig.3a below we see that the large shell diameter is important here.

In order not to burden the picture with too much information, we have not plotted here all the eigenvalues appearing in $[-0.99,0.99]$. To illustrate the full picture, we plot in Fig.2a,b the spectral dimensionality, i.e., the dimension of the projection $E_H([-0.99,\cdot))$ for the two values of Z in

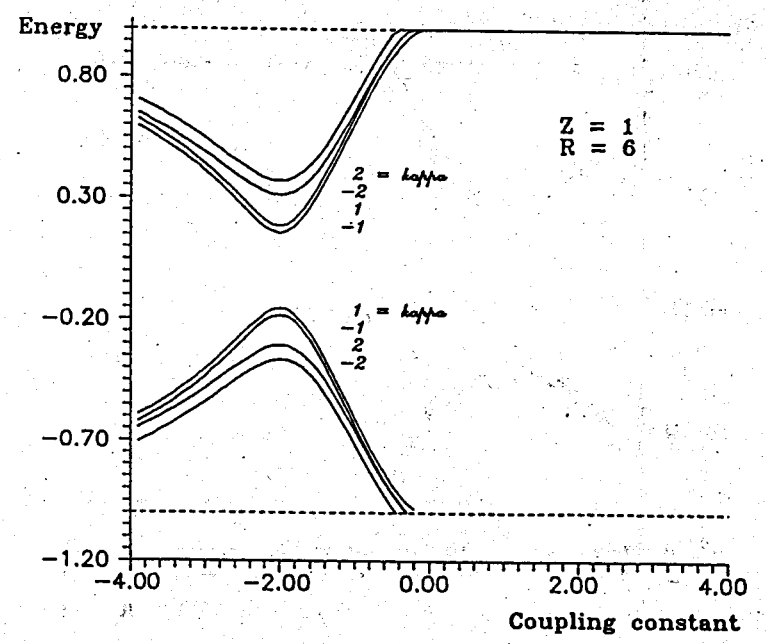

Fig.1a A few "lowest" eigenvalues for the "hydrogen" atom with a scalar δ-shell

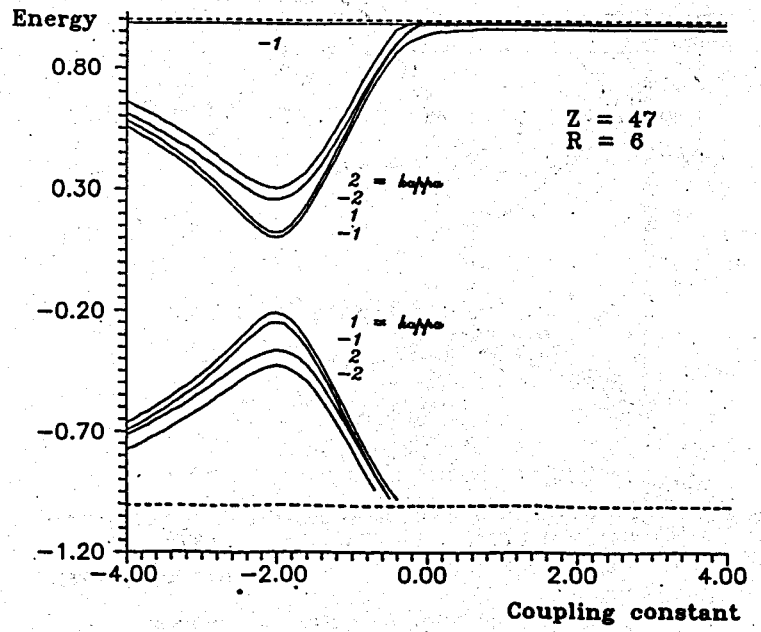

Fig.1b The same for "silver"

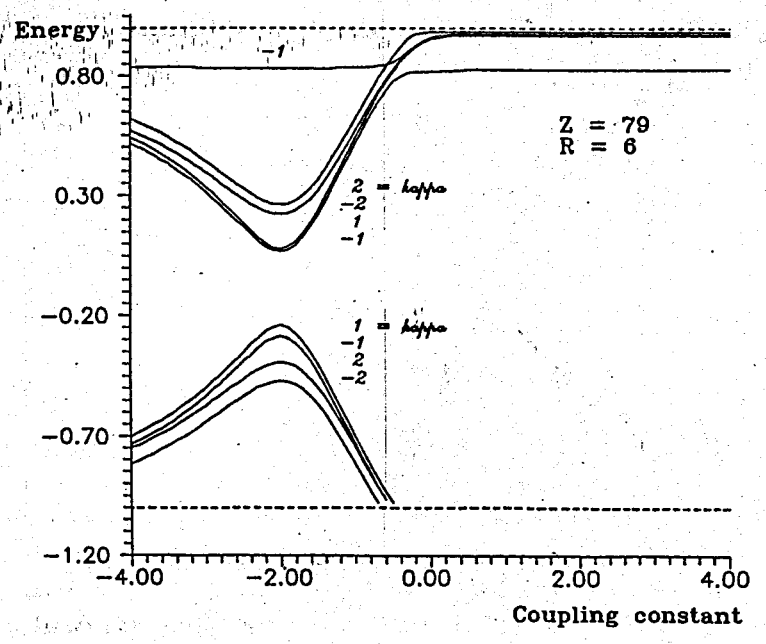

Fig.1c The same for "gold"

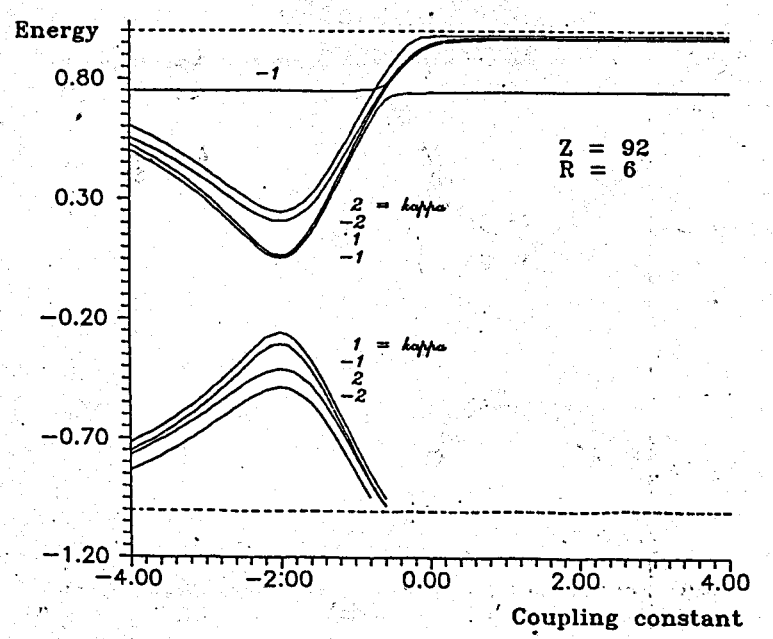

Fig.1d The same for "uranium"

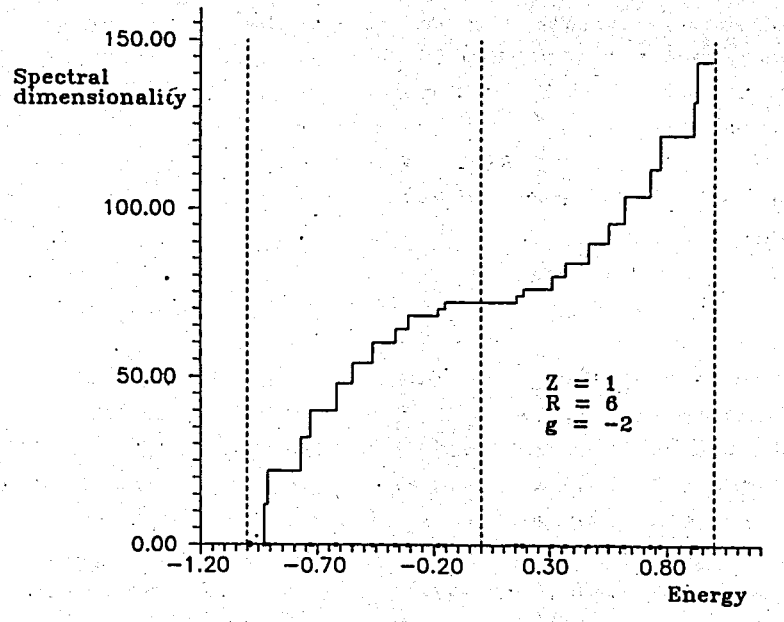

Fig.2a Spectral dimensionality for "hydrogen" in the "maximally attractive" case

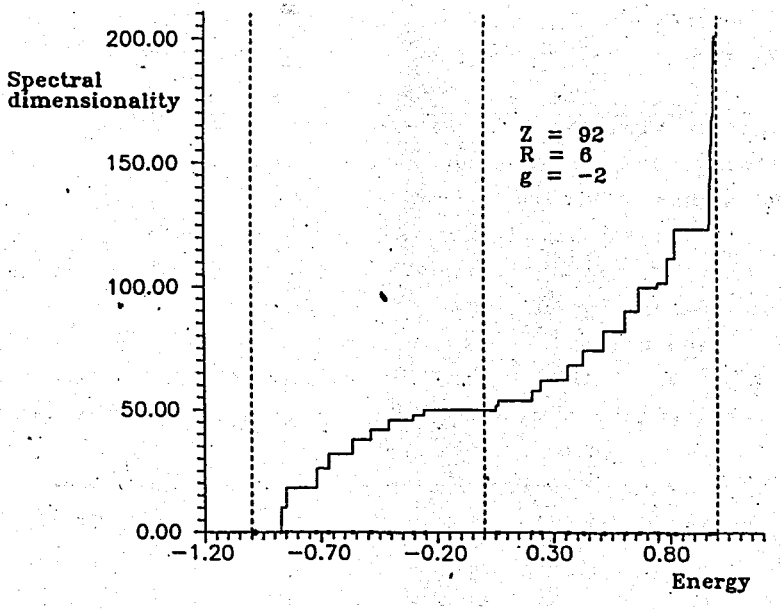

Fig.2b The same for "uranium"

the "maximally attractive" case. We see that while for $Z = 1$ the Coulomb interaction represents a weak perturbation so the picture is nearly symmetric (the difference in modules for the pairs of eigenvalues is $\lesssim 2\cdot 10^{-3}$), in the case of $Z = 92$ the spectrum is obviously asymmetric. Since every eigenvalue is $2|\varkappa|$-times degenerated, these graphs also show to which values of j the eigenvalues belong.

For a smaller sphere, $R = 2.71$, the spectrum is less "dense". We illustrate it showing in Fig.3a the "uranium μ-atom". Another feature which can be seen from this picture as well as from Figs.1a-d is the invariance of the spectrum with respect to the transformation $g \mapsto 4/g$. In order to make the symmetry even more obvious, we show in Fig.3b the positive part of the previous graph but now in a wider scale of g. Looking at the lowest $\varkappa = -1$ level, one can observe that the invariance holds for positive values of g too.

The transformation $g \mapsto 4/g$ is equivalent to the change of sign of the matrix D in (2.13) with (4.2) as can be easily seen. The operators defined by matrices C,D and $C,-D$ are unitarily equivalent and therefore have the same spectra. The unitary equivalence is given by the change of sign of wave function for $r > R$. More generally, all operators corresponding to different θ but the same A in (2.11) are unitarily equivalent (Dittrich *et al*, 1990).

Finally, Fig.3c shows a smaller part of the previous two pictures around g=0. For comparison, the well-known eigenvalues of the relativistic "one-electron" atom are plotted here by dots. We see that the strong interaction removes the degeneracy of these eigenvalues with respect to the sign of $\varkappa$, i.e., with respect to the parity. It is also clear that the levels may cross : for $g \lesssim -0.105$ the $2p_{3/2}$ level is lower than $2s_{1/2}$, and the level crossing can be seen also in the next batch of eigenvalues (where the $3d_{5/2}$ level is not included from technical reasons). This brings Zeldovich effect in mind, however its thorough study in the present model deserves a more detail examination.

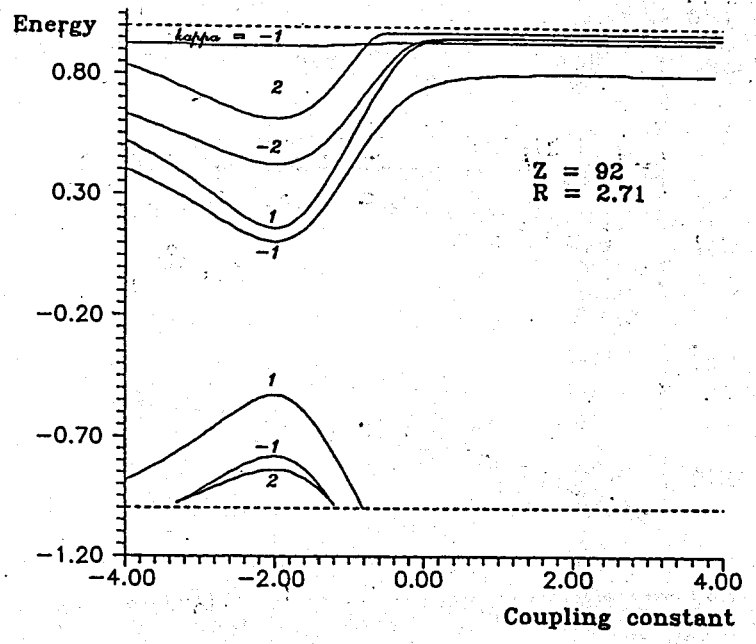

Fig.3a A few "lowest" eigenvalues for the "uranium μ-atom"

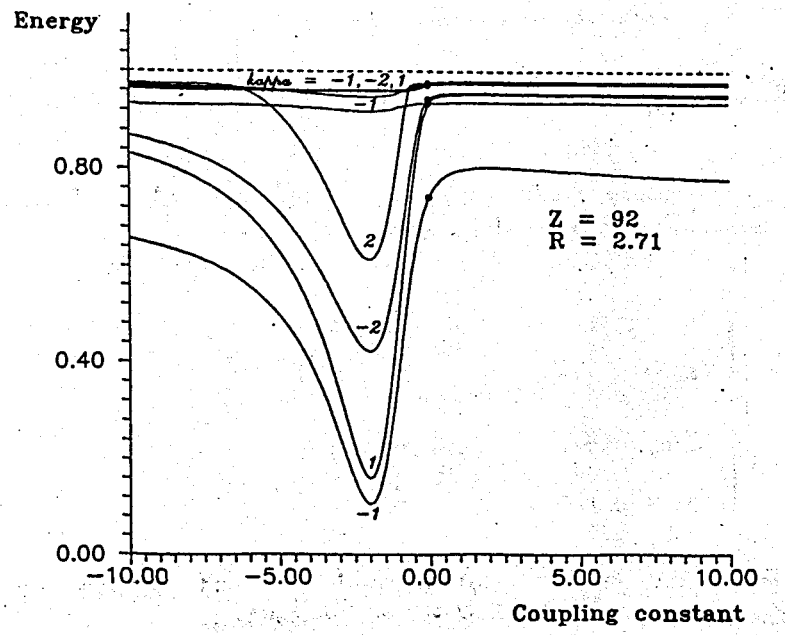

Fig.3b The same in a broader scale of g

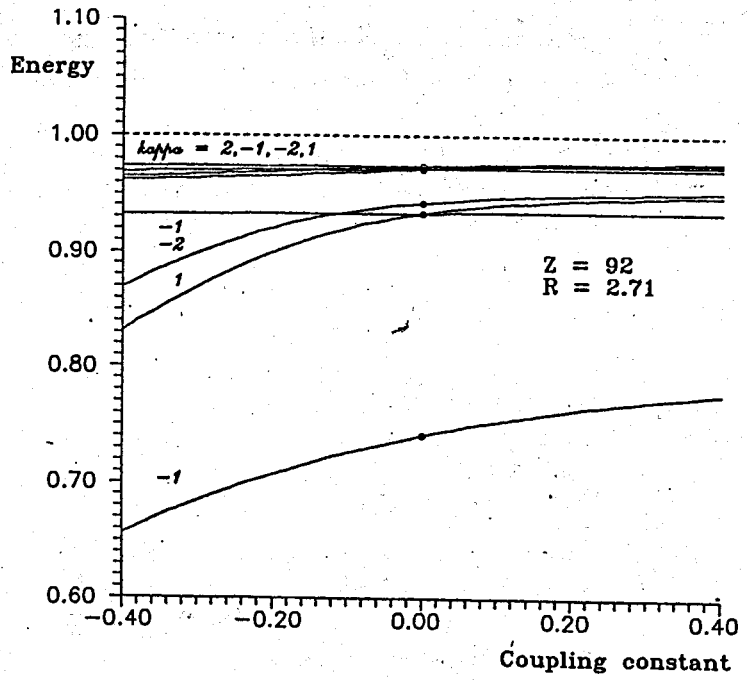

Fig.3c Detail of the previous picture with the purely Coulombic eigenvalues indicated

Appendix: Relation to an alternative definition of δ-shell

Our boundary condition (2.13) with the matrices (4.2), or wmore generally (Dittrich *et al*, 1989) with

$$C = \begin{pmatrix} 1 & (g_S - g_V)/2 \\ (g_S + g_V)/2 & 1 \end{pmatrix} ,$$

$$D = \begin{pmatrix} -1 & (g_S - g_V)/2 \\ (g_S + g_V)/2 & -1 \end{pmatrix} \qquad (A.1)$$

follows from formal integration of the radial equation corresponding to the stationary Dirac equation

$$\left[-i\vec{\alpha}\cdot\vec{\nabla} + \beta m - \frac{Z\alpha}{r} + g_S\beta\delta(r-R) + g_V\delta(r-R)\right]\tilde{\psi} = E\tilde{\psi}$$

using the formal definition

$$\int_{R-\varepsilon}^{R+\varepsilon} \delta(r-R)\,\psi(r)\,dr = \frac{1}{2}\,[\psi(R+) + \psi(R-)] \qquad (A.2)$$

and the limit $\varepsilon \to 0+$.

Dominguez-Adame (1990) proposed recently another definition of δ-shell. Let $F^{(\varepsilon)}_{R+\varepsilon}: \mathbb{R}_+ \to \mathbb{R}_+$ be a function with supp $F^{(\varepsilon)} \subset [R-\varepsilon, R+\varepsilon]$ and $\int_{R-\varepsilon} F^{(\varepsilon)}(r)\,dr = 1$. We consider the stationary Dirac equation

$$\left[-i\vec{\alpha}\cdot\vec{\nabla} + \beta m - \frac{Z\alpha}{r} + s\beta F^{(\varepsilon)}(r) + vF^{(\varepsilon)}(r)\right]\tilde{\psi} = E\tilde{\psi}$$

and the corresponding radial equation

$$\frac{d}{dr}\,\psi(r) = \hat{G}^{(\varepsilon)}(r)\,\psi(r)$$

where $\hat{G}^{(\varepsilon)}(r)$ is a 2×2 matrix. For the radial wave function we then have

$$\psi(r) = U^{(\varepsilon)}(r, r_0)\,\psi(r_0) \quad ,$$

$$U^{(\varepsilon)}(r, r_0) = \hat{P}\,\exp\left(\int_{r_0}^{r} \hat{G}^{(\varepsilon)}(r)\,dr\right) \qquad (A.3)$$

where $\hat{P}$ is the ordering of operator product according to r decreasing from right to left. Now we obtain

$$U^{(0)}(R+, R-) := \lim_{\substack{r\to R+ \\ r_0 \to R-}} \lim_{\varepsilon \to 0+} U^{(\varepsilon)}(r, r_0) \qquad (A.4)$$

in the form

$$U^{(0)}(R+,R-) = \mathrm{ch}[(s^2-v^2)^{1/2}] + \begin{pmatrix} 0 & s-v \\ s+v & 0 \end{pmatrix} \frac{\mathrm{sh}[(s^2-v^2)^{1/2}]}{(s^2-v^2)^{1/2}} =$$

$$= \cos[(v^2-s^2)^{1/2}] + \begin{pmatrix} 0 & s-v \\ s+v & 0 \end{pmatrix} \frac{\sin[(v^2-s^2)^{1/2}]}{(v^2-s^2)^{1/2}} \qquad (A.5)$$

and define (Dominguez-Adame 1990)

$$\psi(R+) = U^{(0)}(R+,R-)\ \psi(R-) .$$

The boundary conditions with (A.1) and with (A.5) are equivalent iff

$$\frac{4 - g_v^2 + g_s^2}{4 + g_v^2 - g_s^2} = \cos[(v^2-s^2)^{1/2}] ,$$

$$\frac{4g_s}{4 + g_v^2 - g_s^2} = s\,\frac{\sin[(v^2-s^2)^{1/2}]}{(v^2-s^2)^{1/2}} , \qquad (A.6)$$

$$\frac{4g_v}{4 + g_v^2 - g_s^2} = v\,\frac{\sin[(v^2-s^2)^{1/2}]}{(v^2-s^2)^{1/2}}$$

i.e., if

$$g_s = 2s\left\{1 + \cos[(v^2-s^2)^{1/2}]\right\}^{-1} \frac{\sin[(v^2-s^2)^{1/2}]}{(v^2-s^2)^{1/2}} ,$$

$$g_v = 2v\left\{1 + \cos[(v^2-s^2)^{1/2}]\right\}^{-1} \frac{\sin[(v^2-s^2)^{1/2}]}{(v^2-s^2)^{1/2}} \qquad (A.7)$$

In these formulas, we assume $4+g_v^2-g_s^2 \neq 0$ and $\cos[(v^2-s^2)^{1/2}] \neq -1$ (for $v^2 = s^2$ they hold if the singularity is removed).

For the case $4+g_v^2-g_s^2 = 0$ when the sphere is impenetrable (Dittrich *et al*, 1989), the finite v, s do not exist but in the limit $4 + g_v^2 - g_s^2 \to 0$ clearly $|s| \to \infty$. The impenetrability condition therefore means infinite coupling constant s of the scalar δ-shell if the definition of Dominguez-Adame is used. For $\cos[(v^2-s^2)^{1/2}] = -1$, the constants g_v, g_s do not exist. The limit $\cos[(v^2-s^2)^{1/2}] \to -1$ corresponds to $|g_v| \to \infty$, $g_v^2 - g_s^2 \to \infty$ (and also $|g_s| \to \infty$ if $|s| > \text{const} > 0$).

For $g_v = v = 0$, (A.7) simplifies to

$$g_s = \frac{2\ \mathrm{sh}\ s}{1 + \mathrm{ch}\ s} .$$

Here $g_s \in (-2,2)$ for $s \in (-\infty,\infty)$ and $g_s \to \pm 2$ for $s \to \pm\infty$. We see that only the set of Hamiltonians with $g_s \in (-2,2)$ is covered by all choices of s but the set with $|g_s| > 2$, which is redundant due to above mentioned symmetry $g_s' = 4/g_s$ leading to unitary equivalent Hamiltonians, has no counterpart. Since the definition of Dominguez-Adame is analogous to the non-relativistic scaling argument (Albeverio *et al*, 1988), the comparison between the two definitions in the non-relativistic limit deserves a deeper study.

Acknowledgement

The authors are indebted to Dr.F.Dominguez-Adame for sending them his paper prior to the publication.

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Received by Publishing Department
on November 23, 1990.