Remarks on the Dirac-Coulomb problem for highly charged ions

Piotr Marecki
II Institut für theoretische Physik
Universität Hamburg
marecki@mail.desy.de

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Plan

The Dirac operator in a Coulomb field exhibits an interesting behavior depending on the charge which produces the field. Whereas small charges cause no particular difficulties the higher the charge the more delicate the situation becomes. In particular from $Z = 119$ on there is a 1-parameter freedom of choosing selfadjoint extensions of the Dirac operator which has significant physical consequences. The talk attempts at presenting the relevant structure.

The plan of the talk is the following:

1. Introduction

2. Coulomb potential; small nuclear charges

3. Strong Coulomb potential

4. How does the extension influence energy levels?

Introduction

The evolution in quantum mechanics is governed by the Hamilton operator. More precisely the Hamiltonian should generate a one-parameter unitary group $U(t)$.

Def. *If an operator operator T is symmetric (i.e. $(\psi, T\chi) = (T\psi, \chi)$) than it is selfadjoint if*

$$D(T) = D(T^*)$$

<u>Only selfadjoint operators generate unitary dynamics.</u>

A theorem[2] says:

T is selfadjoint if $\psi_{\pm i}$ (eigenfuctions to the eigenvalues $\pm i$) do not belong to the domain of the adjoint operator T^*.

If H is not selfadjoint (but symmetric) than it only generates the so-called contraction semi-group (e.g. dynamics of the heat-flow equation in a bounded region with constant temperature at the boundary). Physically this means that the particles escape from the region of interest.

Suppose an operator H is given without its domain and that the corresponding Schrödinger equation has singular points. How do we check the selfadjointness? Typically it is easy to check whether H is symmetric on a certain $\mathcal{C}_0^\infty$ space. If H possesses the property of essential selfadjointness than there exists only one selfadjoint extension to the L^2 and therefore the boundary conditions follow automatically from the square integrability of the wave functions.

Essential selfadjointness has a fascinating connection with the completeness of the classical motion namely, if the Hamilton equations allow a classical particle to leave the region of interest (e.g. hit the boundary) in finite time than the quantum mechanical Hamiltonian almost for sure is not essentially selfadjoint.

The evolution of the Dirac field in some external potential is governed by the Hamiltonian:

$$H = \gamma^0\gamma^i[-i\partial_i + eA_i(t, \mathbf{x})] - eA_0(t, \mathbf{x}) + m\gamma^0.$$

By far the most important question in quantum mechanics is whether the Hamilton operator (for certain external field of interest) is selfadjoint. It leads towards an analysis of the boundary conditions (if the region of interest is bounded) and of the singular points of the potential. The situation may be classified into following hierarchy of difficulty:

- the potential is smooth
- the potential possesses singularities, but H remains essentially selfadjoint
- the singularities cause breakdown of the essential selfadjointness, but selfadjoint extensions of H exist

The first case is covered by a very important theorem:

Thm 1. *If the potential is smooth the Dirac operator* H *defined on* $D(H) = \mathcal{C}_0^\infty(R^3)$ *is essentially selfadjoint.*

Message:

The Hamilton-Dirac operator must be selfadjoint in order to generate a unitary evolution. This is always the case for smooth potentials.

Coulomb potential; small nuclear charges

Separation of angular and radial part leads to the radial Dirac operator:

$$h_\kappa = \begin{pmatrix} 1 - \frac{z}{r} & -\frac{d}{dr} + \frac{\kappa}{r} \\ \frac{d}{dr} + \frac{\kappa}{r} & -1 - \frac{z}{r} \end{pmatrix} \tag{1}$$

which is first defined on $D(h_\kappa) = \mathcal{C}_0^\infty(0,\infty)$ functions. Here z denotes the nuclear charge (rescalled: $z = 1$ corresponds to $Z = e^2/\hbar c = 137,036..$) and $-\kappa$ the eigenvalue of the operator $K = \gamma^0(J^2 - L^2 + 1/4)$. For instance

Level	κ
S	-1
$P_{1/2}$	1
$P_{3/2}$	-2

The separation of variables is justified if all the radial operators are essentially self adjoint on $D(h)$'s. The

Hilbert space is now a L^2 space with scalar product:

$$(\psi, \chi) = \int_0^\infty (\overline{\psi_1}\chi_1 + \overline{\psi_2}\chi_2)\, dr.$$

The further analysis amounts to the investigation of the ordinary differential operator (system) (1). For given κ this operator depends only on one dimensionless parameter (nuclear charge). Therefore all the structure will only depend on κ and Z.

The following theorem holds[1]:

Thm 2. *For nuclear charges not greater than $Z = 118$ the Dirac-Coulomb operator is essentially selfadjoint on $D(H) = \mathcal{C}_0^\infty(R^3\backslash\{0\})$.*

Thus no boundary conditions are needed at $r = 0$ or $r \to \infty$. The extension from $\mathcal{C}_0^\infty$ is unique by the requirement of square-integrability. The domain of the extended operator coincides with the domain of the free Dirac operator.

Strong Coulomb potential

For Z greater than 118 the Dirac operator on $\mathcal{C}_0^\infty(\mathrm{R}\backslash\{0\})$ is not essentially selfadjoint anymore[4]. Indeed there exist eigenfunctions which in both cases $E = \pm i$ are square integrable at $r = 0$ (and vanish quickly at ∞). This corresponds to the von Neumann deficiency indices (1,1) in which case an existance of a 1-parameter family of selfadjoint extensions is expected.

Thus it is possible to restore selfadjointness by means of an extension of the domain of H. Either:

- a boundary condition at $r = 0$ is imposed, or
- a certain linear combination of ψ_i and ψ_{-i} is added to the domain (for each κ)

Also a regularization of the potential at small r has a similar effect.

The spectrum (energy levels) depends strongly on the type of the selfadjoint extension in use[5].

A boundary condition that the solution should vanish at $r = 0$ is acceptable[3] (and also fulfilled for $Z \leq 118$). It leads to the famous Sommerfeld spectrum:

$$E_{n,\kappa} = \frac{1}{\sqrt{1 + \frac{z^2}{\left[\sqrt{\kappa^2 - z^2} + n\right]^2}}}$$

From the usual treatment it is hard to see the breakdown of the essential selfadjointness because:

- one investigates the differential equation without looking at the adjoint problem, or
- a boundary condition/particular extension is a priori chosen which already makes the operator selfadjoint.

Message:

In the case $118 < Z \leq 137$ the Dirac operator is not essentially selfadjoint. Only certain extensions reproduce the usual Sommerfeld spectrum.

How does the extension influence energy levels?

In the case $118 < Z \leq 137$ there exists a particular linear combination of the two independent solutions of the radial Dirac equation which has a property that, after inserting $E = \pm i$ one gets square integrable solutions ψ_i and ψ_{-i}. If a linear combination

$$k \cdot (\psi_{-i} + e^{i\theta}\psi_i) \qquad k \in C,\ \theta \in [0, 2\pi).$$

is added to the domain of the operator a selfadjoint extension is obtained. Clearly as the core was $\mathcal{C}_0^\infty(0,\infty)$ such a solution fixes only the boundary condition at $r = 0$ (at infinity $\psi_{\pm i}$ vanish rapidly, so they add nothing). Now any wavefunction ψ in the domain can be decomposed into

$$\psi = \psi_0 + k(\psi_{-i} + e^{i\theta}\psi_i),$$

where ψ_0 belongs to the old domain. The eigenvalue problem sounds:

$$(h_\kappa - E)\psi_0 = k(E+i)\psi_{-i} + k(E-i)\psi_i.$$

The solution of this inhomogeneous equation (ψ_0) has to vanish at $r=0$. It may be divided into a particular solution (ψ_p) and a homogeneous solution (ψ_h). The particular solution is

$$\psi_p = -k(\psi_{-i} + e^{i\theta}\psi_i),$$

and consequently one obtains a boundary condition for the homogeneous equation:

$$\psi_h(0) = k(\psi_{-i}(0) + e^{i\theta}\psi_i(0)),$$

which certainly produces eigenvalues different from those obtained in the usual treatment:

$$\begin{aligned} (h_\kappa - E)\psi_0 &= 0 \\ \psi_h(0) &= 0 \end{aligned}$$

Conclusions and outlook

The Dirac-Coulomb problem is characterized by a Z-dependent structure:

- for $Z \leq 118$ the Hamiltonian is essentially selfadjoint
- for $118 < Z \leq 137$ there are selfadjoint extensions of the Dirac operator which lead to different energy levels.

The case $Z > 137$ has also received attention. In that case the wavefunctions oscillate rapidly as $r \to 0$, roughly:

$$\psi \sim r^{i\sqrt{z^2-\kappa^2}},$$

so that no usual boundary condition makes sense. An important question arises as to whether the energy levels approach the lower continuum ($E = -1$).

References

[1] B.Thaller, *The Dirac Equation*.

[2] M.Reed, B.Simon, *Methods of modern mathematical physics vol. I and II*.

[3] C.Bunrap et. al., *N. Cimento* **64 B #2** (1981), 407.

[4] H. Narnhofer, *Acta Phys. Aust.* **40** (1974), 306.

[5] V.S. Popov, *Sov. J. Nucl. Phys.* **12 #2** (1971), 235.